THE CLASSICAL CONDENSATES

from Crystals to Fermi-liquids

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CONTENTS

1 Quantum condensed matter physics: the principles.

1.1 Some metaphysics.

This text attempts to be an introduction to the subject which could be called 'conventional quantum condensed matter physics'. Before explaining what is meant with 'conventional', let me first define the discipline as a whole, including its unconventional aspects: quantum condensed matter physics is the subdiscipline of physics focussing on the properties of macroscopic objects in terms of the collective behaviours of (near) infinities of its microscopic, quantum-mechanical constituents.

A student of physics should be nasty reading the preceding paragraph, and ask the question: why should we worry about these macroscopic things which we can see with our own eyes? Isn't it so, that our grandfathers put all their skills in trying to slice this unprofound stuff in smaller and smaller pieces, finally discovering this breath-taking climax of the human pursuit for knowledge: atomic-, nuclear- and particle physics? Not so long ago it was indeed believed that the only alley leading to the most fundamental aspects of nature was by smashing matter into smaller and smaller pieces. Some twenty years ago this attitude changed, not in the last place due to developments in high energy physics. Both at the high energy end (particle physics) as well as at the low energy end (condensed matter physics), nature is of an irreducible many-particle nature - it is only in the middle (atomic-, nuclear physics) that few particles make sense. In the presence of these (near) infinities of interacting constituents the face of physics itself changes. New principles appear of an entirely different nature than the laws governing the behaviours of few-particle systems. These could be called the 'laws of emergent behaviours'.

A first problem facing the novice in this field is to recognize the non-triviality of these laws. They penetrate nature to such an extent that they appear as very familiar and familiar things tend to be taken for granted. A typical example is the 'first' law: 'the whole is more than the sum of its parts', or 'more is different' using Anderson's one-liner[1]. In physics, this principle acts typically in the following way: one starts out considering an 'ultraviolet', a regime of high energy and small spatial dimension, which usually looks rather boring. In condensed matter physics, the ultraviolet typically consists of isolated electrons and atoms having the simple properties as explained in quantum-mechanics textbooks: they have a position and a momentum, and carry internal degrees of freedom like spin. In addition, these elementary constituents have the property that they *interact* with each other. Macroscopic reality is approached by putting more and more of these elementary constituents together. In this process, the 'more is different' law starts to act: the *system* of particles be-

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[1] I refer to a remarkable article by Anderson for a more general discussion: P. W. Anderson, Science **177**, 193 (1972). In addition, Anderson's book 'Basic Notions of Condensed Matter Physics' (Benjamin/Cummings, Menlo Park, 1984) is recommended for further reading. The student is warned: this is not an easy book!

haves in a way which is *qualitatively different* from that of its elementary constituents. By increasing the number of constituents the lowest-lying excitations of the system move down in energy, while the spatial scale increases. *The appearance of nature depends fundamentally on the energy- or length scale which is probed in the experiment.* This 'flow' of physical behaviours as function of particle number and energy (time-, length-) scale is called the *renormalization flow.*

Some general statements can be made about the nature of this scaling flow. One possibility is that the system settles in a *critical state*: every time the size of the system increases by an order of magnitude, the new (bigger) system has the same properties as the old (smaller) system. The system becomes *self-similar*, both in temporal and spatial aspects. This seems the possibility choosen by nature in the high-energy realms: relativistic quantum-field theory can only be consistently formulated if criticality is imposed. Criticality is also quite important in the macroscopic realms: it occurs at finite temperature phase transitions, as well as at the quantum phase transitions taking place at zero-temperature. One of the great triumphs of modern theoretical physics is the invention by Wilson and others of a rigorous mathematical theory of the critical state, the renormalization group theory. This is a rather advanced subject which is deliberately avoided in the present text.

Next to the smooth flow of the critical state, the renormalization process might have a more jumpy character as well. In the jargon this is called 'projective renormalization' and some sophisticated examples of this kind of renormalization will be treated in this text. At some point in the renormalization process 'bound states' might be formed. These are new collective objects with well defined properties, having a special stability so that it costs a finite energy to break them up: an energy scale (or 'gap', also called 'mass') appears. This makes it possible to define a new 'effective' theory describing the system at energies less than this gap in terms of the new composite objects and their mutual interactions. The latter are called 'residual interactions' and can be derived by considering virtual processes involving the (bare) particle states above the energy gap. This is actually quite familiar. Nuclei are bound states of protons and neutrons, atoms are bound states of nuclei and electrons and molecules are bound states of atoms. Atomic physics is the effective theory which remains after the nucleons have been 'integrated out' (the residual interaction is the Coulomb force coming from the nucleus) and chemistry has to do with the effective theory which remains after integrating out the atomic core-electrons[2].

Chemistry, atomic- and nuclear physics have in common that they study bound states of a relatively small number of particles. On the other hand, condensed matter physics and high energy physics both deal with systems build from an *infinity* of constituents[3].

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[2] Notice that nucleons cannot be considered as simple bound states of quarks. In quark confinement, the state of the quantum chromodynamics vacuum plays a crucial role. Although this phenomenon is still not understood, it is believed that it finds its origin in some condensation mechanism.

[3] One could also add statistical mechanics to this list. A problem is that it is nowadays impossible to distinguish the disciplines of statistical mechanics and theoretical condensed matter physics in a reasonable way - it is just the same. On the introductory level, statistical mechanics is presented

In condensed matter physics, one tries to explain the behaviours of macroscopic bodies and every gram of macroscopic matter contains of order 10^{23} particles - closer to infinity than to a few. It turns out that special varieties of emergent phenomena occur in this limit, and these are the subject of quantum condensed matter physics.

A first peculiarity of the 'infrared', the physics of the system at long length scales and small energies, is that one can be suprisingly sloppy in the description of the nature of the microscopic 'ultraviolet'. Starting out from quite different microscopic systems, one ends up with *qualitatively* similar macroscopic physics. For this reason, one might as well start out with the simplest possible *model* for the microscopic physics having the properties which really matter (symmetries, conservation laws, dimension of Hilbert space). It is far easier to establish the qualitative features of the collective system from the model. One is left with the wrong numbers, but the spectrum of qualitative behaviours of macroscopic systems is of such a richness that one can afford to not worry at all about quantitative accuracy. In practice it is even rarely possible to establish these numbers, and one leaves it to the experimentalists to find the parameters of the effective theory. One is sure that in principle it should be possible to 'deform' the model theory in the true (quantitative) theory without changing the qualitative features at all. Anderson calls this *the principle of adiabatic continuity.*

One will be constantly confronted with this general principle studying the remainder of this text. In fact, there is not a single occasion where the starting point will be a precise and fully realistic description of the microscopic reality. Instead one will find, time after time again, highly simplified models. If one is used to the quantitative rigor of e.g. atomic physics, this habit might at first give an impression that one is dealing with some pseudo-science. Keep in mind, however, that the validity of this model appoach rests on the powerful principle of adiabatic continuity.

A next principle emerging in the thermodynamic limit is the highly non-trivial principle of spontaneous symmetry breaking. One learns from quantum mechanics that nature is in first instance organized according to symmetry principles. This has to be learned, because symmetry has a less prominent role in the macroscopic world surrounding us, which obeys the laws of classical physics. This dominating role of symmetry gets lost. A clear way of expressing this difference is as follows: *classical objects do not correspond with quantum-mechanical eigenstates.*

Consider a piece of ordinairy macroscopic matter, like the chair you are sitting on. It is not at all a problem to write down an exact Hamilonian for this chair in terms of the atomic physics effective theory: a near infinity of carbon-, hydrogen atoms, etcetera, with their mutual interactions. This Hamiltonian will be translationally invariant: any of the atoms can be located anywhere in space. Because the Hamiltonian has this invariance, the eigenstates of the Hamiltonian should obey this invariance as well: it should be *impossible* to determine where any of the atoms are from the eigenstates of the Hamiltonian. Reality looks of course very different. In solid matter, the atoms

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with a stronger focus on thermal fluctuations, while condensed matter physics emphasizes zero-temperature quantum aspects.

form a (more or less) regular array and every atom has to keep a fixed distance to its neighbours in order for the solid to exist. Hence, the translational invariance on the level of individual atoms got lost and all what is left is a single invariance for the motion of the body as a whole.

Quantum-mechanics is of course more fundamental than tables and chairs and it should be possible to write down the quantum-mechanical wave functions describing the latter. As I just discussed, these states are not eigenstates and quantum mechanics alone is not sufficient to explain why these states are not eigenstates. We need in addition the help of the laws of the big numbers: *although a few particles cannot break the symmetry spontaneously, an infinity of them can.*

This phenomenon of atoms forming chairs, thereby violating the invariances of the 'fundamental' Hamiltonian (breaking the symmetry), is quite general and the forms of matter it produces are called 'classical condensates' [4]. These classical condensates dominate the macroscopic world. Next to the 'crystalline state' (to which chairs belong), it also occurs in less-familiar situations. Magnets are rather close to crystals. However, the same basic mechanism is also active in truely exotic states of matter, like superconductors and superfluids. Even the Fermi-liquid state, describing the collective state of electrons in metals, belongs to this category. They have all in common that the symmetry breaking brings the condensate in a collective state which obeys the laws of classical physics. A description of the mechanism responsible for this phenomenon will be the main theme of these lectures.

The theory describing the classical condensates was gradually developed during the fifties and sixties. Untill not so long ago, it was believed that *all* macroscopic condensed states belong to this classical category - for this reason I like to call it *conventional* condensed matter physics. During the last two decades or so, the emphasis has been shifting toward systems which do not conform to this classical pattern. The *unconventional* part of quantum condensed matter physics deals with macroscopic systems showing collective behaviours which no longer can be understood within a classical framework. Examples are a variety of quantum critical systems, but also the incompressible quantum liquids which are characterized by an energy scale. Although the research frontier is no longer in the classical sector of reality, a thorough understanding of this sector is a prerequisite for the study of the non-classical states: at the least, one should learn to appreciate the unrobustness of the principles on which our daily world rests.

1.2 Classicalness as an emergent phenomenon.

As I already announced, there is a single unifying mechanism which explains the behaviours of classical condensates, from simple crystals up to fermi-liquids, in terms

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[4] Next to these condensates, the macroscopic world consists also of classical gases and liquids. The classical nature of these disordered states finds it origin in a different mechanism - the difficult concepts of temperature and entropy play here a central role. This is also well understood, but the required formalism puts this issue beyond the limits of the present course.

of special many-particle quantum states. This mechanism is called 'semi-classical mean-field theory', often abbreviated with 'the' mean-field theory (there are others !). Despite its amazing succes, a general mathematical proof for the validity of mean-field theory is not yet delivered - in principle, it should be possible to deliver this proof because the microscopic theory is known. Although it cannot be written as a collection of theorems, it does have the status of physical law in the sense that it accurately describes what nature does. It is a typical example of a theory in physics: without the help of experiment, it would never have been discovered.

Reading this section for the first time, it might appear as rather abstract and incomprehensible. I will try to lessen this by quoting examples derived from the context of the familiar crystalline order. This section is intended as a central reference point for the further reading of this text. You will notice that it will gradually become alive, seeing it at work time after time again.

The classical zero-temperature state of matter is completely specified by a single axiom on the nature of the macroscopic wavefunction (issues (i)-(iii)). Everything else is deduced from quantum-mechanics:
(i) Everything, including macroscopic objects, is described by states in Hilbert space. In many particle problems, the relevant Hilbert space is the Fock space as discussed in chapter II. It appears possible to construct a special kind of many-particle state which describes a classical macroscopic object. *The many-particle wave function* $|\Phi_{Cl}\rangle$, *describing the ground state of a classical condensate, has a finite overlap with a single determinant wave function* $|\Phi^0_{Cl}\rangle$ *which is further specified in (ii) and (iii).* Explicitely (N_H is the dimension of Fock space),

$$|\Phi_{Cl}\rangle = A|\Phi^0_{Cl}\rangle + \sum_{i=2}^{N_H} a_i|\Phi_i\rangle \tag{1.1}$$

with A finite.

This is the (unproven) conjecture on which the whole building rests - the remainder follows by mere deduction. Why is it remarkable? As you might know, the Hilbert space of relevance to many particle problems (Fock space) has a very large dimension (like $N_H = 2^N, N \to \infty$, for the simplest spin problem). The eigenstates should consist of linear superpositions of enormous numbers of the single determinant states, which span Fock-space. In fact, in some cases it can be rigorously shown that not a single basis state has a *finite* weight in the *exact* eigenstates of the macroscopic system. The miracle is now that the *inexact* wave function (1.1), 'dominated' by only one of these basis states, becomes 'correct' as well. As we will discuss in chapter V, this apparent paradox is believed to find its resolution in a subtlety occurring in the approach to the thermodynamic limit.

(ii) The 'classical' state Φ^0_{Cl} is constructed from rather special *single particle* states. These states actually *define* the classical equivalents of the quantum mechanical single particle states, and are best called 'generalized coherent states'. Consider a set of second quantized operators, creating and annihilating microscopic entities $\{\hat{X}_i^\dagger, \hat{X}_i\}$. These describe the physics at the energy scale where the tendency towards classical condensation becomes first visible. For instance, in simple van der Waals crystals, the $\hat{X}^\dagger$ would create complete atoms, and the atoms themselves should be in their precise atomic quantum states. In terms of these operators, wavepackets are formed,

$$\hat{Y}^\dagger(\{\eta_i\}) = \sum_j \alpha_j(\{\eta_i\})\hat{X}_j^\dagger \tag{1.2}$$

corresponding with the 'most classical' version of the particle, where the set of scalars $\{\eta_j\}$ describes the classical phase space variables of the particle. For atoms in crystals, the $Y^\dagger$'s are the familiar wave-packets, localizing the particle as much as possible around an average classical position $\vec{R}_i$. In this step, the special role played by symmetry in quantum mechanics gets lost - the wave packet is constructed in such a way that the position of the atom is determined, although one is still free to choose that position. If the symmetry is more complicated, it is less obvious how to 'translate' the invariances of the quantum system into its remnants on the classical level. This art is called 'generalized coherent states' and we will meet less trivial examples in the context of spin problems and superconductivity.

(iii) The single particle states (1.2) do not make sense on their own. They only relate to nature if an *infinity* of them work together in forming the 'classical' single determinant states,

$$|\Phi^0_{Cl}(\{\eta\})\rangle = \Pi_{i=1}^N \hat{Y}^\dagger(\{\eta_i\})|vac\rangle \tag{1.3}$$

where the set of scalars $\{\eta\}$ describe the classical degrees of freedom of all N particles ($|vac\rangle$ is the 'bare' vacuum). This has to be stressed over and over again: *the classical state of nature is a collective effect.*

(iv) Observable quantities in quantum mechanics correspond with operators which can be expressed in terms of the algebra $\{\hat{X}_i, \hat{X}_j^\dagger\}$. For instance, density and current operators are build from the bilinears,

$$\hat{W}_{ij} = \hat{X}_i^\dagger \hat{X}_j \tag{1.4}$$

The qualitative properties of the classical system follow from calculating the expectation values of these operators with regard to the state (1.3). For instance,

$$W^0_{ij}(\{\eta\}) = \langle\Phi^0_{Cl}(\{\eta\})|\hat{W}_{ij}|\Phi^0_{Cl}(\{\eta\})\rangle \tag{1.5}$$

and the $W(\{\eta\})$'s relate to the classical densities and currents. For instance, the expectation value of the operator measuring the density of atoms in real space would specify the positions of all atoms if the wave function (1.3) would have been constructed from spatially localized wave packets. Alternatively, using spin coherent states, (1.5) would map $su(2)$ (spin-) algebra on its classical 'image': an 'arrow' (classical dipole) of fixed length which can point in any direction, parametrized by the Euler angles $\{\eta\} = \theta, \phi$.

(v) The classical energy of the system is determined by the expectation value of the Hamiltonian,

$$E^0_{Cl}(\{\eta\}) = \langle\Phi^0_{Cl}(\{\eta\})|\mathcal{H}|\Phi^0_{Cl}(\{\eta\})\rangle \tag{1.6}$$

Because the parameters $\{\eta\}$ are still arbitrary, (1.6) defines an energy *landscape* which is in principle quite complicated: the energy as function of the classical phase space parameters $\{\eta\}$ (e.g., positions and momenta of all atoms, or the Euler angles of all spins). However, because the η's are scalars, the classical ground state (state of lowest energy) can be determined by *minimimizing* the classical energy to all η's,

$$\frac{\delta E^0_{Cl}}{\delta \eta_i} = 0. \tag{1.7}$$

which is much easier than diagonalizing the Hamiltonian as is required in quantum-mechanics. Let us label the set of phase space parameters minimizing the classical energy with $\{\eta^0\}$. The classical ground state as appearing in (1.1) is then given by,

$$|\Phi^0_{Cl}\rangle \equiv |\Phi^0_{Cl}(\{\eta^0\})\rangle \tag{1.8}$$

Although often the ground states are emphasized, notice that the Φ^0_{Cl} with arbitrary η's are still genuine classical states, now describing the classical *excitations.*

(vi) The 'classical' states (1.3) do not yet correspond with the proper states (1.1) describing the classical condensates. They are actually no more than 'handles', required to get at the latter. The crucial point is, however, that the true states (1.1) can be reached from the classical state (1.3) by *perturbation theory.* This is implied by the assumption that the overlap between the true state and the classical ansatz is *finite.* In problems with an infinite number of degrees of freedom, perturbation theory acquires a different, more fundamental status than is the case in few body problems. In the latter, perturbation theory acts to gradually improve the numbers. In the former, the zero-th order has to be correct in the sense that the overlap with the true wave function has to be finite, otherwise the perturbation expansion will *diverge.* These infinities cannot be cured within perturbation theory, and the only remedy is to search for a better choice for the zeroth order which is the starting point of the expansion. In practice, perturbation theory is the most important diagnostic tool available. One chooses some collective state as zeroth order and subsequently one looks for infinities in the perturbation expansion around this state. If these occur, one is sure that the state is wrong and that the physics has to be truely different from the expectations which are hard-wired in the choice of zeroth order. Unfortunately, this procedure is not always fool-proof. The infinities might occur in any order, while in practice one is often limited to the evaluation of only the lowest order terms. As we will see, in some special cases it is nevertheless possible to proof that the perturbation expansion is convergent up to all orders - see chapter 7.

(vii) Although the terminology is non-standard, I like to call the state $|\phi_{Cl}\rangle$ (1.1) ('dressed up' with perturbation theory) the 'semiclassical' state, and the single determinant state Φ^0_{Cl} the 'classical' state. In fact, the classical state already yields a *qualitatively correct* description of the physical nature of the system. The reason is simple. All what matters are the expectation values of the operators corresponding with observables,

$$\begin{aligned} \langle \Phi_{Cl} | \hat{W}_{ij} | \Phi_{Cl} \rangle &= A^2 W^0_{ij}(\{\eta\}) + \\ &\sum_i (A^* a_i \langle \Phi^0_{Cl} | \hat{W}_{ij} | \Phi_i \rangle + A a^*_i \langle \Phi_i | \hat{W}_{ij} | \Phi^0_{Cl} \rangle) + \sum_{ii'} a^*_i a_{i'} \langle \Phi_i | \hat{W}_{ij} | \Phi_{i'} \rangle \end{aligned} \tag{1.9}$$

although the terms in the second line will usually average out to zero, this does not really matter as long as the overlap A between the semi-classical and classical states is finite. The magnitude of the classical property W^0_{ij} will get *reduced* by an amount A^2, but it will remain *finite*, and its finiteness is what really matters. For instance, in the classical crystal the atoms are precisely at their crystalline positions, but in the semiclassical crystal the atoms show zero point motions. However, as long as all atoms spend a finite amount of time at their classical lattice positions, the crystal as a whole still exists.

What did we actually achieve? The above is a precise description of the relationship between quantum physics and classical physics: the latter is a special case of the former, realized as a *collective* effect in the limit where the number of constituents approaches infinity. Notice that this is quite different from the way this relationship appears in elementary quantum-mechanics textbooks. The inventors of quantum mechanics exploited some *analogies* with classical mechanics to get some guidance in the process of formulating quantum-mechanics. The founding fathers did not know about the far more difficult many particle quantum-mechanics, needed to understand the above. In this historical setting, it becomes understandable that great minds (like Einstein) got seriously confused. This confusion propagates untill the present day in the field calling itself 'foundations of quantum-mechanics': it is insisted on that classicalness is more fundamental than quantum-mechanics, and one should somehow force quantum-mechanics to conform with the laws of classical physics. This is silly: classicalness is nothing more than a *collective effect* of quantum mechanics and, in a rigorous sense, quantum mechanics is more complete than classical physics: information concerning the fully quantum-mechanical system gets lost if the special case 'classical physics' is realized (e.g., the state (1.1) is not an eigenstate)[5]. This observation is actually not at all generally appreciated, and only recently attempts are undertaken to reformulate the foundations of quantum mechanics taking classical condensation into account[6].

A first advantage of this modern, many-particle view on the phenomenon 'classical physics' is that it shows that the classical nature of macroscopic bodies is actually *not at all self-evident*: there exists no theorem implying that the construction (i)-(vii) holds without exceptions. I already pointed at the existence of a number of exceptions (the 'unconventional' part), and I will present some cases in the text where one actually can proof that whatsoever is realized is something different from a classical entity. A requirement for the stability of the classical state is that the classical energy landscape (1.6) is characterized by a *a global minimum.* This is easy to understand. Imagine that this energy landscape is characterized by an infinite degree of

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[5] This issue becomes actually rather acute in the context of quantum-gravity: the classical limit (general relativity) seems here to be so far removed from the full quantum theory that the former yields no guidance at all with respect to the formulation of the latter.

[6] For instance, it appears unnecessary to introduce separate axioms concerning the collapse of the wave function in the measurement process (Copenhagen interprtation). This can be understood as a many-particle effect already contained in the basic axioms of quantum-mechanics: the exact wavefunctions of the test particles have to become part of the inexact wavefunction describing the measuring machine, which itself is a classical condensate.

degeneracy: there exists an infinity of classical states of a different appearance, which nevertheless have the same energy. One directly infers a problem with the finiteness of the perturbation theory. The system will tunnel from one classical minimum to the next and all these degenerate states would end up, having the same weight in the ground state wavefunction: the overlap with any particular classical state would be rigorously zero!

It is a specialty of classical nature, that the existence of such an unique global minimum always goes hand in hand with *regularity*. Stronger, classical ground states seem always to show the property of *long range order*: the condensate consists of a basic unit which repeats itself, filling up physical space. A typical example of long range order is the periodic arrangements of atoms in crystals[7].

The presence of long range order allows for a further characterization of classical condensates in general terms. The quantity specifying the magnitude of the long range order is the *order parameter*. In simple cases, it is directly clear how to define the order parameter. For instance, in the case of crystalline order it measures to what extent all primitive cells of the crystal are centered on points of the Bravais lattice. However, the nature of the long range order can be much harder to recognize and the identification of the order parameter is often a key step in the process of understanding a problem. This will be more than once illustrated in these notes - see the chapter on superconductivity.

A central physical property of classical condensates is the property of 'rigidity' (or 'hardness'). This is nothing else than the familiar property of solid objects to respond as a unity to external perturbations, as long as the perturbation is not too severe. Rigidity has a fundamental reason: because the ground state corresponds with the global minimum of the classical energy, a finite amount of energy has to be paid to change anything *inside* the system. Despite its familiarity, keep in mind that it is not obvious: *exact quantum eigenstates do not seem to carry rigidity.*

The global minimum of energy occurs in the phase-space of all constituents. It is therefore possible to consider *collective* motions where all constituents are brought out of their equilibrium positions by an infinitisimal amount. These excitations are called *collective modes* and it turns out that these modes dominate in many cases the low energy end of the excitation spectrum. They correspond with minimal perturbations of the long range order, and they are also called 'order parameter modes'. These have some universal properties in common, which do not depend on the specific kind of long range order. These are tied to the symmetries in the problem.

Symmetries of central importance are *continuous* symmetries, like translational- and rotational invariance. I already described how their dominance in the quantum-mechanical sense got lost in the classical condensation process. In the end product (the long range ordered state) very little is left of these original invariances. For instance, in a crystal all atoms have to keep a fixed distance from their neighbours

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[7] Glasses are not characterized by long range order. However, they do not correspond with thermodynamic ground states either.

which rather precisely specifies their positions in space. However, there is still something left: *we cannot specify the position of the whole crystal in space.* More generally, instead of the freedom to place the constitents 'anywhere' we are left with the freedom to place the condensate as a whole 'anywhere'. It appears now possible to consider this uniform displacement as a limiting case of an order parameter mode. These order parameter modes correspond with periodic modulations of the order parameter with a wavelength λ. Quite generally, if $\lambda \to \infty$ there is at least one mode which will exactly correspond with the uniform displacement. Hence, *if a continuous symmetry is spontaneously broken, at least one mode exists with a frequency (energy) tending to zero in the long wavelength limit.* In addition, the frequency of his mode will approach this limit linearly ($\sim k \sim 1/\lambda$), and the lifetime of the mode will become infinitely long in the long wavelength limit. This should already be familiar from the behaviour of sound waves (acoustic phonons) in crystals. However, it is a very general phenomenon which can be rigorously proven (the so-called Goldstone theorem), and these modes are called 'zero-modes' or 'Goldstone modes'. Again, awareness of the general principle will be of much help in recognizing what is going on in less familiar situations.

The attentive reader should now protest: Why do classical condensates exist at all? Wasn't it argued that the minimum of the classical energy should be unique in order to prohibit quantum melting? We now learn that the ground state is always highly degenerate when a continuous symmetry is into play, because it does not cost energy to uniformly shift the order parameter. Part of the answer is straightforward: moving the whole crystal involves a macroscopic (kilogram-like) mass and it is easy to estimate that such a quantum fluctuation will take longer than the age of the universe to have any measurable impact. This is, however, not the full answer. In contrast to the infinite wavelength case (uniform displacement), the finite wave-length Goldstone modes are truely internal excitations and they produce a high density of alternative classical states at low energies. Although systems characterized by broken continuous symmeries are non-degenerate, they are not so far away from being degenerate, and they should be considered as border line cases. In fact, the existence of classical order is decided by secondary factors like spatial dimensionality and/or magnitude of the microscopic quantum fluctuations. This is the fundamental reason why it is so difficult to prove the existence of classical condensation in general terms.

1.3 Touring the classical world.

The remainder of these notes is devoted to putting flesh on the general framework introduced in the previous section. If crystalline order would have been all, this text would have become fairly short. However, the paradigm is powerful and applies to far more remote and exotic corners of physical reality. The strategy is to start out with the familiar: the crystalline order as discussed in chapter IV. From this 'home-base', we will climb towards the more distant summits of the classical sector.

The problem with chapter IV is that 'classicalness' works too well in worlds made out of atoms. Atoms are fairly heavy objects and there is little quantum-mechanics left already in the 'ultraviolet' of this problem - this tends to obscure what is problematic about the classical world. For this reason, we shift attention as soon as possible to matter made out of *electrons.* The quantum-mechanics of individual electrons is much harder to 'collectivize' in classical states and the questions appear here in a more natural setting. In addition, electron systems also show a more interesting spectrum of classical condensations than atoms do, not in the last place due to the more interesting ultraviolet.

Much of the hard work is done in chapter V, dealing with electron systems dominated by hard-core repulsive interactions. Here we meet *magnetism.* Electron spins have the advantage that they are relatively easy to handle mathematically. For this reason, spin problems have always played an important role in the development of many particle physics, and they continue to do so. The starting point will be the *strong coupling limit* where the electron-electron interactions dominate over the kinetic energy. Under certain conditions, it is possible to localize the electrons while their spins are still free to move: the magnetic (or 'Mott-Hubbard') insulators. This turns out to be an interesting excercise in projective renormalization: I will present the rigorous way of turning electrons into spins.

This will yield the so-called Heisenberg spin problems. The classical condensates, associated with these spin systems, are the *Néel states* or *anti-ferromagnets* - ferromagnets have a very special status, as will be explained. In this context, the questions of principle are most easily adressed, and in this regard the discussion of the Néel state is the most important part of this text.

As a next step, it will be shown how to handle classical condensation if the *kinetic energy* is dominating in the ultraviolet, the so-called *weak coupling limit.* This is a true miracle: despite the fact that the system of electrons is in the quantum-limit, it still appears possible to form classical condensates, such as the *spin density waves* and *charge density waves.* The key insight is that one no longer attempts to 'make' the system classical (in the sense of (1.2)) by forming wave-packets in real-space, but instead one constructs wave packets in *momentum space*, satisfying first the kinetic energy. In fact, one can connect real space and momentum space condensation smoothly without affecting the macroscopic properties qualitatively - the principle of adiabatic continuity is seen at work.

Chapter VI deals with *superconductivity and superfluidity.* In technical respects, this is a repetition of chapter V. Conceptually, it is a different matter. Up to spin ordering, we tend to accept classical matter as it is: it is somehow in the line of our expectations. Superconductivity is different. One really needs the general principles in order to accept this phenomenon - the reason seems to be that a counter-intuitive symmetry is broken: local gauge symmetry. The strategy in this chapter will be unconventional: it will follow precisely the same pattern as used to explain magnetism. First the strong coupling limit is considered where it is much easier to get a clear view on what is going on. Subsequently, these results will be continued to weak coupling, where nature is in the form of the *Bardeen-Cooper-Schrieffer theory.*

At the very edge of the classical universe, the *Fermi-liquid* state is found: the collective state of electrons in normal metals. As will be discussed in chapter VII, it is even not quite clear if calling this state a classical one is still meaningful. Next to genuine classical features (like an order parameter, a 'classical wavefunction', and zero-modes), this state is also characterized by low lying excitations which are not quite classical: the quasiparticles. Also in technical respects, it becomes manifest that one is balancing on the outer edge of the classical world. The relatively unsophisticated mathematical machinery as introduced in the introductory chapters II and III no longer suffices, and much of chapter VII is spent on giving a first impression of the powerful machinery of quantum field theory.

2 The foundations: quantum-mechanics.

In this chapter some basic facts of quantum-mechanics, as needed in the remainder of this course, will be recollected. This is mostly old news.

The main focus of this chapter will be on the two level problem. The other standard problems of basic quantum mechanics, like the particle in the box (with and without simple potentials) and the hydrogen atom, are well exposed in the standard textbooks. For unknown reasons, this is usually not the case with the two level problem and I believe it is impossible to master condensed matter physics if one does not exercise the most minimal problem of quantum mechanics.

What you need to know at this point: the quantum aspects of at least the classical sector of reality are made out of three basic constituents: collective modes which are like harmonic oscillators, and particles which either behave like non-interacting particles (mostly electrons) or like spins. The basic behaviors of these objects are the corner stones of most quantum-mechanics books. Let us start with the very basics, the efficient and profound way of looking at quantum-mechanics due to Dirac.

2.1 The basics.

The wave function of a particle with spin 1/2

A particle with spin-$\frac{1}{2}$ is described by a wave function $\psi(\vec{r}, s)$. Here, $\vec{r}$ is the position in physical space of the particle and s its spin component, defined with respect to an arbitrary reference axis, usually called the z-axis $(s = \pm\, \frac{1}{2})$.
Interpretation:

$$|\psi(\vec{r}, s)|^2 \; d\vec{r} \;=\; \begin{array}{l}\text{probability to find the particle with spin } s \\ \text{in an infinitesimal volume } d\vec{r} \text{ around } \vec{r}.\end{array}$$

Given this probabilistic interpretation, the wave function has to be normalized according to:

$$\sum_{s=\pm\,\frac{1}{2}} \int d\vec{r}\; |\psi(\vec{r}, s)|^2 = 1 \; . \tag{2.1}$$

One can also write $\psi(\vec{r}, \frac{1}{2})$ and $\psi(\vec{r}, -\frac{1}{2})$ as the two components of a *spinor* (vector in the internal spin-space):

$$\psi(\vec{r}) = \begin{pmatrix} \psi(\vec{r}, \frac{1}{2}) \\ \\ \psi(\vec{r}, -\frac{1}{2}) \end{pmatrix} \; . \tag{2.2}$$

Dirac formalism for an arbitrary quantum system

Nature consists of a linear space (Hilbert space) spanned up by vectors ('states') $|\psi >$. The label ψ might refer to any meaningful property of the system, like its

spatial/temporal position, its internal spin state, its energy, etcetera. $|\psi>$ is called *ket*. To every $|\psi>$ a *bra* $<\psi|$ is associated (in fact, a vector in the dual Hilbert space). It is then possible to form the scalar product of two states $|\psi_1>$ and $|\psi_2>$: $<\psi_1|\psi_2>$, a "*bra-cket*". This can also be considered as a projection of $|\psi_2>$ on $|\psi_1>$, or as the overlap of $|\psi_2>$ and $|\psi_1>$.
Property:

$$<\psi_1|\psi_2>=<\psi_2|\psi_1>^* \quad . \tag{2.3}$$

In addition, brackets have to be normalized

$$<\psi|\psi>=1 \quad . \tag{2.4}$$

spin-$\frac{1}{2}$ particle in Dirac notation

$|\vec{r},s>$ is the state describing a particle at position $\vec{r}$ in physical space with spin s. The scalar product of two states of this type is

$$<\vec{r}\,'s'|\vec{r}s>=\delta(\vec{r}-\vec{r}\,')\;\delta_{ss'} \quad . \tag{2.5}$$

(2.5) shows that the vectors $\{|\vec{r},s>\}$ form an *orthonormal* system. It is also *complete*, an arbitrary state $|\psi>$ describing a spin-$\frac{1}{2}$ particle can be written as a linear combination of states $|\vec{r},s>$; the expansion coefficients are the projections $<\vec{r},s|\psi>$. Hence:

$$|\psi>=\sum_s\int d\vec{r}\;|\vec{r},s><\vec{r},s|\psi> \quad . \tag{2.6}$$

The wave function, as introduced under (i), has the meaning

$$\begin{aligned} <\vec{r},s|\psi> &= \psi(\vec{r},s) \quad , \\ <\psi|\vec{r},s> &= \psi^*(\vec{r},s) \quad . \end{aligned} \tag{2.7}$$

$<\vec{r},s|\psi>$ is called the wavefunction of the particle in the position representation.

$\Longrightarrow$ exercise 2.1

(1.2) can also be written in the mixed form

$$\psi(\vec{r})=\psi(\vec{r}\,,\tfrac{1}{2})|\tfrac{1}{2}>+\psi(\vec{r}\,,-\tfrac{1}{2})|-\tfrac{1}{2}> \quad . \tag{2.8}$$

with different ways of writing the kets of the spin-1/2:

$$\begin{aligned} |\tfrac{1}{2}> \;&\equiv\; |\uparrow> \;\equiv\; |+> \;\equiv\; \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \\ |-\tfrac{1}{2}> \;&\equiv\; |\downarrow> \;\equiv\; |-> \;\equiv\; \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad . \end{aligned} \tag{2.9}$$

Representation free notation

$|\psi>$ has the advantage that one does not have to specify what physical question one asks from the system - for instance, $|\psi>$ has the same information content as $\psi(\vec{r}\,, s)$ if one asks for position information. If one wants to know about momentum, one can use $|\psi>$ as well. $|\vec{p}\,, s>$ is the state of a particle with momentum $\vec{p}$ and spin s , and

$$\hat{\psi}(\vec{p}\,, s) =< \vec{p}\,, s|\psi > \tag{2.10}$$

is the wavefunction in the momentum representation.

$\Longrightarrow$ exercise 2.2

Complete orthonormal systems

Since (2.6) is true for all $|\psi>$, we might as well define the identity operator

$$\sum_s \int d\vec{r}\ |\vec{r}s> \quad <\vec{r}s| = 1 \tag{2.11}$$

obviously so, because the system $\{|\vec{r}, s>\}$ is complete. There are many other complete systems, like $\{|\vec{p}, s>\}$. Any quantum-mechanical system is characterized by a complete orthonormal system,

$$< j|i >= \delta_{ij} \quad , \tag{2.12}$$

and

$$\sum_i |i> \quad <i| = 1 \ . \tag{2.13}$$

An arbitrary state $|\psi>$ can therefore be written as

$$|\psi> \quad = \sum_i |i> \quad <i|\psi> \quad = \sum_i \psi(i)|\ i> \tag{2.14}$$

the expansion of ψ in terms of states $|i>$. If i refers to a continuous variable, one should use a Dirac delta-function on the right hand side of ref. (2.12) instead of the Kronecker delta [compare with (2.5)].

Operators

A is an operator with matrixelements $A_{ij} \equiv< i|A|j>$.
The hermitian conjugate $A^\dagger$ of A is defined by

$$\left(A^\dagger\right)_{ij} = A^*_{ji} \ . \tag{2.15}$$

$$A \text{ is } \textit{hermitian} \text{ if } \qquad A = A^\dagger \ ; \tag{2.16}$$

$$A \text{ is } \textit{unitary} \text{ if } \qquad AA^\dagger = 1 \ . \tag{2.17}$$

$\Longrightarrow$ exercise 2.3

In quantum-mechanics, A is a linear operator in Hilbert space, and $|i>$ is a state in the orthonormal system $\{|j>\}$. $A|i>$ is a different state, which is sometimes written as $|Ai>$ (with bra $<Ai|$) . A might be expanded as:

$$A|i> \quad = \sum_j \; |j> \quad <j|A|i> \quad = \sum_j \; A_{ji} \; |j> \quad . \tag{2.18}$$

Since

$$<j|A|i> = <j|Ai> = <Ai|j>^* \tag{2.19}$$

and

$$<j|A|i> = <i|A^\dagger|j>^* = <i|A^\dagger j>^* = <A^\dagger j|i> \tag{2.20}$$

it follows that A acting on a ket is equivalent to $A^\dagger$ acting on a bra: $<j|Ai> = <A^\dagger j|i>$.

Observables

Every measurable quantity (observable) corresponds with a hermitian operator acting in Hilbert space. If A is hermitian, the eigenvalues $\lambda = \alpha_1 \; , \alpha_2 \; , \cdots$ as determined by

$$A|\psi> = \lambda|\psi> \tag{2.21}$$

are *real* quantities, with a spectrum which can be either discrete or continuous. This equation also defines the eigenstates $|\alpha_1> \;\; , |\alpha_2> \;\; , \cdots$, such that $A|\alpha_i> = \alpha_i|\alpha_i>$.

$\Longrightarrow$ exercise 2.4

α_i are the only possible outcomes for the measurement of the observable A. In a simultaneous measurement of two physical quantities A and B, the outcomes for both quantities can only be completely determined if the operators commute,

$$[A, B] \equiv AB - BA = 0 \quad . \tag{2.22}$$

The Hamiltonian

The Hamiltonian $\mathcal{H}$ is the operator for the total *energy*. Its eigenstates are determined by (see (2.21))

$$\mathcal{H} \; |\psi> \quad = E \; |\psi> \tag{2.23}$$

and these play a special role: Eq. (2.23) is the time independent Schrödinger equation, the object which keeps nature in a good shape - for some reason time and/or energy are very important quantities. We define its eigenvalues and eigenstates by

$$E = \varepsilon_1 \; , \varepsilon_2 \; , \cdots \quad , \tag{2.24}$$

$$|\psi> \quad = |\varepsilon_1 \; > \; , \; |\varepsilon_2 \; > \; , \cdots \; . \tag{2.25}$$

This eigenvalue-spectrum can of course be continuous.
If we start out at $t = 0$ with

$$|\psi>_{t=0} \quad = | \; \varepsilon_j \; > \quad , \tag{2.26}$$

it follows from the time-dependent Schrödinger equation

$$i\hbar \; \frac{\partial|\psi>}{\partial t} = \mathcal{H}|\psi> \quad , \tag{2.27}$$

that

$$|\psi>_t \quad = e^{-i\varepsilon_j t/\hbar} \; | \; \varepsilon_j \; > \quad . \tag{2.28}$$

$\Longrightarrow$ exercise 2.5

To solve the Schrödinger-equation (2.23) it can be convenient to execute the calculations in a specific representation, for instance the position representation,

$$\mathcal{H} \; \psi(r) = E \; \psi(r) \quad ,$$

where we recognize the Schrödinger equation as presented in introductory textbooks. Keep in mind that this is in fact a special case of the more general expression (2.23).

$\Longrightarrow$ exercise 2.6

Examples of single particle Hamiltonians

Quantum-mechanics started out with the exploration of one particle problems, mostly because these problems can be exactly solved in a variety of cases. In a strict sense, problems in nature are *never* precisely of a single particle nature. Fortunately, it appears that in a number of cases *effective* single particle problems can be extracted from the full many-particle reality, as you will frequently encounter in this lecture series.

The Hamiltonian of an isolated particle moving in an external, time-independent potential $V(\vec{r})$ is,

$$\mathcal{H} = \frac{\vec{p}^{\;2}}{2m} + V(\vec{r}) \quad , \tag{2.29}$$

where

$$\begin{aligned} \vec{p} \quad &\equiv \quad (p_x \; , p_y \; , p_z) \equiv (p_1 \; , p_2 \; , p_3) \qquad \text{momentum operator} \quad , \\ \vec{r} \quad &\equiv \quad (x \; , y \; , z) \equiv (x_1 \; , x_2 \; , x_3) \qquad \text{position operator} \quad , \\ \vec{p}^{\;2} \quad &= \quad p^2 \equiv p_x^2 + p_y^2 + p_z^2 = p_1^2 + p_2^2 + p_3^2 \quad . \end{aligned} \tag{2.30}$$

Notice the two ways of labeling physical space. In position representation, the momentum operator becomes,

$$p_j = -i\hbar \, \frac{\partial}{\partial x_j} \quad , \quad j = 1, 2, 3 \tag{2.31}$$

The single particle Hamiltonian becomes

$$\mathcal{H} = -\frac{\hbar^2}{2m} \, \Delta + V(\vec{r}) \ , \tag{2.32}$$

$$\Delta \equiv \nabla^2 = \frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} + \frac{\partial}{\partial z^2} = \sum_j \frac{\partial^2}{\partial x_j^2} \ . \tag{2.33}$$

Some examples of textbook potentials:

$V(\vec{r}) = 0$	particle in the vacuum
$V(\vec{r}) = -\frac{e^2}{r}$	electron in the electric field of a point charge
$V(\vec{r}) = \frac{1}{2} m\omega_0^2 r^2$	3-dimensional harmonic oscillator with characteristic frequency ω_0
$V(\vec{r}) = \begin{cases} 0 & r < r_0 \\ \infty & r > r_0 \end{cases}$	particle in a spherical box with radius r_0
$V(\vec{r}) = \begin{cases} 0 & \lvert z \rvert > z_0 \\ -V_0 & \lvert z \rvert < z_0 \end{cases}$	electron in the neighborhood of an attractive interface (width $2z_0$, depth $-V_0$), e.g., in between two semiconductors

The last three cases are examples of model potentials. Even on the single particle level it is rarely possible to obtain closed, analytic solutions for realistic potentials which are usually rather complicated. However, in the absence of disorder and chaotic behavior, it appears possible nowadays to obtain numerical solutions to any desired accuracy for every $V(\vec{r})$ one can imagine. This will be further discussed in the chapter on band structure.

$\Longrightarrow$ exercise 2.7

The two level problem.

Another very useful toy problem is the so-called two level problem. In most elementary textbooks it is rather underexposed (with the notable exception of Feynman's 'lectures in physics'), despite the fact that it is at the core of a large variety of physically interesting problems.

We assume that the world consists of two states, $|1>$ and $|2>$. In the spirit of Dirac, $|1>$ and $|2>$ could be anything (which makes this toy so widely applicable) but to help the imagination we consider it here to be a simplified version of the H_2^+ molecule: $|1>$ labels the atomic s-state of the electron centered on one proton and $|2>$ denotes the s-state around the other proton. It is assumed that these states form a small, but nevertheless complete orthonormal set,

$$|1><1| + |2><2| = 1 \tag{2.34}$$

Since this set is complete, we can project the Hamiltonian to find, in full generality,

$$\mathcal{H} = |1> \varepsilon_1 <1| + |2> \varepsilon_2 <2| + |1> t <2| + |2> t^* <1| \quad , \tag{2.35}$$

with matrix elements

$$\begin{aligned} \varepsilon_1 &= <1|\mathcal{H}|1> \quad , \\ \varepsilon_2 &= <2|\mathcal{H}|2> \quad , \\ t &= <1|\mathcal{H}|2> \quad , \\ t^* &= <2|\mathcal{H}|1> \end{aligned} \tag{2.36}$$

This is the general structure of the two level problem. Applied to the H_2^+ molecule, we imagine that we start out assuming that both protons are on different sides of the universe so that their electronic wavefunctions do not overlap: t is zero. The atomic states are of course degenerate (in the absence of electric fields etcetera) such that $\varepsilon_1 = \varepsilon_2 = \varepsilon$. We move the two protons closer together so that the atomic wavefunctions begin to overlap: *an electron can tunnel from one proton to the other* and this is parametrized by a finite 'tunneling amplitude', or 'hopping', or 'transfer matrix element' t. Of course, doing so the states $|1>$ and $|2>$ should be in principle be non-orthogonal ($<1|2> \neq 0$) but we assume that in the process the states are constantly re-orthogonalized - this will only change the values of ϵ and t and these we do not want to calculate anyhow.

If $\varepsilon_1 = \varepsilon_2 = \varepsilon$ and choosing for convenience t to be real, (2.35) the eigenvalues are determined from

$$\begin{vmatrix} \omega - \varepsilon & t \\ t & \omega - \varepsilon \end{vmatrix} = 0 \tag{2.37}$$

with solutions $\omega_\pm = \varepsilon \pm t$ and the eigenvectors are

$$\begin{aligned} |-> &= \frac{1}{\sqrt{2}}(|1> - |2>) \\ |+> &= \frac{1}{\sqrt{2}}(|1> + |2>) \end{aligned} \tag{2.38}$$

and $|\pm>$ forms of course again a complete orthonormal system. The Hamiltonian has a diagonal form in this new basis,

$$\mathcal{H} = |-> (\varepsilon - t) <-| + |+> (\varepsilon + t) <+| \quad , \tag{2.39}$$

Hence, assuming that $t > 0$, we find that the tunneling has lowered the energy of the $|->$ state and raised the energy of the $|+>$ state. This can be summarized in a picture (figure 2.1).

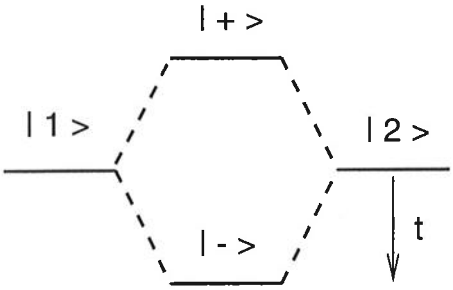

Figure 2.1: *Level diagram for the two level problem. The dashed lines indicate how the 'hybridized' states* $|\pm >$ *evolve from the 'pure' states* $|1, 2 >$.

One recognizes one of the laws of quantum mechanics. By allowing the electron to hop from one proton to the other it can explore a larger region of space and thereby increase its position uncertainty: the box becomes larger and the electron can reduce its average momentum and thereby reduce its kinetic energy. Hence, the energy of the lowest lying state ($|- >$) goes down. It actually means that if we prepare the H_2^+ system in its electronic ground state ($|- >$ occupied) it can gain energy by letting the protons come closer together, forming a molecule! This is quite a realistic picture of the glue which keeps molecules together: in chemistry it is called covalent binding. For this reason, the state $|- >$ is called a 'bonding' state. It is less obvious that this bonding state has a 'partner' ($|+ >$) which looks quite similar except that the signs are reversed - starting out with plane waves, this kind of states is completely invisible. States of this nature are called 'anti-bonding': if one puts the electron in the $|+ >$ state by exciting the H_2^+ molecule with a laser pulse or so, the protons have a good reason to unbind. Finally, it sometimes happens that eigenstates do not know about quantities like t, and these states are called 'non-bonding', for obvious reasons.

Next to explaining lots of molecules (in chemistry, the generalization of this toy problem is called the 'linear combination of atomic orbitals' method), its extensions play an important role in solid state physics as well, where it is called the 'tight-binding method' which will be explained in further detail in chapter 3. For further two-level based entertainment I refer to the book by Feynman.

$\Longrightarrow$ exercise 2.8

2.2 Harmonic oscillators.

Harmonic oscillators have a very special status in physics. For whatsoever reason, the force-mediating 'fields' both in the high energy realms, as in the macroscopic condensed state (where they correspond with the 'collective modes'), have a mathematical structure which can be expressed in terms of an *ensemble* of harmonic oscillators. Here the single harmonic oscillator is discussed. It is a first example of a quantum problem where the notion of a single 'particle' (better: 'quantum of something') is rather meaningless - only the relationships between states with different numbers of quanta really matter. Accordingly, it can also be considered as a first glimpse on the second quantization formalism. It is about operators creating and annihilating stuff, where all the work is done by algebraic relations (commutators).

The Schrödinger equation for a particle with mass m moving in a harmonic oscillator potential is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right]\psi(x) \;=\; E_n\psi(x) \quad . \tag{2.40}$$

This equation can be viewed as a differential equation which can be solved in terms of Hermite polynomials. Doing so, one finds the energy eigenvalues

$$E_n \;=\; (n+\frac{1}{2})\hbar\omega \quad . \tag{2.41}$$

If the particle is excited into the n-th quantum state, it is indicated with the ket $|n>$. The eigenfunction in terms of the Hermite polynomials, $\psi_n(x)$, is the projection of $|n>$ on the position coordinate $\psi_n(x) =< x|n>$.

This problem might as well be solved by manipulating operators. This is much more efficient, and yields a deeper insight in the nature of the problem. First, rescale the operators

$$\begin{aligned} p &= \sqrt{m\hbar\omega}\,\bar{p} \quad , \\ x &= \sqrt{\hbar/m\omega}\,\bar{x} \quad , \end{aligned} \tag{2.42}$$

and the Hamiltonian becomes

$$\mathcal{H} \;=\; \frac{1}{2}\hbar\omega(\bar{p}^2+\bar{x}^2) \quad . \tag{2.43}$$

The key idea is to introduce the operators,

$$\begin{aligned} b &= \frac{1}{\sqrt{2}}(\bar{x}+i\bar{p}) \quad , \\ b^\dagger &= \frac{1}{\sqrt{2}}(\bar{x}-i\bar{p}) \quad . \end{aligned} \tag{2.44}$$

These operators obey an interesting algebra, the so-called boson-Heisenberg algebra

$$[b,b] \;=\; 0 \quad , \qquad [b^\dagger,b^\dagger] \;=\; 0 \quad , \qquad [b,b^\dagger] \;=\; 1 \quad . \tag{2.45}$$

$\Longrightarrow$ exercise 2.9

In terms of b en $b^\dagger$ the Hamiltonian becomes

$$\mathcal{H} \;=\; \hbar\omega(b^\dagger b+\frac{1}{2}) \quad . \tag{2.46}$$

Diagonalization of the Hamiltonian is equivalent to finding the eigenstates of the 'bilinear' operator $b^\dagger b$,

$$b^\dagger b|n> \;=\; \hat{n}|n> \;=\; n|n> \quad . \tag{2.47}$$

and we recognize from (2.41) that $\hat{n}$ measures actually the occupation number n. Next to $\hat{n}$ measuring the number of quanta, it turns out that $b^\dagger$ *creates* one quantum of oscillation while b *annihilates* a quantum. We find this out by doing algebraic manipulations using the Heisenberg algebra, keeping track of the action of the operators in Hilbert space.

Let us consider what happens when b and $b^\dagger$ act separately on the state space $|n>$. Especially

$$\begin{aligned} \left(b^\dagger b\right) b^\dagger |n> &= b^\dagger \left(1 + b^\dagger b\right) |n> \quad , \\ &= (n+1) b^\dagger |n> \quad . \end{aligned} \tag{2.48}$$

is revealing. We only used (2.44) and the algebra (2.45) to find out that $b^\dagger |n>$ is proportional to $|n+1>$,

$$b^\dagger |n> = e_n |n+1> \quad . \tag{2.49}$$

with an unknown constant of proportionality e_n. We find that $b^\dagger$ has the effect of *creating* a quantum of energy - if we let $b^\dagger$ act on $|n>$ we end up in a state $|n+1>$ and using (2.46,2.47) we find that the energy of the system has increased by an amount $\hbar\omega$. Repeating this calculation for b, it is found that b has precisely the opposite effect of *annihilating* quanta, $b|n> \sim |n-1>$.

The constant of proportionality has still to be determined. On the one hand,

$$\begin{aligned} <n|b b^\dagger|n> &= e_n <n|b|n+1> = e_n <n+1|b^\dagger|n>^* = \\ &= |e_n|^2 <n+1|n+1>, \end{aligned} \tag{2.50}$$

and on the other hand

$$<n|b b^\dagger|n> = <n|1 + b^\dagger b|n> = n+1 \quad . \tag{2.51}$$

and it follows that $e_n = \sqrt{n+1}$ (e_n can be choosen to be real). Repeating this for b we arrive at the final result,

$$\begin{aligned} b^\dagger |n> &= \sqrt{n+1} |n+1> \quad , \\ b|n> &= \sqrt{n} |n-1> \quad . \end{aligned} \tag{2.52}$$

These simple manipulations teach us two important lessons: (i) a formal lesson, it appears possible to calculate entirely in terms of the operators themselves. We can leave wavefunctions implicit and all we need is an abstract conception of Hilbert space. All the hard work is done by algebraic manipulation in the space of operators, and this becomes quantum mechanics because the algebra has a non-commutative (non-abelian) structure. (ii) A lesson about physics. We find, buried in this simple potential problem, a new notion of particle. One can as well say that $b^\dagger$ creates a particle carrying an energy $\hbar\omega$ while b annihilates it. As we will later find, the commutation relations (2.45) imply that these particles are *bosons.* This is actually the sense of the 'particle-ness' of the particles carrying the forces, like the photons, gluons and vector bosons. In quantum-field theory, the harmonic oscillator nature of the fundamental fields is a matter of hypothesis. In condensed matter, the precise equivalents of these field-particles show up as well, where they carry names like phonons, magnons, plasmons, etcetera all of which will be encountered in these lectures. There is one big difference with the fundamental fields: in the condensed state, they are the quantized version of the collective modes which are themselves implied by the rigid nature of the classically ordered state.

2.3 Many particles: quantum statistics.

The formalism as explained up to now is not sufficient since nature never consists of one particle in isolation. Dealing with more particles, one needs additional axioms and these are the axioms of quantum statistics. In three-dimensional space the basic statement is: in a system of indistinguishable particles, the states of the many-particle system have to be either symmetric under exchange of two single particle quantumnumbers, Q, Q': $|Q(1)Q'(2).... > = |Q'(1)Q(2).... >$, or antisymmetric: $|Q(1)Q'(2).... > = -|Q'(1)Q(2).... >$. Here $1, 2, \cdots$ labels the particles. If the wavefunction is symmetric the particles are called bosons, if it is antisymmetric the particles are called fermions.

$\Longrightarrow$ exercise 2.10

These statements were originally introduced by Pauli as mere physical hypothesis. It turns out that one can actually prove mathematically (using the topology of world-lines in the Feynman path integral formalism) that these two are the only possibilities in the three dimensional world. This is different in lower dimensions. Assuming that the particles have a hard-core, so that they cannot pass each other, it can be shown that statistics looses its meaning in one space dimension, while in two dimensions statistics becomes arbitrary in the sense that nature could in principle interpolate between fermion and boson statistics: the subject of anyons.

On a fundamental level, the particles carrying a mass are always fermions, while the force mediating fields are described by bosons. In the macroscopic realm this is still true, except that one can now also find bosonic, massive particles which are bound states of an even number of fermions, like for instance ^4He. In addition, the spin-statistics theorems of relativistic quantum-mechanics tell that fermions carry half-integer spin while bosons carry integer spin. In so far particles play a role in condensed matter physics, these are in most cases either $s = 1/2$ electrons or 'massless' bosons, like the phonons etcetera.

Even if the fermions or bosons are non-interacting, the symmetry properties of the many particle wavefunction give rise to special *collective* behaviors: the particles do not act any longer as if they are independent of each other, in the way they are in a classical ideal gas. One could also say that the behaviors of individual particles become *correlated* with that of all other particles in a manner which is beyond classical intuition. Massive, non-interacting bosons are subject to Bose-Einstein condensation: the ground state of the N-particle system consists of a N-fold occupied lowest lying single-particle eigenstate. Fermions do precisely the opposite: every single-particle eigenstate can be at most occupied by one fermion, the Pauli exclusion principle. One of the consequences is the different behavior at finite temperatures,

$$\begin{aligned} n_B(j) &= \frac{1}{e^{\beta(\varepsilon_j - \mu)} + 1} \\ n_F(j) &= \frac{1}{e^{\beta(\varepsilon_j - \mu)} - 1}, \end{aligned} \tag{2.53}$$

the Bose and Fermi factors, expressing how excited single particle states (ε_j) get occupied at finite temperature ($\beta = 1/k_B T$), differently for bosons and fermions. In the case of the Fermi systems, the thermodynamic potential μ becomes at zero temperature equal to the Fermi-energy E_F, for non-interacting problems given by the sum of the energies of the N lowest lying single particle states. For non-interacting bosons, μ becomes N times the energy of the lowest lying single particle state.

Slater determinants

H_N is the the Hilbert space of all possible N particle wave functions. This contains a subspace H_N^A spanned by all antisymmetric solutions, corresponding with indistinguishable fermions. One first considers the case that only one particle is present ($N = 1$). This defines a complete and orthonormal basis $|k_i>$ - notice that this basis is in principle arbitrary, it does not have to be the one which diagonalizes the single particle Hamiltonian. In many cases the choice of such a diagonal basis is even inconvenient. The full Hilbert space H_N of the N-particle problem is spanned by the set of all products of N single particle states,

$$|k_1(1)>|k_2(2)> \cdots |k_N(N)> \;\equiv\; |k_1(1)k_2(2)k_3(3) \cdots k_N(N)> \quad , \tag{2.54}$$

$|k_1(1)>$ means: particle 1 occupies single particle state $|k_1>$, etcetera. Exchanging for instance particle 1 and 3,

$$|k_1(3)k_2(2)k_3(1) \cdots k_N(N)> \quad ,$$

and (2.54) is obviously not anti-symmetric. Notice that we could as well have permuted the quantum numbers instead of the particle labels. Anti-symmetry can be restored by taking a special linear combination of product states. An arbitrary permutation of all particles is symbolically written as $\mathcal{P}$,

$$\mathcal{P}\,|k_1(1)k_2(2)k_3(3) \cdots k_N(N)> \;=\; |k_1(\mathcal{P}1)k_2(\mathcal{P}2)k_3(\mathcal{P}3) \cdots k_N(\mathcal{P}N)> \tag{2.55}$$

$\mathcal{P}n$ labels the particle which ends up after all the exchanges in the state, initially occupied by particle n. *Every* ordering of particles can be constructed from a series of *pair* permutations. Although there are different ways of arriving at the same overall permutation using pair permutations, the number of pair permutations is even or odd regardless the sequence in which the pair permutations are carried out. This makes it possible to introduce the number $\eta_P = \pm 1$, the 'parity' of the permutation: $\eta_P = +1$ if the number of permutation is even, and $\eta_P = -1$ if it is odd.

$\Longrightarrow$ exercise 2.11

The Pauli-Principe requires the wavefunction to change sign under the exchange of two unspecified fermions. In terms of η_P,

$$\mathcal{P}|\Psi(1,2,\cdots,N)> \; = \; \eta_P|\Psi(1,2,\cdots,N)> \quad . \tag{2.56}$$

The linear combinations of product states which fulfills this requirement ($\sum_P$ sums over all permutations),

$$\begin{aligned} |k_1k_2k_3\cdots k_N> \; &\equiv \; \frac{1}{\sqrt{N!}}\sum_P \eta_P|k_1(\mathcal{P}1)k_2(\mathcal{P}2)\cdots k_N(\mathcal{P}N)> \quad , \\ &\equiv \; \sqrt{N!}\mathcal{A}|k_1(1)k_2(2)k_3(3)\cdots k_N(N)> \end{aligned} \tag{2.57}$$

where we defined the antisymmetrization operator,

$$\mathcal{A} = \frac{1}{N!}\sum_P \eta_P\,\mathcal{P} \quad , \tag{2.58}$$

which projects an arbitrary state of $\mathcal{H}_N$ into the antisymmetric subspace $\mathcal{H}_N^A$.

$\Longrightarrow$ exercise 2.12

These expressions are not easy to visualize. The following form is much more convenient,

$$|k_1k_2k_3\cdots k_N> = \frac{1}{\sqrt{N!}}\begin{vmatrix} |k_1(1)> & |k_1(2)> & \cdots\cdots & |k_1(N)> \\ |k_2(1)> & |k_2(2)> & \cdots\cdots & |k_2(N)> \\ \vdots & \vdots & & \vdots \\ |k_N(1)> & |k_N(2)> & \cdots\cdots & |k_N(N)> \end{vmatrix} . \tag{2.59}$$

The so-called Slater determinants which span the antisymmetrical part of the N particle Hilbert space H_N^A. The determinant form is very convenient. Exchange of rows (or columns) in a determinant gives rise to a sign changes: for instance, $|k_1k_2\cdots k_N> \; = \; - \; |k_2k_1\cdots k_N>$, and we recognize (2.56). In addition, $|k_1k_2k_2k_3k_4\cdots k_N> \; = \; 0$, two fermions cannot occupy the same single particle state.

There is one complication. If we do not take precautions, the basis $|k_1k_2\cdots k_N>$ is overcomplete, because the same state is obtained, except for a minus sign, if two particles are exchanged. One has to add an additional constraint to prevent this double counting. The remedy is to choose an order for the quantum numbers k, such that either $k < k'$, or $k > k'$ - for instance, if the states k are eigenstates of the single particle Hamiltonian, the natural ordering is according to increasing single particle energy. By allowing only the subset of states

$$\{|k_1k_2k_3\cdots k_N>\} \quad \text{under the condition that} \quad k_1 < k_2 < \cdots < k_N \tag{2.60}$$

overcompleteness is avoided and (2.60) is a complete and orthonormal basis for the many-fermion Hilbert space H_N^A.

$\Longrightarrow$ exercise 2.13

It is special to the problem of non-interacting particles that all N-particle eigenstates can be directly derived from the eigenstates of the one particle problem by simply using the single particle quantum numbers for the k_i's in (2.60). At the moment that particles start interacting with each other, the N-particle eigenstates can no longer be written in terms of single Slater determinants, because interactions will give rise to non-zero matrix elements between different Slater determinants which cannot be transformed away by transforming single particle states. Instead, one has to solve the problem in the full H_N^A space and the eigenstates will have the form,

$$\Psi_i = \sum_{k_1<k_2<\cdots<k_N} C^i_{k_1,k_2,\cdots,k_N} |k_1 k_2 \cdots k_N> \quad . \tag{2.61}$$

In the chemistry literature this is called 'configuration interaction' (every Slater determinant is a 'configuration' of electrons), while physicist call it 'the many-body problem'. As will be further illustrated, this Hilbert space has the nasty property of having an enormous size, even for the simplest problems. 'Exact' solutions (or even accurate approximate solutions) are out of reach for physically interesting systems even if one uses the fastest computers. Nevertheless, something can be said about the qualitative features of this problem and this is the main theme of this lecture series.

Two levels and two electrons: non-interacting H_2.

To obtain some intuition regarding Slater determinants and the many-body Hilbert space, it is instructive to consider the two (non-interacting) fermion variant of the two level problem discussed at the end of section 2.1. This could be a caricature of the neutral hydrogen molecule (H_2) - it is actually a rather poor model because interaction effects are quite important in this molecule. A much better toy-model for H_2 will be presented in chapter V.

Including spin, the single particle basis can be choosen to be the unhybridized site basis $\{|i\sigma>\}, i = 1, 2; \sigma = \uparrow, \downarrow$ (2.34). We define ($\{i, i'\}\epsilon\{1, 2\}$)

$$|j>_2 \equiv |i\sigma i'\sigma'> \equiv \sqrt{2!}\mathcal{A}\ |i(1)>|\sigma(1)>|i'(2)>|\sigma'(2)> \tag{2.62}$$

and the complete *two* particle basis is, including the double counting constraint (2.60),

$$\begin{aligned} |1>_2 &= |1\uparrow 2\downarrow> \ , \ |2>_2 = |2\uparrow 1\downarrow> \ , \ |3>_2 = |1\uparrow 1\downarrow> \\ |4>_2 &= |2\uparrow 2\downarrow> \ , \ |5>_2 = |1\uparrow 2\uparrow> \ , \ |6>_2 = |1\downarrow 2\downarrow> \end{aligned} \tag{2.63}$$

The two particle Hilbert space is 6-dimensional, still of the same order as the 4-dimensional one particle space - this looks already quite different when we attach one more site and one more electron (see chapter V). By writing these states explicitely, and using the single particle Hamiltonian (2.35,2.36, $\varepsilon_1 = \varepsilon_2 = \varepsilon$, t real), one finds that the Hamiltonian becomes in two particle Hilbert space,

$$\begin{aligned} \mathcal{H} &= 2\varepsilon \sum_{j=1}^{6} |j>_2 \ <j|_2 \ + \\ & \quad t\ (\ |1>_2 \ <3|_2 \ + \ |1>_2 \ <4|_2 \ + \ |2>_2 \ <3|_2 \ + \ |2>_2 \ <4|_2 \ + \ h.c.) \end{aligned} \tag{2.64}$$

$h.c.$ means hermitian conjugate. The Hamiltonian is diagonalized by,

$$\begin{aligned} |a>_2 &= \frac{1}{2}(-|1>_2 -|2>_2 +|3>_2 +|4>_2) \\ |b>_2 &= \frac{1}{2}(|1>_2 +|2>_2 +|3>_2 +|4>_2) \\ |c>_2 &= \frac{1}{\sqrt{2}}(|1>_2 -|2>_2) \\ |d>_2 &= \frac{1}{\sqrt{2}}(|3>_2 -|4>_2) \end{aligned} \tag{2.65}$$

and the diagonalized Hamiltonian becomes,

$$\begin{aligned} \mathcal{H} &= 2\varepsilon\ (|5>_2 \ <5|_2 \ + \ |6>_2 \ <6|_2 \ + \ |c>_2 \ <c|_2 \ + \ |d>_2 \ <d|_2) \ + \\ & \quad |a>_2 \ (2\varepsilon - 2t) \ <a|_2 \ + \ |b>_2 \ (2\varepsilon + 2t) \ <b|_2 \end{aligned} \tag{2.66}$$

Hence, we find four non-bonding two particle states ($|5>_2, |6>_2, |c>_2, |d>_2$), one bonding state ($|a>_2$), yielding twice as much kinetic energy as the single-particle bonding state, and one antibonding state ($|b>_2$).

⟹ exercise 2.14

Of course, we could have saved the effort of diagonalizing in the 'big' two particle Hilbert space: this is a non-interacting problem, and in this case we can profit fully from the solution of the one particle problem. Spanning the two-particle Hilbert space using the one particle eigenstates (2.38) instead, the problem is directly solved. We leave it to the reader to show that

$$\begin{aligned} |-\uparrow - \downarrow> &= |a>_2 \\ |+\uparrow + \downarrow> &= |b>_2 \\ |-\uparrow + \downarrow> &= \frac{1}{\sqrt{2}}(|c>_2 +|d>_2) \\ |+\uparrow - \downarrow> &= \frac{1}{\sqrt{2}}(-|c>_2 +|d>_2) \\ |+\uparrow - \uparrow> &= -|5>_2 \\ |+\downarrow - \downarrow> &= -|6>_2 \end{aligned} \tag{2.67}$$

while from the left hand side of (2.67) and the one particle result (2.39) the eigenvalues of the two-particle problem can be directly inferred.

⟹ exercise 2.15

Writing the Slater determinants of the bonding state explicitely in product wave functions,

$$|+\uparrow+\downarrow>=|+(1)>|+(2)>\frac{1}{\sqrt{2}}(|\uparrow(1)>|\downarrow(2)>-|\downarrow(2)>|\uparrow(1)>) \tag{2.68}$$

The 'orbital' part is symmetric and indicates that both particles are found in exactly the same region in space. The total wavefunction is kept antisymmetric by the spin part, which is recognized to be a two particle singlet state (see also section 2.5). This is quite different for the non-bonding combination characterized by parallel spin

$$|+\uparrow-\uparrow>=-\frac{1}{\sqrt{2}}(|1(1)>|2(2)>-|1(2)>|2(1)>)|\uparrow(1)>|\uparrow(2)> \tag{2.69}$$

Now the spin part is symmetric, corresponding with a two particle triplet. This forces the orbital part to be antisymmetric. As a consequence, the particles *avoid* each other: if particle 1 is on atom 1, particle 2 is *always* on atom 2 and vice versa. This is a simple example of the 'exchange hole': fermions with the same spin tend to avoid each other, regardless the interactions. This is a very general principle which has a variety of physical ramifications. In the present example, it forbids the electrons to hop (this triplet is quite literally 'non-bonding') and we will see in chapter 4 that precisely this phenomenon gives rise to the kinetic exchange interactions in magnetic insulators. At the opposite end one encounters the Hund's rule exchange known from atomic physics which is also the driving force behind itinerant magnetism: the exchange hole keeps the electrons from approaching each other to closely and this *yields* energy because they repell each other less, on average.

2.4 Second quantization.

It should be clear from the previous section that manipulations involving wavefunctions of the Slater determinant type tend to be rather tedious. In the evaluation of matrix elements, etcetera, one has to work him/herself through complicated sums, finding out at the end that the answers are simple, suggesting the existence of a more efficient algorithm. Even worse, one would like to write down expressions for the Hamiltonian and other properties, given that N particles are around. If one tries to do this in the 'first quantized' formalism (using operators like $|i>_N<j|_N$, $|i>_N$ is the N particle Hilbert space), one finds out that (i) for every N the Hamiltonian looks different (see the 'H_2' molecule) and (ii) this expression would become very lengthy indeed for any truly interesting problem, because of the gigantic size of the Hilbert space.

The way out is second quantization. This follows the same general pattern as was exposed in section (2.2) (harmonic oscillator). One only needs an abstract notion of the Hilbert space, and all the hard work is done in terms of operators. The physics is encoded in the non-abelian structure of the algebra. This includes the statistics; for bosons in general one recovers the algebra (2.45)) while the result for fermions is similar, except that the operators *anti-commute*. In first instance, second quantization can be considered as a convenience. However, one can wonder if there are deeper meanings behind this formalism. Certain tricks have been invented using second quantization, which solve the problem in a couple of lines. If one tries to do the same calculation using Slater determinants, one would get entangled in algebraic manipulations for years and most likely one would loose track, even knowing the answer. A good example is the Bogoliubov transformation, explained at the end of this section, which is the key mathematical operation needed in both the theory of superconductivity (chapter VI) and the semiclassical theory of spin condensation (chapter V).

The Fockspace H

Second quantization is about operators which act on yet another Hilbert space: the *Fockspace* H, defined as the direct sum of the N particle Hilbert spaces H_N of the previous section, H_0, H_1, H_2, $\cdots$,

$$H \;\equiv\; H_0 \;\oplus H_1 \;\oplus H_2 \;\oplus \;\;\cdots\;\; \oplus H_N \;\oplus\;\; \cdots \quad . \tag{2.70}$$

H_0 has a special status, it is the Hilbert space of the 'problem' with no particles. This is spanned by one normalized state: $|0>$, describing nothingness, called the 'bare vacuum' in the jargon of physics.

The *antisymmetric Fockspace* H^A is constructed from the anti-symmetric subspaces H_N^A (2.70):

$$H^A \;\equiv\; H_0 \;\oplus H_1 \;\oplus H_2^A \;\oplus \;\;\cdots\;\; \oplus H_N^A \;\oplus\;\; \cdots \quad . \tag{2.71}$$

Antisymmetrization is of course irrelevant for the bare vacuum and the one particle sector H_1. Because of (2.61),

$$\{|0>, |k_1>, |k_1k_2>, \cdots, |k_1k_2\cdots k_N>, \cdots, \qquad \text{with } k_1 < k_2 < \cdots\} \quad .$$

The completeness relation in Fock space is,

$$\sum_{N=0}^{\infty} \sum_{k_1<k_2<\cdots<k_N} |k_1k_2\cdots k_N> < k_1k_2\cdots k_N| \;=\; 1 \quad . \tag{2.72}$$

Creation and annihilation operators.

Creation and annihilation operators are operators which act on Fock space with the effect to move the system from the N particle sector to the $N+1$ particle sector (creation operator), or from the N to $N-1$ sector (annihilation operator). The creation operator $a_k^\dagger$ is defined by its action on Fock space. Starting with the bare vacuum,

$$a_k^\dagger|0> \;\;=\;\; |k> \quad , \tag{2.73}$$

$a_k^\dagger$ creates one particle in state k. If more than one particle is around, one has to worry about the ordering (2.60). For fermions,

$$a_k^\dagger|k_1> \;\;=\;\; \begin{cases} |kk_1> & \text{for } k < k_1 \quad , \\ \\ -|k_1k> & \text{for } k_1 < k \quad . \end{cases} \tag{2.74}$$

or for arbitrary particle number N

$$a_k^\dagger|k_1k_2\cdots k_N> \;=\; \begin{cases} |kk_1k_2\cdots k_N> & , \\ \\ (-1)^i\;|k_1\cdots k_ikk_{i+1}\cdots k_N> & , \end{cases} \tag{2.75}$$

The rule is to place the quantum number of the newly created particle to the far left and then shift the quantum number to its proper locus in the ordered sequence of quantum numbers, multiplying the wave function with -1 every time one passes a single particle quantum number of the N particle state (the fermion sign). In the case of fermions, one cannot create a particle in a state which is already occupied,

$$a_k^\dagger|k_1k_2\cdots k\cdots k_N> \;=\; 0 \tag{2.76}$$

Applying (2.74,2.75) repeatedly, one can construct any state in the antisymmetric Fock space starting from the bare vacuum,

$$|k_1k_2\cdots k_N> \;=\; a_{k_1}^\dagger a_{k_2}^\dagger\cdots a_{k_N}^\dagger|0> \quad . \tag{2.77}$$

The *annihilation operator* a_k is defined in a similar way,

$$a_k|0> \;=\; 0 \quad , \tag{2.78}$$

$$a_k|k> \;=\; |0> \quad , \tag{2.79}$$

$$a_k|k_1k_2\cdots k_N> \;=\; 0 \qquad \text{for } k\neq k_1, k\neq k_2,\cdots,k\neq k_N \quad , \tag{2.80}$$

while for $k \;=\; k_{i+1}$

$$\begin{aligned} a_k|k_1\cdots k_N> &= (-1)^i\; a_k|kk_1\cdots k_ik_{i+2}\cdots k_N> \quad , \\ &= (-1)^i|k_1\cdots k_ik_{i+2}\cdots k_N> \quad . \end{aligned} \tag{2.81}$$

summarized in the expression,

$$a_k|k_1\cdots k_N> \;=\; \sum_{i=0}^{N-1}(-1)^i\;\delta_{k,k_{i+1}}|k_1\cdots k_ik_{i+2}\cdots k_N> \quad . \tag{2.82}$$

for $N \;=\; 0$ the right hand side of (2.82) is of course zero. In the notation we have already anticipated on the fact that a is the hermitian conjugate of $a^\dagger$.

$\Longrightarrow$ exercise 2.16

By using these definitions it is easily checked that the fermion creation and annihilation operators obey the so-called fermion Heisenberg algebra

$$\left\{a_k^\dagger, a_\ell^\dagger\right\} \;=\; 0 \quad , \qquad \{a_k, a_\ell\} \;=\; 0 \quad , \qquad \left\{a_k, a_\ell^\dagger\right\} \;=\; \delta_{k\ell} \quad . \tag{2.83}$$

which is *anti-commuting*: for any pair of operators A and B, $\{A,B\} \;\equiv\; AB+BA$. In this way, the antisymmetry of the many particle wave functions gets coded into the algebra. The derivation of the second quantization formalism for bosons (symmetric wave functions) goes along similar lines, except that one does not have to worry about the sign factors $(-1)^i$. One finds that the boson creation ($b_k^\dagger$) and annihilation (b_ℓ) operators satisfy the *commutation* relations (compare with (2.45)),

$$\left[b_k^\dagger, b_\ell^\dagger\right] = 0 \quad , \qquad [b_k, b_\ell] = 0 \quad , \qquad \left[b_k, b_\ell^\dagger\right] = \delta_{k\ell} \quad . \tag{2.84}$$

The algebraic relations (2.83) and (2.84) will turn out to be central parts of the machinery of many-body quantum-mechanics.

$\Longrightarrow$ exercise 2.17

Operators in second quantization.

Because any state in Fock space can be constructed using creation operators, it is also possible to re-express any operator entirely in terms of creation and annihilation operators. This yields particularly convenient forms. Next to many-particle wave functions, one also deals with many-particle operators in many-body physics, of the general form

$$\mathcal{B} = \sum_{i<j<n\cdots=1}^{N} \mathcal{B}(i,j,n\cdots) \quad . \tag{2.85}$$

expressing for instance the interactions between particles $i, j, n, \cdots$. In practice, one encounters most frequently one particle operators (only i in the sum; kinetic energy, external potentials, current- and density operators) or two particle operators (i, j; pair interactions).

Let us consider what happens when $\mathcal{B}$ acts on a Slater determinant. Using the antisymmetrization operator $\mathcal{A}$ (2.58) we can write

$$\begin{aligned} \mathcal{B}|k_1k_2\cdots k_N> &= \mathcal{B}\sqrt{N!}\,\mathcal{A}|k_1(1)k_2(2)\cdots k_N(N)> \quad , \\ &= \sqrt{N!}\,\mathcal{A}\mathcal{B}|k_1(1)k_2(2)\cdots k_N(N)> \quad . \end{aligned} \tag{2.86}$$

We have assumed that $\mathcal{B}$ commutes with $\mathcal{A}$ - this condition is in practice always satisfied. The effect of $\mathcal{B}$ on the simple product state is easy to obtain. Use the completeness relation in the (unsymmetrized) subspace H_N,

$$\mathcal{B}|k_1k_2\cdots k_N> = \sqrt{N!}\mathcal{A} \sum_{\ell_1,\ell_2,\cdots,\ell_N} |\ell_1(1)\cdots\ell_N(N)> \mathcal{B}(\{l\};\{k\}) \tag{2.87}$$

introducing the shorthand,

$$\mathcal{B}(\{l\};\{k\}) = <\ell_1(1)\cdots\ell_N(N)|\mathcal{B}|k_1(1)\cdots k_N(N)> \tag{2.88}$$

Subsequently,

$$\begin{aligned} \mathcal{B}(\{l\};\{k\}) &= \sum_{i<j<n\cdots=1}^{N} <\ell_1(1)\cdots\ell_N(N)|\mathcal{B}(i,j,n\cdots)|k_1(1)\cdots k_N(N)> \\ &= \sum_{i<j<n\cdots=1}^{N} \prod_{p=1}^{N,*} \delta_{\ell_p,k_p} <\ell_i(i)\ell_j(j)\ell_n(n)\cdots|\mathcal{B}(i,j,n\cdots)|k_i(i)k_j(j)k_n(n)\cdots> \\ &\equiv \sum_{i<j<n\cdots=1}^{N} \prod_{p=1}^{N,*} \delta_{\ell_p,k_p} B(\ell_i\ell_j\ell_n\cdots;k_ik_jk_n\cdots) \end{aligned} \tag{2.89}$$

where $*$ means: exclude $i, j, n, \cdots$ in taking the product. Because of the Kronecker delta's the sums over the ℓ's can be executed,

$$\begin{aligned}
\mathcal{B}|k_1k_2\cdots k_N> \quad &= \quad \sum_{i<j<n\cdots=1}^{N}\ \sum_{\ell_i,\ell_j,\ell_n,\cdots} B(\ell_i\ell_j\ell_n\cdots;k_ik_jk_n\cdots)\times \\
&\qquad |k_1,\cdots,\ell_i,\cdots,\ell_j,\cdots,\ell_n,\cdots,k_N> \\
&= \quad \sum_{i<j<n\cdots=1}^{N}\ \sum_{\ell_i,\ell_j,\ell_n,\cdots} B(\ell_i\ell_j\ell_n\cdots;k_ik_jk_n\cdots)\times \\
&\qquad a^\dagger_{\ell_i}a^\dagger_{\ell_j}\cdots a_{k_j}a_{k_i}\cdots|k_1\,k_2,\cdots,k_N> \quad .
\end{aligned} \tag{2.90}$$

The work has been done. We can rewrite this result in terms of summations over quantum numbers. For an N_i point interaction, we can make the replacement

$$\sum_{i<j<n\cdots=1}^{N} \quad = \quad \frac{1}{N_i!}\sum_{i}\sum_{j\neq i}\sum_{n\neq i,j}\cdots . \tag{2.91}$$

This is possible, because interchanging two creation operators in (2.90) yields the same sign as interchanging two annihilation operators. The factor $1/N_i!$ now takes care of the double counting. We can forget about the constraints on the summations, because $a_qa_q = 0$. We rename $l_il_jl_n\cdots \rightarrow p_1p_2p_3\cdots$. Since the annihilation operators give only a non-zero result if the states k_i, $k_j\cdots$ are occupied, we can as well sum over all quantum-numbers instead $(q_1, q_2\cdots)$. Doing this, we obtain the following second quantized expression for $\mathcal{B}$:

$$\mathcal{B} \;=\; \frac{1}{N_i!}\sum_{p_1,p_2\cdots,q_1,q_2\cdots} B(p_1p_2\cdots;q_1q_2\cdots)a^\dagger_{p_1}a^\dagger_{p_2}\cdots a_{q_2}a_{q_1} \;. \tag{2.92}$$

This expression is valid in all sectors of Fock space.

The single particle problem.

A one particle operator

$$\mathcal{V}_1 \;=\; \sum_{i=1}^{N} V(i) \tag{2.93}$$

can be written according to (2.92)

$$\mathcal{V}_1 \;=\; \sum_{p,q} V_{pq}a^\dagger_p a_q \quad , \tag{2.94}$$

$$V_{pq} \;=\; <p(1)|V(1)|q(1)> \quad . \tag{2.95}$$

For instance, the standard one particle problem (2.32) has the second quantized form

$$\mathcal{H} = \sum_{p,q}\langle p| - \frac{\hbar^2}{2m}\,\Delta + V(\vec{r})|q\rangle a^\dagger_p a_q \tag{2.96}$$

the states $|p\rangle$ and $|q\rangle$ are arbitrary, as long as they form a complete and orthonormal one particle basis.

$\Longrightarrow$ exercise 2.18

The number operator

$$\hat{n}_k = a_k^\dagger a_k \quad . \tag{2.97}$$

has a special status. $\hat{n}_k$ is the observable which measures if the single particle state $|k>$ (not necessarily an eigenstate of the single particle problem) is occupied or not in a many-particle wave function. It is easily checked that every Slater determinant $|k_1 k_2 \cdots k_N>$ corresponds with an eigenvector of $\hat{n}_k$ with eigenvalue $n_k = 0$ or $n_k = 1$:

$$\hat{n}_k |k_1 k_2 \cdots k_N> = \left\{ \begin{array}{l} 0 \quad \text{if } k \text{ not in } \{k_1, k_2, \cdots, k_N\} \quad , \\ |k_1, k_2, \cdots, k_N> \;\text{ if } k \in \{k_1, k_2, \cdots, k_N\} \quad . \end{array} \right. \tag{2.98}$$

and one calls the eigenvalues n_k the occupation numbers.

$\Longrightarrow$ exercise 2.19

These occupation numbers also suggest an alternative representation. Instead of indexing the state explicitely with the occupied k's, one lists all possible k's and indicates instead if they are occupied or not with the n_k's,

$$|k_1 k_2 \cdots k_N> \quad \Longleftrightarrow \quad |0,0,\cdots,0,\underset{\substack{\uparrow \\ \text{position } k_1}}{1},0,\cdots,0,\underset{\substack{\uparrow \\ \text{position } k_2}}{1},0,\cdots,0,\underset{\substack{\uparrow \\ \text{position } k_N}}{1},0\cdots> \tag{2.99}$$

or alternatively

$$|n_1, n_2, n_3, \cdots> = \left(a_1^\dagger\right)^{n_1} \left(a_2^\dagger\right)^{n_2} \left(a_3^\dagger\right)^{n_3} \cdots |0> = \prod_{n_k} \left(a_k^\dagger\right)^{n_k} |0> \quad . \tag{2.100}$$

Diagonalizing single particle problems.

In a couple of cases it makes sense to do perturbation theory in the strength of the interactions. The diagonalized single particle problem is considered to be the zeroth order, and the effects of the interactions can be treated with perturbation theory (e.g. the weak coupling theories in chapter V and VI, and the Fermi-liquid of chapter VII). In these cases it make sense to work in the single particle basis which diagonalizes the single particle Hamiltonian - knowing about the occupation numbers, one can directly read off the single particle energies. In terms of the eigenvalues ε_k and eigenstates $|k>$ of the single particle Hamiltonian, the diagonalized problem is

$$\mathcal{H} = \sum_k \varepsilon_k \hat{n}_k \tag{2.101}$$

One could of course diagonalize the Hamiltonian first and then define the creation- and annihilation operators associated with the eigenstates. It is, however, also possible to diagonalize the problem directly in terms of the operators. The single particle Hamiltonian has the form

$$\mathcal{H} = \sum_p \sum_r h_{pr} a_p^\dagger a_r \quad . \tag{2.102}$$

It is now possible to transform the operators *themselves.* U is an unitary matrix ($U^\dagger = U^{-1}$),

$$c_k = \sum_p U_{kp} a_p \quad , \qquad c_k^\dagger = \sum_p U_{kp}^* a_p^\dagger = \sum_p a_p^\dagger U_{pk}^\dagger \quad . \tag{2.103}$$

with the inverse

$$a_p = \sum_k U_{pk}^\dagger c_k \quad , \qquad a_p^\dagger = \sum_k \left(U_{pk}^\dagger\right)^* c_k^\dagger = \sum_k c_k^\dagger U_{kp} \quad . \tag{2.104}$$

This transformation respects the fermion anticommutation relations

$$\{c_k^\dagger, c_\ell^\dagger\} = 0 \quad , \qquad \{c_k, c_\ell\} = 0 \quad , \qquad \{c_k, c_\ell^\dagger\} = \delta_{k\ell} \quad . \tag{2.105}$$

which should be the case because one cannot change the statistics of the particles on the single particle level,

$\Longrightarrow$ exercise 2.20

Using (2.104), the Hamiltonian might as well be written as,

$$\begin{aligned} \mathcal{H} &= \sum_p \sum_r \; \sum_k \sum_\ell c_k^\dagger U_{kp} h_{pr} U_{r\ell}^\dagger c_\ell \quad , \\ &= \sum_{k,\ell} \left(\sum_p \sum_r U_{kp} h_{pr} U_{r\ell}^\dagger \right) c_k^\dagger c_\ell \quad , \\ &= \sum_k \varepsilon_k c_k^\dagger c_k \quad . \end{aligned} \tag{2.106}$$

In the third line, the diagonal form is imposed and one recognizes the eigenvalue problem

$$\sum_p \sum_r U_{kp} h_{pr} U_{r\ell}^\dagger = \tilde{h}_{k\ell} = \delta_{k\ell} \varepsilon_k \quad . \tag{2.107}$$

the same problem as we would have to solve in first quantization.

$\Longrightarrow$ exercise 2.21

$\Longrightarrow$ exercise 2.22

The Bogoliubov transformation.

Up to this point, second quantization does not yield any advantage over the familiar diagonalization carried out in first quantization. It turns out, however, that the second quantization formalization allows for a generalization of the notion of 'the single particle problem'. *Any* Hamiltonian which can be written in terms of products of two creation operators, two annihilation operators and/or one creation and one annihilation operator,

$$\mathcal{H} = \sum_p \sum_r \left[A_{pr} a_p a_r + 2B_{pr} a_p^\dagger a_r + A_{rp} a_r^\dagger a_p^\dagger \right] \tag{2.108}$$

($\underline{A}, \underline{B}$ are Hermitian) can be brought in a diagonal form

$$\mathcal{H} = \sum_k \varepsilon_k c_k^\dagger c_k + const. \tag{2.109}$$

by the so-called Bogoliubov transformation,

$$c_k = \sum_p \left[U_{kp} a_p + V_{kp} a_p^\dagger \right] \quad . \tag{2.110}$$

The matrices $\underline{U}$ and $\underline{V}$ can be choosen such that the c_k's again satisfy the fermion Heisenberg algebra, if the a's are fermions, or the boson algebra if the a's are bosons.

Problems of the form (2.108) arise in a physical context where the total number of particles is no longer a conserved quantity. Mathematically, the Hamiltonian no longer commutes with the operator counting the total number of 'bare' particles,

$$\hat{N} = \sum_p a_p^\dagger a_p \tag{2.111}$$

The message of the Bogoliubov transformation is that even in this situation it is possible to identify new, precisely defined particles which automatically include this number fluctuation, as long as the Hamiltonian only contains bilinears of the bare creation and annihilation operators. These new particles are 'composites' of the bare particles, in the sense that they can be for instance partly electrons and partly holes.

These non-number conserving problems arise in a variety of physical situations. The bosonic variety shows up if one requantizes condensed states by dressing them up with quantized collective modes - a typical example will be discussed in chapter V (Holstein-Primakoff). On the fermionic side, the invention of this mathematical fact gave Schrieffer his place in the list 'Bardeen-Cooper-Schrieffer': the Bogoliubov transformation is doing the hard work in the microscopic theory of superconductivity (chapter VI).

Although (2.110) can be proven in general, we will save this effort because we will only need the Bogoliubov generalization of the two level problem,

$$\mathcal{H} = \varepsilon_a a^\dagger a + \varepsilon_b b^\dagger b + t a^\dagger b^\dagger + t^* b a \tag{2.112}$$

Instead of two levels $|1>$ and $|2>$ we consider now two fermions, a and b, having a coupling t in the 'particle-particle channel'. The Bogoliubov transformation for this case is,

$$\begin{aligned} c_1^\dagger &= u^* a^\dagger + v^* b \\ c_2 &= v a^\dagger - u b \end{aligned} \tag{2.113}$$

and by conjugation,

$$\begin{aligned} c_1 &= ua + vb^\dagger \\ c_2^\dagger &= v^* a - u^* b^\dagger \end{aligned} \tag{2.114}$$

⟹ exercise 2.23

One should now determine the inverse transformation, yielding expressions for a, b etcetera in terms of the the c_i's. The Hamiltonian is expressed in the c_i's and one demands that all scalars multiplying the operator products vanish, except for the terms in front of the number operators of the new fermions $c_1^\dagger c_1$ and $c_2^\dagger c_2$. This becomes particularly simple if one assumes $\varepsilon_a = \varepsilon_b = 0$ and real t. One anticipates that the particle and the hole will appear with equal and real amplitudes, $u = v = 1/\sqrt{2}$,

$$\begin{aligned} c_1^\dagger &= \frac{1}{\sqrt{2}}(a^\dagger + b) \\ c_2 &= \frac{1}{\sqrt{2}}(a^\dagger - b) \end{aligned} \tag{2.115}$$

Substituting the inverse

$$\begin{aligned} a^\dagger &= \frac{1}{\sqrt{2}}(c_1^\dagger + c_2) \\ b &= \frac{1}{\sqrt{2}}(c_1^\dagger - c_2) \end{aligned} \tag{2.116}$$

in the Hamiltonian

$$\begin{aligned} \mathcal{H} &= t(a^\dagger b^\dagger + ba) \\ &= t(c_1^\dagger c_1 + c_2^\dagger c_2 - 1) \end{aligned} \tag{2.117}$$

The Bogoliubov-problem is not quite the same as the ordinary diagonalization problems which we studied before. The eigenstates are now superposition of states with different numbers of particles. Also, there is a new vacuum state. It is defined by $c_{1,2}|\text{vac}>= 0$, while the original vacuum had $a|\text{vac}>= b|\text{vac}>= 0$. The new single particle states remain degenerate but move up in energy with an amount t, while the new vacuum shifts down by t. This vacuum shift is related to the energy source stabilizing superconductivity - see chapter VI.

⟹ exercise 2.24

⟹ exercise 2.25

Pair interactions.

Let us now turn to interactions. It is nearly always assumed that the constituents interact via *pair* interactions. This is in some important cases justifiable: electrons interact via Coulomb interactions and He atoms via van der Waals forces. However, it is not necessarily always the case and the truth of the matter is that many particle phenomena driven by multi-particle interactions are largely unexplored.

A pair interaction looks like

$$\mathcal{V}_2 = \sum_{i<j=1}^{N} V(i,j) \quad . \tag{2.118}$$

where the two particle potential might depend on the positions, velocities, spins etcetera of the particles i and j. For indistinguishable particles, we can directly use the recipe (2.85-2.90) to write the interaction term in second quantization

$$\mathcal{V}_2 = \frac{1}{2} \sum_{r,s} \sum_{p,q} V_{pqrs}\, a_p^\dagger a_q^\dagger a_s a_r \quad . \tag{2.119}$$

With the 'interaction matrix elements',

$$V_{pqrs} = < p(1) q(2) | V(1,2) | r(1) s(2) > \quad . \tag{2.120}$$

Notice that one has to keep track of the order in which the operators appear, because of the fermion sign. The most common interactions (e.g. Coulomb, van der Waals) only depend on the distance between the particles: $V(i,j) = V(r_i - r_j)$. Using (no spin-orbital coupling)

$$< \vec{r} | p > = \psi_p(\vec{r}) | s_p > \tag{2.121}$$

we find

$$\begin{aligned} V_{pqrs} &= \int d\vec{r_1}' d\vec{r_2}' \int d\vec{r}_1 d\vec{r}_2 < pq | \vec{r_1}' \vec{r_2}' >< \vec{r_1}' \vec{r_2}' | V(1,2) | \vec{r}_1 \vec{r}_2 >< \vec{r}_1 \vec{r}_2 | rs >, \\ &= \int d\vec{r_1}' d\vec{r_2}' \int d\vec{r}_1 d\vec{r}_2 < s_p s_q | \psi_p^*(\vec{r_1}') \psi_q^*(\vec{r_2}')\; V(\vec{r}_1 - \vec{r}_2) \delta(\vec{r_1}' - \vec{r}_1) \quad , \\ &\qquad\qquad \times\; \delta(\vec{r_2}' - \vec{r}_2) \psi_r(\vec{r}_1) \psi_s(\vec{r}_2) | s_r s_s > \quad , \\ &= \delta_{s_p s_r} \delta_{s_q s_s} \int d\vec{r}_1 d\vec{r}_2 \psi_p^*(\vec{r}_1) \psi_q^*(\vec{r}_2) V(\vec{r}_1 - \vec{r}_2) \psi_r(\vec{r}_1) \psi_s(\vec{r}_2) \quad . \end{aligned} \tag{2.122}$$

In principle these can be calculated from the full knowledge of the single particle sector. In practice, one often only considers simplified ('model') forms for these interaction matrix elements.

Nursery school diagrams.

In the course of this lecture series several ways of dealing with the many-particle problem will unfold. One of these alleys is the diagrammatic perturbation theory which will be treated in the final chapter, in a kindergarten style. Already earlier on it will turn out to be convenient to draw diagram-like pictures. A typical example will be the 'diagram' for (2.119). One imagines time running from left to right and space from bottom to top. The 'history' implied by (2.119) can be pictorially represented by the diagram as shown in figure 2.2.

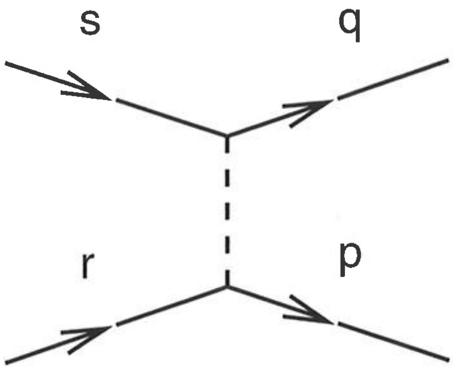

Figure 2.2: *'Nursery school diagram' of the pair interaction. the incoming particles in states s and r are annihilated by the interaction (dashed line) to be subsequently created in the states q and p.*

Equations of motion.

Besides exact diagonalization and a couple of perturbative methods, it will turn out to be particularly convenient to set up calculations using the equations of motion for the operators. Next to the Schrödinger picture (2.26-2.28), where the time evolution of the system is described in terms of the time dependence of the states, one can as well ascribe the time evolution entirely to the operators (Heisenberg picture). For instance, the time dependence of an observable A with operator $\hat{A}$,

$$\begin{aligned} A(t) &= <\psi(t)|\hat{A}|\psi(t)> \\ &= <\psi|\hat{A}(t)|\psi> \end{aligned} \qquad (2.123)$$

with $|\psi(t)>$ as given by (2.28) and

$$\hat{A}(t) = e^{-i\mathcal{H}t}\hat{A}e^{i\mathcal{H}t} \qquad (2.124)$$

The time-evolution of the operator can be calculated using the operator equation of motion (using units $\hbar = 1$, such that frequency is measured in units of energy),

$$i\frac{\delta A(t)}{\delta t} \equiv i\dot{A} = [A(t), \mathcal{H}] \qquad (2.125)$$

This equation applies to any operator, including the creation- and annihilation operators. The advantage is that one can stay in 'operator space', figuring out the physics by doing algebraic manipulations.

If a problem can be diagonalized, it is of course also possible to solve the system of differential equations implied by Eq. (2.125). For instance, given the single particle problem (2.102), the time evolution of a bare creation operator is determined by,

$$\begin{aligned} i\dot{a}_q^\dagger &= \sum_{pr} h_{pr}\left[a_q^\dagger, a_p^\dagger a_r\right] \\ &= -\sum_p h_{pq}a_p^\dagger \end{aligned} \qquad (2.126)$$

where the second line is derived by using the fermion algebra. This yields a system of linear, first order differential equations with the same dimension as Hilbert space. To solve this system, one looks for new operators obeying

$$i\dot{c}_k^\dagger = -\varepsilon_k c_k^\dagger \tag{2.127}$$

such that ($c_k^\dagger(0)$ is the operator at $t = 0$)

$$c_k^\dagger = e^{i\varepsilon_k t} c_k^\dagger(0) \tag{2.128}$$

while $a_q^\dagger$ can be written as

$$a_q^\dagger = \sum_k e^{i\varepsilon_k t} c_k^\dagger(0) U_{kq} \tag{2.129}$$

where ε_k of course corresponds with the eigenvalues (2.106) and $\underline{U}$ with the transformation (2.104) of the time-independent formalism.

$\Longrightarrow$ exercise 2.26

In many cases one is not so much interested in the time evolution of a single particle, but instead in expectation values of density or current operators which relate to bilinears in terms of the particle operators of the kind $\hat{\rho}_{kq} = a_k^\dagger a_{k+q}$. In the special case of a single particle problem these are easily calculated using (2.129). However, it will turn out that in the presence of interactions it is often convenient to study the time dependence of $\hat{\rho}_{kq}$ directly. For instance, considering the 'diagonal' density $\hat{n}_q = a_q^\dagger a_q$, its time evolution as determined by the single particle Hamiltonian is,

$$\begin{aligned} i\dot{\hat{n}}_q^\dagger &= \sum_{pr} h_{pr} \left[a_q^\dagger a_q, a_p^\dagger a_r\right] \\ &= \sum_p \left(-h_{pq} a_p^\dagger a_q + h_{qp} a_q^\dagger a_p\right) \end{aligned} \tag{2.130}$$

again yielding a system of differential equations which in principle can be solved.

$\Longrightarrow$ exercise 2.27

The equation of motion method does not cause miracles - if the problem cannot be solved exactly by e.g. direct diagonalization, the equations of motions are also of little help. Using equations of motions, the kind of trouble caused by interaction terms can be seen easily. The time dependences due to the interactions are caused by the commutator with the interaction term in the Hamiltonian (2.119), for instance

$$\begin{aligned} \left[a_l^\dagger, \mathcal{V}_2\right] &= \frac{1}{2} \sum_{r,s,p,q} V_{pqrs} \left[a_l^\dagger, a_p^\dagger a_q^\dagger a_r a_s\right] \\ &= \frac{1}{2} \sum_{r,p,q} \left(V_{pqrl} - V_{pqlr}\right) a_p^\dagger a_q^\dagger a_r \end{aligned} \tag{2.131}$$

Next to changing its own quantum-number, the particle l now also causes another fermion to change its quantum number: the particle 'scatters against an electron-hole pair'. The 'nursery school' diagram of this process is indicated in figure 2.3.

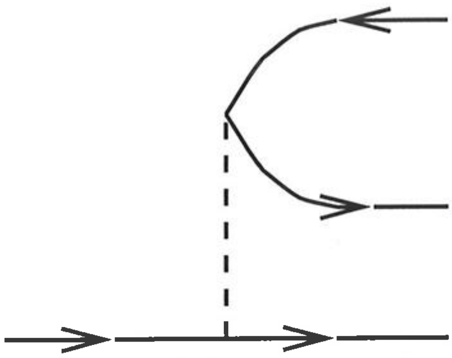

Figure 2.3: *'Nursery school diagram' of the scattering of a particle against a particle hole pair, due to the pair interaction.*

The operator $a^\dagger_p a^\dagger_q a_r$ has of course also a time evolution of its own, connecting it via the interaction term with operators composed of five fermion operators, and so on. In this way one has to explore the full N particle Hilbert space in order to establish the time evolution of even the simplest object, the single particle. I already announced that an exact solution is per default not possible.

$\Longrightarrow$ exercise 2.28

Although exact solutions are out of the picture, equations of motion are often used in this lecture series. The reason is that this method fits quite well to a highlight of quantum condensed matter physics: if classical condensation occurs, it becomes *qualitatively* correct to 'decouple' the equations of motion in the very beginning, by approximating $a^\dagger_p a^\dagger_q a_r \rightarrow O a^\dagger_p$ (schematically), where O is a scalar quantity, the 'order parameter amplitude'. Doing so, one obtains an effective single particle problem which can be solved, yielding the 'collective modes'. This is called the 'random phase approximation', or 'RPA'.

2.5 The $su(2)$ Lie algebra: spin.

Up to now we have encountered two types of algebra, the fermion- and boson Heisenberg algebra's, which we have learned to appreciate as the mathematical language underlying the concept of particle. These algebra's are implicitly tied to a fundamental symmetry of nature: translational invariance which allows for the concept of linear momentum. Nature also exhibits more complicated continuous symmetries, which are associated with more complicated Lie algebra's. Physically, these imply other 'particles' which behave quite differently from free bosons and fermions.

In most of condensed matter physics one only encounters the $su(2)$ algebra, describing spin.[1]. In chapter V it will be explained under which circumstances spin becomes a

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[1] Some exceptions: the mysterious order parameters of superfluid ^3He become immediately obvious if one realizes that one is dealing with a nearly $SO(4)$ symmetric problem. In addition, it often turns out to be mathematically convenient to 'enlarge' a quantum spin problem to $SU(N)$,

physical object. It is the spin of the electron as explained by Dirac, except that it occurs on its own: due to an interesting collective process (projective renormalization), the electron looses all its properties except its spin and the problem is completely described in terms of the $su(2)$ algebra.

The algebra.

The $su(2)$ Lie algebra should be familiar

$$\left[\hat{S}^x, \hat{S}^y\right] = i\hat{S}^z \ , \ \left[\hat{S}^z, \hat{S}^x\right] = i\hat{S}^y \ , \ \left[\hat{S}^y, \hat{S}^z\right] = i\hat{S}^x \tag{2.132}$$

and the identity. (2.132) is sometimes written in the shorthand notation

$$\left[\hat{S}^a, \hat{S}^b\right] = i\epsilon^{abc}\hat{S}^c \tag{2.133}$$

where ϵ^{abc} is the Levi-Civita symbol. In contrast to the larger Lie algebra's, $su(2)$ does not contain mutually commuting elements. The Cartan subalgebra (the subset of commuting elements) contains therefore only one element, usually choosen to be $\hat{S}^z$: the z component of the spin does not fluctuate. In addition, the algebra has one Casimir operator, the 'total spin':

$$\hat{S}^2 \equiv \vec{\hat{S}} \cdot \vec{\hat{S}} \equiv (\hat{S}_x)^2 + (\hat{S}_y)^2 + (\hat{S}_z)^2 \tag{2.134}$$

commuting with all elements

$$\left[\hat{S}^2, \hat{S}^a\right] = 0 \ , \ a = x, y, z \tag{2.135}$$

The Hilbert space of a globally invariant $SU(2)$ problem can therefore be divided up into sectors characterized by the two spin quantum numbers S, M_s,

$$\begin{aligned} \hat{S}^z|i; S, M_s> &= M_s|i; S, M_s> \\ \hat{S}^2|i; S, M_s> &= S(S+1)|i; S, M_s> \end{aligned} \tag{2.136}$$

From representation theory it follows that S can be a positive (half) integer and

$$M_s = -S, -S+1, \cdots, S-1, S \tag{2.137}$$

A state with 'total spin' S is therefore $2S+1$-fold degenerate, and the state with $M_s = S$ ($M_s = -S$) is called the 'maximum (minimum) weight' state. In addition, the 'step' or 'flip' operators,

$$\begin{aligned} \hat{S}^+ &= \hat{S}^x + i\hat{S}^y \\ \hat{S}^- &= \hat{S}^x - i\hat{S}^y \end{aligned} \tag{2.138}$$

have the useful property of changing the M_s quantum numbers according to ($A(S, M_s)$ is a normalization constant),

$$\begin{aligned} A(S, M_s)\ \hat{S}^+|i; S, M_s> &= |i; S, M_s+1> \ , \ \hat{S}^+|i; S, S>= 0 \\ A(S, M_s)\ \hat{S}^-|i; S, M_s> &= |i; S, M_s-1> \ , \ \hat{S}^-|i; S, -S>= 0 \end{aligned} \tag{2.139}$$

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subsequently defining a perturbation theory controlled by $1/N$. See, e.g., A. Auerbach 'Interacting electrons and quantum magnetism' (Springer, New York, 1994).

Another way of writing $su(2)$,

$$\left[\hat{S}^+, \hat{S}^-\right] = 2\hat{S}^z \;, \quad \left[\hat{S}^z, \hat{S}^+\right] = \hat{S}^+ \;, \quad \left[\hat{S}^-, \hat{S}^z\right] = \hat{S}^- \tag{2.140}$$

$\Longrightarrow$ exercise 2.29

The electron spin ($S = 1/2$).

The electron is a doublet under $su(2)$ ($S = 1/2, 2S+1 = 2$). In terms of the spinor representation (2.2) the spin operators can be expressed by Pauli-matrices,

$$\hat{S}^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \;, \quad \hat{S}^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \;, \quad \hat{S}^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{2.141}$$

Alternatively, the spin operators might as well be expressed in terms of the fermion Heisenberg algebra,

$$\begin{aligned} \hat{S}^z_i &= \frac{1}{2}(c^\dagger_{i\uparrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c_{i\downarrow}) \;, \quad \hat{1}_i = c^\dagger_{i\uparrow} c_{i\uparrow} + c^\dagger_{i\downarrow} c_{i\downarrow} \\ \hat{S}^+_i &= c^\dagger_{i\uparrow} c_{i\downarrow} \;, \quad \hat{S}^-_i = c^\dagger_{i\downarrow} c_{i\uparrow} \end{aligned} \tag{2.142}$$

where i is an arbitrary label. Spin is an example of a density-like quantity, corresponding with a bilinear in the fermion operators: $\sim a^\dagger_k a_l$

$\Longrightarrow$ exercise 2.30

Many spins: vector addition.

We will be interested in problems of many interacting spins, of the form,

$$\mathcal{H} = \sum_{ij} J_{ij} \vec{\hat{S}}_i \cdot \vec{\hat{S}}_j + \sum_{ijkl} J_{ijkl} \left(\vec{\hat{S}}_i \cdot \vec{\hat{S}}_j\right)\left(\vec{\hat{S}}_k \cdot \vec{\hat{S}}_l\right) + \cdots \tag{2.143}$$

where the $\hat{S}$'s themselves typically refer to electron spins. This class of problems is *globally* $su(2)$ *invariant.* This has the following meaning: define operators for the spin components of the whole system

$$\hat{S}^a_{tot} = \sum_{i=1}^{N} \hat{S}^a_i \;, \quad a = x, y, z \tag{2.144}$$

and for the total spin of the whole system,

$$\hat{S}^2_{tot} = \vec{\hat{S}}_{tot} \cdot \vec{\hat{S}}_{tot} \tag{2.145}$$

Global $su(2)$ invariance means that the eigenstates of the many-spin problem can be labeled by S_{tot} and M_{tot} according to

$$\begin{aligned} \hat{S}^z_{tot}|i; S_{tot}, M_{tot}> &= M_{tot}|i; S_{tot}, M_{tot}> \\ \hat{S}^2_{tot}|i; S_{tot}, M_{tot}> &= S_{tot}(S_{tot}+1)|i; S_{tot}, M_{tot}> \end{aligned} \tag{2.146}$$

The many-spin eigenstates can be constructed using the rules of *vector addition* as discussed in elementary textbooks. The eigenstates of $\hat{S}^z$ are easy. One writes product states of the elementary spins, of the form

$$|k; M_{tot} >= |M_s(1) > |M_s(2) > \cdots |M_s(N-1) > |M_s(N) > \tag{2.147}$$

and the total z component is given by the sum of the z components of the individual spins,

$$M_{tot} = \sum_{i=1}^{N} M_s(i) \tag{2.148}$$

The determination of the eigenstates of $\hat{S}^2_{tot}$ is much harder. Although one gets some help from group theory (Clebsch-Gordon coefficients, etcetera), group theory alone is not powerful enough to allow for the construction of precise eigenstates of $\hat{S}^2_{tot}$ if the system contains a macroscopic number of spins. The quantum spin problems are generically unsolvable as well.

$\Longrightarrow$ exercise 2.31

Two interacting electron spins.

The simplest example of an interacting spin problem is the 'two-spin Heisenberg problem',

$$\mathcal{H} = J\vec{\hat{S}}_1 \cdot \vec{\hat{S}}_2 \tag{2.149}$$

where $\vec{\hat{S}}$ describes a doublet - this is the analogue in spin space of the two level problem. Let me illustrate how to solve this problem, using the bare minimum of group theory. A basis for this problem is

$$\begin{aligned} |1,1> &= |\uparrow(1)>|\uparrow(2)> \ , \ |a,0>=|\uparrow(1)>|\downarrow(2)> \\ |b,0> &= |\downarrow(1)>|\uparrow(2)> \ , \ |1,-1>=|\downarrow(1)>|\downarrow(2)> \end{aligned} \tag{2.150}$$

(2.149) is globally $su(2)$ invariant and we already made use of this fact in the labeling of the states (2.150): in so far possible, we indicate $|S_{tot}, M_{tot}>$. The largest S_{tot} which can be constructed from two spin 1/2's is $S_{tot} = 1$, the three-fold degenerate triplet. The maximum and minimum weight states $|1,1>$ and $|1,-1>$ of this triplet are automatically also eigenstates of $\hat{S}^2_{tot}$. The $M_{tot} = 0$ states $|a,0>$ and $|b,0>$ are not eigenstates of total spin. One linear combination of these two states should correspond with the $M_{tot} = 0$ triplet state and the state orthogonal to this triplet state is non-degenerate and should therefore correspond with a singlet ($S_{tot} = 0$). Starting out with the maximum weight state of the fully polarized state, one can systematically work 'downwards' to smaller S_{tot} by using (2.139) to determine the non-maximum weight states belonging to the large S_{tot} states and finding subsequently the states which are orthogonal to those, corresponding with smaller S_{tot}. For the present example,

$$S^-|1,1>=|a,0>+|b,0> \tag{2.151}$$

and the $M_{tot} = 0$ triplet and the singlet are therefore,

$$|1,0>= \frac{1}{\sqrt{2}}(|a,0> + |b,0>) \ , \ |0,0>= \frac{1}{\sqrt{2}}(|a,0> - |b,0>) \tag{2.152}$$

These states diagonalize the Hamiltonian,

$$\mathcal{H} = -\frac{3J}{4}|0,0><0,0| + \frac{J}{4}\sum_{k=-1,0,1}|1,k><1,k| \tag{2.153}$$

$\Longrightarrow$ exercise 2.32

$\Longrightarrow$ exercise 2.33

$\Longrightarrow$ exercise 2.34

2.6 Exercises chapter 2

2.1 a) Use (2.7) to show that the normalization conditions (2.1) and (2.4) are identical.

b) Write $<\psi_2|\psi_1>$ in the notation of section 2.1 (i).

2.2 The wave function of a free particle is given by $\hat{\psi} =<\vec{r}|\vec{p}>\propto \exp(\imath\vec{p}\cdot\vec{r}/\hbar)$, as we shall see further on. Show that $\hat{\psi}$ is the fourier transform of ψ.

Hint: use the completeness relation.

2.3 Show that, for a unitary matrix, $A^\dagger A = 1$ is also true. This implies that the inverse of a unitary matrix is the same as its hermitian conjugate.

2.4 Show that the eigenvalues α_i of a hermitian operator A are real numbers. Show furthermore, that it is possible to choose an orthonormal basis of eigenstates $\{|\alpha_i>\}$ if the eigenvalues are nondegenerate.

2.5 Derive the time-evolution of an arbitrary state $|\psi>_\circ$, using the fact that the eigenstates of $\mathcal{H}$ form a complete orthonormal set.

2.6 a) The causal relation between $\psi(t)$ ant $\psi(t_0)$ can be written in the form $\psi(t) = U(t,t_0)\psi(t_0)$, where ψ is a solution of the time-dependent Schrödinger equation (we assume $\mathcal{H}$ to have no explicit time dependence). Express U in terms of the Hamiltonian. What is the causal relation in state-space? Give the matrix representation of U with respect to the basis of energy eigenstates.

b) Consider two observables A and B with $[A,B] \neq 0$. Is the matrix representation of A with respect to the basis of eigenstates of B diagonal?

c) Proof that the following definitions are identical: $<A_t>= \sum_i A_i|<A_i|\psi>(t)|^2$, $<A_t>=<\psi|A|\psi>$.

d) What determines whether a set of commuting observables describing a quantum system is complete?

e) A spinless particle is in an orbital momentum state $2|1,1> +\imath|1,0> -2|1,-1>$ (notation $|1,m>$). Normalize this state.

f) The operator A satisfies the relation $A^2 = 1$ (the unity operator). What are the possible eigenstates of A?

g) The operator B satisfies the anticommutation relation $AB + BA = 0$, where A is the operator from excercise 2.6f. What is the eigenvalue of B, belonging to the common eigenstate $|\psi>$ of A and B?

h) Proof the relation $[AB, C] = A[B, C] + [A, C]B$, where A, B and C are arbitrary operators.

2.7 a) Proof $[p^2, x_j] = -2\imath\hbar p_j$.

b) Show that the single particle Schrödinger equation with Hamiltonian (2.29) implies the following relations

$$\begin{aligned}\frac{d}{dt} < x_j >_t &= \frac{1}{m} < p_j >_t \quad , \\ \frac{d}{dt} < p_j >_t &= - < \frac{\partial V}{\partial x_j} >_t \quad ,\end{aligned}$$

where $< x_j >_t \; =< \psi|x_j|\psi >_t$, etc. This is Ehrenfest's theorem.

2.8 Solve the two-level problem with $\varepsilon_1 \neq \varepsilon_2$ and t real. We will need this further on.

2.9 Check the commutation relations (2.45).

2.10 Show that two identical fermions cannot have the same value for all of their quantumnumbers, while this is possible for an arbitrary number of identical bosons.

2.11 Write the ordering 342165 as a series of pair-permutations performed on the ordering 123456. What is η_p for this case?

2.12 Proof that $\mathcal{A}$ is a projection operator by showing that $\mathcal{A}^2 = \mathcal{A}$. Use the fact that $\mathcal{P}$ is unitary and that $\eta_{pp'} = \eta_p\eta_{p'}$.

2.13 a) Proof the orthogonality and the completeness of the set of states (2.60).

b) In most cases where we use an explicit representation (i.e. position, momentum), k is used as a label for both the spatial and the spin part of the wavefunction , $k = (\vec{k}, \sigma)$. Suppose we work in position representation, the single particle state $|k>$ can be written as,

$$\begin{aligned}< \vec{r}_1 s_1|k > &= < \vec{r}_1 s_1|\vec{k}\sigma > \quad , \\ &= < \vec{r}_1|\vec{k} >< s_1|\sigma > \; = \; \psi_{\vec{k}}(\vec{r}_1)\delta_{s_1,\sigma} \quad .\end{aligned}$$

In an analogous way, we obtain for an N-particle state.

$$\begin{aligned}
&< \vec{r}_1 s_1 \cdots \vec{r}_N s_N | k_1 \cdots k_N > \\
&= \frac{1}{\sqrt{N!}} \sum_P \eta_P < \vec{r}_1 s_1 \cdots \vec{r}_N s_N | \vec{k}_1(\mathcal{P}1)\sigma_1(\mathcal{P}1) \cdots \vec{k}_N(\mathcal{P}N)\sigma_N(\mathcal{P}N) > \quad , \\
&= \frac{1}{\sqrt{N!}} \sum_P \eta_P < \vec{r}_1 s_1 \cdots \ \vec{r}_N s_N | \vec{k}_{\mathcal{P}1}(1)\sigma_{\mathcal{P}1}(1) \cdots \vec{k}_{\mathcal{P}N}(N)\sigma_{\mathcal{P}N}(N) > \quad , \\
&= \frac{1}{\sqrt{N!}} \sum_P \eta_P \, \delta_{s_1,\sigma_{\mathcal{P}1}} \cdots \delta_{s_N,\sigma_{\mathcal{P}N}} \, \psi_{\vec{k}_{\mathcal{P}1}}(\vec{r}_1) \cdots \psi_{\vec{k}_{\mathcal{P}N}}(\vec{r}_N) \quad .
\end{aligned}$$

Rewrite this last result in the mixed notation (2.8).

2.14 Use the decomposition $\mathcal{H} = \sum_{i,j=1}^{6} |i >_2 < i|_2 \mathcal{H} |j >_2 < j|_2$ to express the Hamiltonian in terms of two-particle Slater determinants. Diagonalize the Hamiltonian.

2.15 Derive (2.67) by writing everything out in terms of single-particle states. Proof that the eigenvalues of a non-interacting N-particle Hamiltonian are sums of eigenvalues of the corresponding single-particle Hamiltonians.

2.16 Show that a and $a^\dagger$ are each other's hermitian conjugate.

2.17 a) Proof the anticommutators (2.83).

b) Derive the equivalent of (2.71), (2.72), (2.75) and (2.83) for the bosons. Use as input that $b_k^\dagger b_k$ should count the number of bosons in state k.

2.18 Write the two-level Hamiltonian in second quantization. Construct the two particle basis by applying fermion creation operators to the vacuum.

2.19 a) Show that, for fermions, $\hat{n}_k^2 = \hat{n}_k$: $\hat{n}_k$ is a projection operator.

b) Verify $[\hat{n}_k, \hat{n}_l] = 0$.

2.20 a) Check that the operators c and $c^\dagger$ as defined by (2.103) satisfy fermion anticommutation relations.

b) Obtain the transformation of the kind (2.103) for bosons.

2.21 The operator $\hat{N} = \sum_k \hat{n}_k$ counts the total number of particles, which is a conserved quantity. Hence, $\hat{N}$ must be invariant under unitary transformations of the form (2.103). Check that this is indeed the case.

2.22 Diagonalize the two-level problem with $\varepsilon_1 \neq \varepsilon_2$, t real, using the second quantization formalism.

2.23 Show that the c-operators obey the fermion anticommutation relations if the transformation is unitary.

2.24 Diagonalize (2.112) with the Bogoliubov transformation for the case $\varepsilon_a = \pm\varepsilon_b$, t real.

2.25 For bosons, a transformation of the form can be performed

$$\begin{aligned} c_1^\dagger &= \cosh\chi e^{-\imath\phi_1} a^\dagger + \sinh\chi e^{-\imath\phi_2} b, \\ c_2 &= \sinh\chi e^{\imath(\phi-\phi_1)} a^\dagger + \cosh\chi e^{\imath(\phi-\phi_2)} b. \end{aligned} \tag{2.154}$$

a) Derive this by starting with the general transformation

$$\begin{aligned} c_1^\dagger &= \alpha_1^* a^\dagger + \alpha_2^* b, \\ c_2 &= \alpha_3 a^\dagger + \alpha_4 b, \end{aligned} \tag{2.155}$$

and imposing Heisenberg commutation relations on the c's. Is this transformation unitary? Derive the inverse transformation.

b) This transformation is not the most general Bogoliubov transformation. There is no guarantee that it will diagonalize the Hamiltonian. For what case ($\varepsilon_a = \varepsilon_b$, or $\varepsilon_a = -\varepsilon_b$) is it possible to diagonalize (2.112) through this transformation? For what values of t (real) and ε_a ?

2.26 a) Derive (2.126), (2.127), (2.129) and (2.130).

b) Solve $a^\dagger(t)$ for the two-level problem with $\varepsilon_1 = \varepsilon_2$, t real.

2.27 a) Derive (2.130)

b) Consider the two-level problem with degenerate energy-levels one and two. Feynman introduces this as a toy model for the ammonia molecule: level 1 corresponds to the nitrogen atom being located below the plane spanned by the hydrogen atoms, and level 2 with the nitrogen located above this plane. Suppose that the system is in level 1 at $t = 0$. Calculate the expectation value $< n_1(t) >$ using (2.129).

c) Calculate $< n_1(t) >$ using the equation of motion: calculate the time derivative of the operators which occur in the equation of motion of $n_1(t)$. Solve the resulting set of coupled first order differential equations.

2.28 a) Derive (2.131). What is the meaning of the Hund's rule exchange-term $-V_{pqlr}$?

b) Calculate the time derivative of $a_i^\dagger a_j^\dagger a_k$ for a Hamiltonian consisting of the interaction-term (2.119).

2.29 Write the two-spin Heisenberg Hamiltonian $\mathcal{H} = J\vec{\hat{S}}_1 \cdot \vec{\hat{S}}_2$ in terms of the spin raising and lowering operators $\hat{S}^\pm$. Derive the equation of motion of $\hat{S}_1^+$ with respect to this Hamiltonian.

2.30 Check that the operators in (2.142) form an $su(2)$ algebra using the fermion algebra.

2.31 Derive the exact ground state wavefunction and energy of the Hamiltonian (2.143) for the special case that all exchange couplings (J's) are negative. Is this state realized in nature?

2.32 a) Write the Hamiltonian of the Heisenberg triangle, $\mathcal{H} = J\vec{S}_1 \cdot \vec{S}_2 + J\vec{S}_2 \cdot \vec{S}_3 + J\vec{S}_2 \cdot \vec{S}_1$, in terms of the total spin operator.

b) Repeat (2.150) to (2.153) for the case of the Heisenberg triangle.

2.33 Consider a two-site Heisenberg problem. Calculate the time-dependence of $< S_1^z(t) >$ by solving its equation of motion, for the case that the system is (i) in state $|0, 0>$ at $t = 0$, (ii) in state $|a, 0>$ at $t = 0$.

2.34 a) What is the statistics of a spin $S = \frac{1}{2}$: fermion, boson ?

b) Consider $S = 1$. A spinor representation can be introduced,

$$\psi(\vec{r}) = \begin{pmatrix} \psi(\vec{r}, s = 1) \\ \psi(\vec{r}, s = 0) \\ \psi(\vec{r}, s = -1) \end{pmatrix}, \tag{2.156}$$

in analogy with (2.2). The $S = 1$ basis-spinors are given by

$$|1,1>= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1,0>= \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |1,-1>= \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{2.157}$$

Derive explicit expressions of the $su(2)$ operators in this representation.

c) Using the notation (2.142), the $S = 1$ states can be represented as follows

$$\begin{aligned} |1,1> &= c_{1\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} |\text{vac}> \equiv b_1^{\dagger} |\text{vac}>, \\ |1,0> &= \frac{1}{\sqrt{2}} \left(c_{1\uparrow}^{\dagger} c_{2\downarrow}^{\dagger} + c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} \right) |\text{vac}> \equiv b_0^{\dagger} |\text{vac}>, \\ |1,-1> &= c_{1\uparrow}^{\dagger} c_{2\uparrow}^{\dagger} |\text{vac}> \equiv b_{-1}^{\dagger} |\text{vac}> . \end{aligned}$$

The operators $b_{1,0,-1}^{\dagger}$ are called *hard-core bosons*: operators acting on different sites commute, while no more than one boson can be present on the same site (the 'hard core'). Write the $S = 1$ spin operators in terms of these hard-core bosons.

d) Solve the two-particle Heisenberg problem for the case of $S = 1$ spins.

3 Pragmatic Band Structure

Most of the remainder of these lecture notes will deal with electrons. Fact is that for the majority of electron systems encountered in solids, a description exists which is not only qualitatively correct, but also accurate enough to allow for the quantitative calculation of properties of the whole solid, like the cohesive energy, lattice parameters and even structural phase diagrams as function of pressure and temperature. This is called 'band structure theory on basis of the local approximation to density functional theory', or 'LDA (=local density approximation) band structure theory', or simply 'band structure theory'.

The qualitative success of this approach rests in last instance in the principles behind Fermi-liquid theory as discussed in chapter VII: in a rigorous sense, the electron states in a metal can be calculated in terms of other entities, called quasiparticles, which resemble electrons in all aspects except that they do not interact, while each of them contributes to an average, static potential felt by all other quasiparticles. All you have to know at this moment is that, instead of the solving the interacting electron problem, one might as well solve a problem of non-interacting quasiparticles moving in the static potential coming from the other quasiparticles and the lattice of ions if you are dealing with electrons in a normal metal, a normal semiconductor or a normal insulator. Nowadays, such a problem can always be handled, thanks to the computer.

Another matter is to translate this into a *quantitative* theory - Fermi-liquid theory does not tell anything about numbers, let alone it could address the magnitude of the cohesive energy which is a sensitive function of everything in the solid. To get the numbers, one needs the LDA part: this is a way to obtain accurate estimates for the aforementioned averaged, static quasiparticle potential. Historically, it has been an outcome of a process of trial and error. Although it has been called 'a triumph of parameter fitting', there is a way to rationalize its success to some extent, as I will sketch in chapter VII. The bottomline is that LDA works far too well, even taking these considerations into account, and all what remains is to accept it with a critical attitude, knowing that one is on shaky grounds.

To my opinion, band structure theory does not deserve a substantial exposure in a treatise dealing with the *principles* of the condensed state, despite its practical importance. For this reason I will limit the discussion here to the bare minimum: (i) the generalities of quantum-mechanics in the presence of static, periodic potentials (section 3.2). (ii) A technical part, teaching you how to handle simple band structure problems as will show up later in this course. Band structure becomes simple in two limits, which will both be discussed: (iia) the weak potential limit, described in terms of perturbation theory in terms of plane waves (section 3.3). (iib) The strong scattering limit, which is described in terms of slightly perturbed atomic states: the tight binding case (section 3.4). This latter part will evolve into a tutorial, learning you to read the outcomes of real live band structure calculations. Finally an appendix (section 3.5), listing the high-tech band structure methods available on the market, with their weaknesses and their strengths.

3.1 Electrons in a periodic potential.

We are interested in a problem of electrons moving in a lattice of ions. Having done the LDA part correctly, this will give rise to a problem of non-interacting fermions described by a Schrödinger equation,

$$\hat{H}\psi(\vec{r}) = \left[-\frac{\hbar^2}{2m}\Delta + U(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}) \quad , \tag{3.1}$$

where the potential U is set by both the ion cores and the average LDA potentials, originating in the electron-electron interactions. We will be in first instance interested in systems characterized by long range crystalline order. The ions form a periodic structure and the LDA potentials have the same symmetry as the lattice. A crystalline structure can be constructed from a Bravais lattice, the set of all points $\vec{R}$ given by

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \quad , \qquad n_1, n_2, n_3 \text{ integer} \quad . \tag{3.2}$$

and a basis, centered on every site of the Bravais lattice. In this case, the potential $U(\vec{r})$ will have the same periodicity as the Bravais lattice,

$$U(\vec{r} + \vec{R}_i) = U(\vec{r}) \quad , \qquad i = 1, 2, 3 \quad . \tag{3.3}$$

To fully profit of this symmetry, reciprocal space is needed. This space is spanned by the wave-numbers (or 'crystal momenta') $\vec{k}$, and the Bragg peaks of the periodic lattice are centered on the sites of the reciprocal lattice $\vec{K}$, satisfying

$$e^{i\vec{K}\cdot\vec{R}} = 1 \tag{3.4}$$

It follows that

$$\vec{K} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3 \quad , \qquad m_1, m_2, m_3 \text{ integer} \quad , \tag{3.5}$$

while the vectors $\vec{b}_i$ can be deduced from those in real space by

$$\begin{aligned} \vec{a}_i \cdot \vec{b}_j &= 2\pi\delta_{ij} \quad , && (i, j = 1, 2, 3), \\ \vec{b}_i &= \frac{2\pi}{v}(\vec{a}_j \times \vec{a}_k) \quad , && (i, j, k \text{ cyclic}), \\ v &= \text{vol}(a_1, a_2, a_3) \quad , \\ &= \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) && (\text{en cyclic}) \qquad (3.6) \\ \vec{K} \cdot \vec{R} &= \text{a multiple of } 2\pi \quad . && \qquad (3.7) \end{aligned}$$

For instance, the reciprocal lattice of a cubic lattice is itself a cubic lattice.

It is often convenient to assume that the crystal is of a finite extent, letting the size of the crystal go to infinity at the end of the calculation. The boundary conditions of choice are the periodic ones. For an arbitrary function f,

$$f(\vec{r}) = f(\vec{r} + N_i\vec{a}_i) \quad , \qquad (i = 1, 2, 3) \quad . \tag{3.8}$$

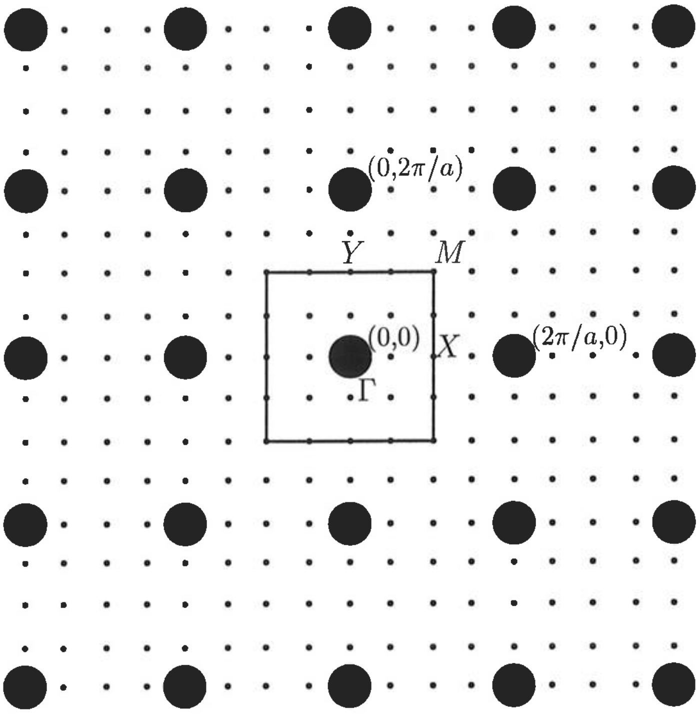

Figure 3.1: *The reciprocal lattice, and the mesh of k-points using periodic boundary conditions, of the two dimensional square lattice in real space. The first Brillouin zone is indicated, including the standard labeling of the high symmetry points.*

and the wavevectors $\vec{k}$ are then also defined on a mesh, with a much finer spacing than the reciprocal lattice $\vec{K}$ (lattice constant $\sim \pi/(N_i a)$),

$$\vec{k} \;=\; \frac{m_1}{N_1}\vec{b}_1 \;+\; \frac{m_2}{N_2}\vec{b}_2 \;+\; \frac{m_3}{N_3}\vec{b}_3 \quad , \tag{3.9}$$

$\Longrightarrow$ Exercise 3.1

The lattices encountered in these notes will always be of the simplest kind: square lattices in two dimensions, cubic lattices in three dimensions, and hypercubes in higher dimensions (sometimes summarized with 'cubic lattices'). The reciprocal space of the square lattice, including the standard labeling of the first Brillioun zone, is shown in figure 3.1.

Bloch-theorem

Having identified the remnants of translational invariance in the periodic crystal, let us now exploit the ramifications of the remaining discrete symmetry in the context of the quantum-problem (3.1, 3.3): the Bloch theorem. This states that the eigenstates of (3.1, 3.3) can be written as,

$$\psi_{\vec{k}}(\vec{r}) \;=\; e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r}) \quad , \tag{3.10}$$

$\vec{k}$ is a vector in reciprocal space, and $u_{\vec{k}}(\vec{r})$ a function with the periodicity of the Bravais lattice,

$$u_{\vec{k}}(\vec{r}) \;=\; u_{\vec{k}}(\vec{r}+\vec{R}) \quad . \tag{3.11}$$

A function like $\psi_{\vec{k}}(\vec{r})$ is called a Bloch function.

The Bloch theorem (3.10, 3.11) is a typical example of the role of symmetry in quantum-mechanics, in this case the (abelian) group of discrete translations. The proof of the theorem follows the same lines as used in the derivations of linear- and angular momentum. For every vector $\vec{R}$ of the Bravais lattice a translation operator $\hat{T}$ is defined, shifting the argument of an arbitrary function $f(\vec{r})$ over a distance $\vec{R}$: $\hat{T}_{\vec{R}}f(\vec{r}) = \ f(\vec{r}+\vec{R})$. Because the Hamiltonian is periodic, it commutes with $\hat{T}_{\vec{R}}$,

$$\hat{T}_{\vec{R}}\mathcal{H}\psi \ = \ \hat{H}(\vec{r}+\vec{R})\psi(\vec{r}+\vec{R}) \ = \ \hat{H}(\vec{r})\psi(\vec{r}+\vec{R}) \ = \ \hat{H}\hat{T}_{\vec{R}}\psi \quad . \tag{3.12}$$

because ψ can be taken to be any function,

$$\hat{T}_{\vec{R}}\hat{H} = \hat{H}\hat{T}_{\vec{R}} \quad . \tag{3.13}$$

The order of the translations does not matter if they are applied repeatedly,

$$\hat{T}_{\vec{R}}\hat{T}_{\vec{R}'}f(\vec{r}) = \hat{T}_{\vec{R}'}\hat{T}_{\vec{R}}f(\vec{r}) = f(\vec{r}+\vec{R}+\vec{R}') \tag{3.14}$$

and different $\hat{T}$'s commute with each other

$$\hat{T}_{\vec{R}}\hat{T}_{\vec{R}'} = \hat{T}_{\vec{R}}\hat{T}_{\vec{R}'} = \hat{T}_{\vec{R}+\vec{R}'} \tag{3.15}$$

Because $\hat{H}$ and $\hat{T}_{\vec{R}}$ commute for all $\vec{R}$, the eigenstates of $\hat{H}$ are also eigenstates of the set $\hat{T}$,

$$\begin{aligned} \hat{H}\psi &= \varepsilon\psi \quad , \\ \hat{T}_{\vec{R}}\psi &= c(\vec{R})\psi \quad . \end{aligned} \tag{3.16}$$

It is easy to deduce the eigenvalues $c(\vec{R})$ of $\hat{T}_{\vec{R}}$. Using (3.14)

$$c(\vec{R}+\vec{R}') \ = \ c(\vec{R})c(\vec{R}') \quad . \tag{3.17}$$

and $c(\vec{R})$ has to be of the form,

$$c(\vec{R}) \ = \ e^{i\vec{k}\cdot\vec{R}} \quad , \tag{3.18}$$

Together with (3.16) this implies that the eigenstates ψ of $\hat{H}$ can be chosen, such that for every vector $\vec{R}$ of the Bravais lattice,

$$\hat{T}_{\vec{R}}\psi(\vec{r}) \ = \ \psi(\vec{r}+\vec{R}) \ = \ e^{i\vec{k}\cdot\vec{R}}\psi(\vec{r}) \quad . \tag{3.19}$$

and this result is equivalent to (3.10,3.11).

$\Longrightarrow$ Exercise 3.2.

$\Longrightarrow$ Exercise 3.3.

$\Longrightarrow$ Exercise 3.4.

The functions $u_{\vec{k}}$

Substituting the wave-functions (3.10) in the Schrödinger equation (3.1) for the periodic crystal, we find that $u_{\vec{k}}$ satisfies the eigenvalue equation,

$$\hat{H}_{\vec{k}}u_{\vec{k}}(\vec{r}) \ = \ \left[\frac{\hbar^2}{2m}\left(-i\nabla+\vec{k}\right)^2 + U(\vec{r})\right]u_{\vec{k}}(\vec{r}) \ = \ \varepsilon_{\vec{k}}u_{\vec{k}}(\vec{r}) \quad , \tag{3.20}$$

with the boundary condition

$$u_{\vec{k}}(\vec{r}) \;=\; u_{\vec{k}}(\vec{r}+\vec{R}) \quad . \tag{3.21}$$

Because of the factor $e^{i\vec{k}\cdot\vec{R}}$ in (3.19), we directly infer that (3.20,3.21) are the same if an arbitrary vector $\vec{K}$ of the reciprocal lattice is added to the wavenumber $\vec{k}$: whatsoever the outcome, it will repeat itself in $\vec{k}$ space, much in the same way as the structure of the crystal repeats itself in real space. In real space one can describe the crystal by drawing a picture of the unit cell, subsequently stating that these unit cells have to be packed onto the Bravais lattice. Alternatively one can draw a picture (build a model) of a larger chunk of the crystal. In the same way, in reciprocal space one can consider the solutions of (3.20, 3.21) in the first Brillouin zone, stating that such a picture can be extended to the whole of $\vec{k}$ space by 'packing' those on the reciprocal lattice ('reduced-zone scheme'). Alternatively, one can draw the picture in a larger chunk of reciprocal space (the 'repeated-zone scheme')[1]. Such a picture contains redundant information. However, as in the case of the crystal structure, it is sometimes helpful in the process of visualizing the band structure.

The quantum problem (3.20, 3.21) is the difficult step in the band structure problem. In principle, it is clear what to do: choose periodic boundary conditions, such that the mesh of $\vec{k}$ points is sufficiently dense that clear pictures of the bands are obtained. Subsequently, solve (3.20) for all $\vec{k}$-points independently, and plot as many of them you need in order to get an impression of the bands. In essence, (3.20) amounts to solving a molecule-like problem, where the role of the molecule is played by the unit cell. It is of course not quite a molecule, because $\vec{k}$ enters into the kinetic term in (3.20). The problem is different for every wavevector, and in addition one has to take care of the boundary condition (3.21). Although the problem has been enormously simplified by exploiting the remaining translational invariance, it is still a formidable task to obtain accurate solutions for the 'quasi-molecules' (3.20). Because molecular-like single particle problems cannot be solved in closed form, the strategy is to choose some basis of single particle states which usually is rather large - the art of doing these calculations is in trying to keep this basis as small as possible, as will be further discussed in section (3.4). In this basis, a Hamiltonian matrix is obtained (compare 2.34-2.39) which is numerically diagonalized, and because many basis states are needed, many eigenstates are obtained.

$\Longrightarrow$ Exercise 3.5

These calculations are repeated for many $\vec{k}$-points and the energies of the different eigenstates are plotted as function of $\vec{k}$: the band structure. For a three dimensional crystal, one would need a four dimensional space (k_x, k_y, k_z, energy) to get a full view on all the bands. This is of course not possible, and instead one plots the bands along representative directions (high symmetry lines) in the first Brillioun zone.

In the figure, the full band structure of La_2CuO_4 is shown. La_2CuO_4 is directly related to the oxide materials in which the phenomenon of high T_c superconductivity

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[1] In addition, one can follow the remnant of the free dispersion in all of $\vec{k}$ space: 'the extended-zone scheme'.

occurs.

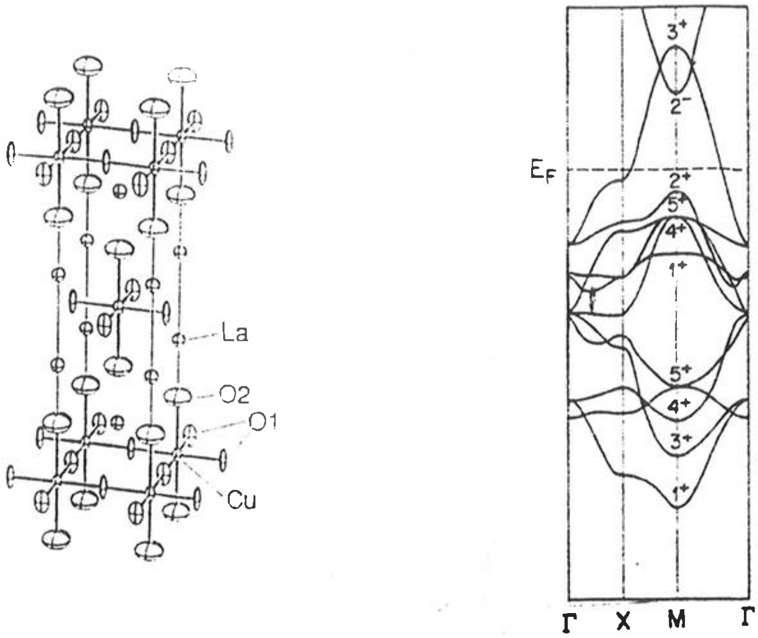

Figure 3.2: *Unit cell of La_2CuO_4, a parent material of the high T_c superconductors and the LAPW/LDA band structure of $CaCuO_2$ (L. F. Mattheiss and D. R. Haman, Phys. Rev. B* **40**, *2217 (1989)) - the band structure of La_2CuO_4 is virtually indistinguishable of that of $CaCuO_2$ in the valence band region. The dashed line indicates the Fermi-energy. The labeling of the (square) Brillioun zone follows the convention of Fig. (3.1).*

In the figure, the full unit cell of this material is shown as well, and this cell is very large - the high T_c cuprates belong to the most complex inorganic crystalline materials ever studied in detail. On a closer look, it can be seen that this material consists of layers of CuO, separated by layers of LaO. This greatly simplifies the problem: the LaO layers are inert,in the sense that the valence electrons (the ones close to the Fermi-energy) cannot penetrate these layers at all. Instead, the valence electrons are confined to the CuO ('perovskite') layers. These are nothing else than

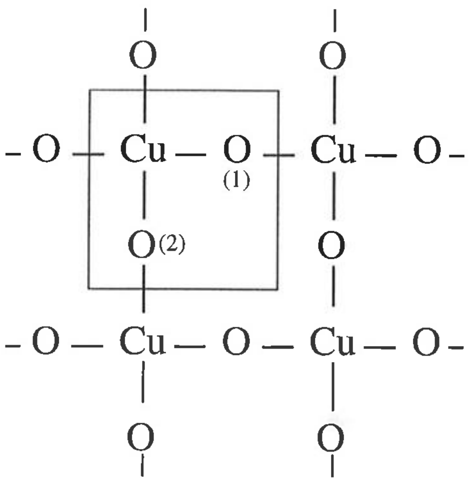

Figure 3.3: *The two dimensional perovskite planes of the high T_c superconductors, corresponding with CuO_2 unit cells stacked on a square Bravais lattice. The valence bands of Fig. 3.2 originate in these planes.*

simple two dimensional square Bravais lattices with a unit cell consisting of one Cu- and two O atoms (figure 3.3). It turns out that nearly all bands shown in the figure are derived from the above simple perovskite layer. Only the bands near E_F (Fermi energy) are shown and the band gap associated with the electronic states in the LaO layers is so large that none of these states fit in the energy frame of Fig. 3.2, except for the unoccupied La $s-$like free-electron like bands ($E \sim k^2$), dipping down at the M point. Hence, all other 'spaghetti's' seen in the band-picture are derived from the simple CuO_2 lattice. This is the reason to show this picture - at the end of this chapter you will have a fair feeling where all these bands come from. Concerning physics, the true electronic structure of La_2CuO_4 is a completely different story than the 'simple' band structure of Fig. (3.2), because of electron-electron interaction effects.

Statement of the problem.

The difficulty in calculating (3.20) arises from the form of the potential $U(\vec{R})$, which is depicted in figure 3.4. Near the ion cores, deep potential wells are found which

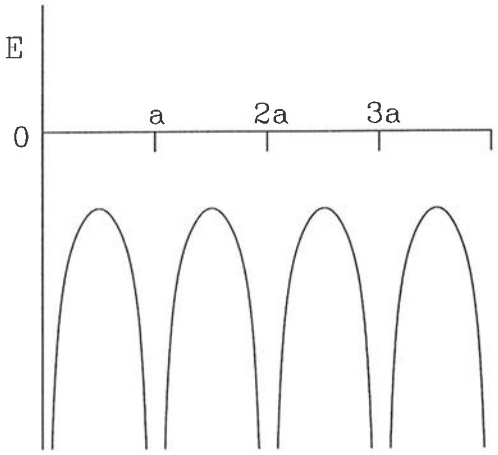

Figure 3.4: *Sketch of the typical shape of the periodic potential felt by the electrons in crystals. This consists of a superposition of deep potential wells, separated by flat pieces in the interstitial regions.*

are quite close the atomic potentials. In this region, the states will look atomic-like and a natural basis would be in terms of the familiar $ns, np, nd, ...$ atomic orbitals (n is the radial quantum number). Increasing the energy, the potential starts to vary until one reaches the regime where the electrons start to see a rather flat potential corresponding with the regions in between the atoms: the 'interstitial' regions. The electron states in these regions are much better described in terms of weakly perturbed plane waves, as are the states with a large total energy. The problem is that the valence bands (bands in the neighbourhood of the Fermi-energy) usually correspond with states which lie in the transition region between the 'atomic-core' and 'plane wave' regimes. It is a fact of mathematics that it is very hard to *interpolate* between atomic wavefunctions and plane waves: one needs a large numbers of plane waves to obtain an accurate expansion for an atomic wave function, and vice versa. A number of sophisticated tricks has been invented to overcome (or at least lessen) this problem - a summary of this 'orbital engineering' program will be given in the last section. Fact is, that your eyes have much less difficulty with this interpolation than the computer has. The two limits are the subject of the next two sections: first the weak potential limit (the plane waves), and subsequently the atomic limit, which is called 'tight binding'.

3.2 Weak potential scattering.

We start out assuming that the potential energy is very small compared to the kinetic energy, which is always the case if the total energy is large enough - the findings in this section always apply to high lying *unoccupied* states. This limit can be treated with perturbation theory. The Hamiltonian in real space representation is divided in a zero-order part $\hat{H}_0$ and a small perturbation $\hat{H}_1$ (σ is spin),

$$\begin{aligned}
\hat{H} &= \sum_\sigma \int d\vec{r} |\vec{r}\sigma\rangle \left(\hat{H}_0 + \hat{H}_1\right) \langle \vec{r}\sigma| \\
\hat{H}_0 &= -\frac{\hbar^2}{2m}\Delta \\
\hat{H}_1 &= U(\vec{r}),
\end{aligned} \tag{3.22}$$

and the small potential can be treated perturbatively.

Plane waves.

The eigenstates of H_0 are of course the plane wave states $|\vec{k}\sigma\rangle$, such that

$$\langle \vec{k}|\vec{r}\rangle = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}}, \tag{3.23}$$

and the energy eigenvalues are given by the 'free dispersion',

$$\varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} \quad . \tag{3.24}$$

$\Longrightarrow$ Exercise 3.6.

In order to simplify the counting, the electrons are thought to be confined in a (hyper)cube of linear dimension L with periodic boundary conditions, such that the volume needed for the normalization constant $\Omega = L^d$ (d is space dimension), while the wave-vectors lie on a mesh in $\vec{k}$ space with coordinates,

$$k_j = \frac{2\pi\ n_j}{L}\ , \qquad\qquad n_j = 0,\ \ \pm 1,\ \ \pm 2\ \ ,\cdots . \tag{3.25}$$

and at the end of the calculation one can take $L \to \infty$.

$\Longrightarrow$ Exercise 3.7.

$\Longrightarrow$ Exercise 3.8.

Since the plane waves form a complete set of single particle wavefunction, the unity is resolved by ($|\vec{k}\sigma\rangle$ is (3.23) in Dirac notation),

$$\sum_{\vec{k},\sigma} \left|\vec{k}\sigma\right\rangle \left\langle\vec{k}\sigma\right| = 1 \ . \tag{3.26}$$

The system characterized by the absence of any potential scattering is called the 'Jellium', and this plays a central role in the theory of the metallic state - the effects of the lattice potentials are secondary with regard to the effects of electron-electron interactions and can be left out in first instance (in the sense of the principle of adiabatic continuation). This jellium of interacting electrons will be the main actor in chapter VII.

$\Longrightarrow$ Exercise 3.9..

Periodic potentials and plane waves.

Only in some exceptional cases the problem with $U(\vec{r}) \neq 0$ can be solved analytically. A typical example is the Kronig-Penney model (a periodic array of delta functions) in $d = 1$, as treated in quantum-mechanics textbooks.

$\Longrightarrow$ Exercise 3.10.

Luckily, one does not need these closed solutions because perturbation theory works quite well, as long as the potential is weak. As a first step, we write the Hamiltonian in the basis of plane waves. Using (3.24, 3.26),

$$\hat{H} \ = \ \sum_{\vec{k},\sigma} |\vec{k}\sigma\rangle \ \varepsilon_{\vec{k}} \langle\vec{k}\sigma| \ + \sum_{\vec{k},\vec{k}',\sigma} |\vec{k}\sigma\rangle \ \left[\int d\vec{r} \langle\vec{k}\sigma|\vec{r}\sigma\rangle U(\vec{r}) \langle\vec{r}\sigma|\vec{k}'\sigma\rangle\right] \langle\vec{k}'\sigma| \tag{3.27}$$

We have to evaluate the expectation value of the potential with regard to the plane wave states. This simplifies for a periodic potential because its Fourier components are only non-zero on the reciprocal lattice $\vec{K}$, at the positions in $\vec{k}$ space where the Bragg peaks appear. Hence,

$$U(\vec{r}) = \sum_{\vec{K}} U(\vec{K}) e^{i\vec{K}\cdot\vec{r}} \tag{3.28}$$

where $U(\vec{K})$ are the Fourier components of the potential. The matrix elements between the plane wave states become,

$$\begin{aligned} \int d\vec{r} \langle\vec{k}|\vec{r}\rangle U(\vec{r}) \langle\vec{r}|\vec{k}'\rangle \ &= \ \frac{1}{\Omega} \int d\vec{r} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} U(\vec{r}) \\ &= \ \sum_{\vec{K}} U_{\vec{K}} \frac{1}{\Omega} \int d\vec{r} e^{i(\vec{K}-\vec{k}'+\vec{k})\cdot\vec{r}} \\ &= \ \sum_{\vec{K}} U_{\vec{K}} \delta(\vec{K} - \vec{k} + \vec{k}') \end{aligned} \tag{3.29}$$

and (3.27) simplifies to,

$$\hat{H} = \sum_{\vec{k},\sigma} \left|\vec{k}\sigma\rangle\, \varepsilon_{\vec{k}} \langle\vec{k}\sigma\right| + \sum_{\vec{K},\vec{k},\sigma} \left|\vec{k}\sigma\rangle\, U(\vec{K}) \langle\vec{k}+\vec{K}\sigma\right| \tag{3.30}$$

Hence, the Hamiltonian blocks into subproblems, each of which is spanned by a basis of plane wave states characterized by $\vec{k}$ plus all states obtained by adding to $\vec{k}$ an arbitrary vector of the reciprocal lattice.

One dimension.

The essence of the problem can already be inferred from the one dimensional crystal. We imagine that we first let the strength of the potential go to zero. The bandstructure in the periodic-zone scheme is depicted in figure 3.5. It has free dispersions centered around the reciprocal lattice vectors. Switching on the potential, the states intersected by the dashed-dotted line will start to mix according to (3.30): the states $|k\rangle$, $|k+K\rangle$, $|k-K\rangle$, $|k+2K\rangle \cdots$, with off-diagonal matrix elements like

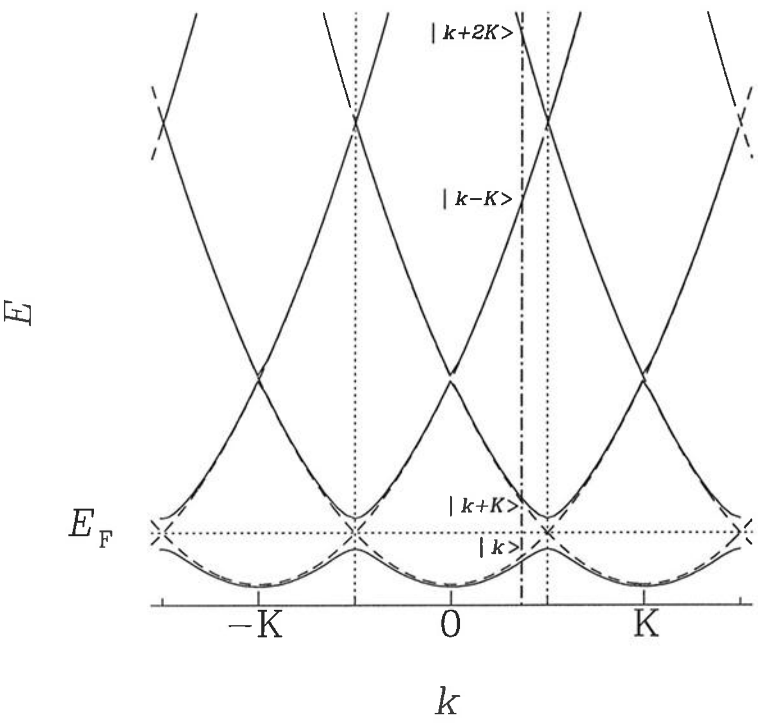

Figure 3.5: *Free (dashed lines) and nearly-free (full lines) electron dispersions in he repeated zone scheme. The first Brillouin zone is indicated with the dotted line, as well as the Fermi-energy for a filling of two electrons per unit cell. The states crossed by the dashed-dotted line will start to mix if the potential is switched on.*

$\langle k|H_1|k+K\rangle = U_K$, $\langle k-K|H_1|k+2K\rangle = U_{3K}$, etcetera. Because the spectrum of free electron states is unbounded from above, we would have to diagonalize an infinitely large matrix to obtain the exact solution and this is of course not feasible[2]. It turns out, that even in the case that the potential is rather strong, it appears possible to terminate this infinite progression at some large value of $\vec{K}$ if the interest is in the states at low energies. The problem is that one has to go to really large values of $\vec{K}$ (like $1000K$ in the present example) in order to have a reasonable description of the atomic states.

This is different in weak coupling. If $U_K << \varepsilon_K = \frac{(\hbar K)^2}{2m}$ (the typical kinetic energy difference) and we are interested in the lowest lying band we have only to consider the states $|k\rangle$ and $|k+K\rangle$, neglecting the states with higher K's ($|k+2K\rangle, |k+3K\rangle$) altogether. All what is left is a two level problem, with determinant[3],

$$\begin{vmatrix} \varepsilon_k - \omega & U_K \\ U_K & \varepsilon_{k+K} - \omega \end{vmatrix} = 0 \tag{3.31}$$

with solutions,

$$\omega_{\pm,k} = \frac{1}{2}(\varepsilon_{k+K} + \varepsilon_k) \pm \frac{1}{2}\sqrt{(\varepsilon_{k+K} - \varepsilon_k)^2 + 4U_K^2} \tag{3.32}$$

As long as we are not too close to the Brillioun zone boundary (dotted lines in the figure), the potential will give rise to insignificant corrections of order U_K^2/ε_K. A specialty arises right at the zone-boundary. The kinetic energy difference vanishes: $\varepsilon_k = \varepsilon_{k+K}$ and the two eigenstates of kinetic energy become *degenerate*. Hence, regardless the smallness of U, the potential energy will 'dominate' and the 'bonding' state will shift downward with U_K while the 'antibonding' state will shift upward with the same amount: at the zone-boundary, a gap opens up with the exact magnitude $2U_K$ due to the scattering against the lattice (see figure 3.5)! We will find in chapters V and VI that this behaviour of the gap will play an important role in the weak coupling theory of classical condensation.

The above can be repeated for every pair of free bands. In fact, perturbation theory becomes better and better if the energy increases because the kinetic energy differences increase quadratically with $\vec{K}$, while the $U_{\vec{K}}$'s decrease: at large enough energies, electron states always become plane-wave like. The net result is indicated with the full lines in figure (3.5): away from the zone-boundaries the bands follow the free dispersions closely. Only at the zone boundaries the potential scattering changes the situation drastically: gaps appear, which decrease in magnitude if the energy increases. The physical interpretation is as follows: starting in the limit $\vec{k} \rightarrow 0$, the wavelength of the electron is much larger than the lattice constant and on this length scale the crystal looks like the uniform vacuum because the potential is averaged away. Accordingly, the electron has a k^2 dispersion. When momentum increases,

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[2] This problem is circumvented in the formalism using phase shifts - see the exact solution of the Kronig-Penney model, exercise 3.10

[3] notice that the potential now appears on the off-diagonal, instead of the kinetic energy in the H_2 molecule example of section 2.1

the wavelength decreases until the electron-wave precisely fits into the unit cell at wavenumber $\vec{K}/2$. Here the influence of the potential is at maximum, diffraction occurs and the result is the band gap. In particle language, as a ramification of the breaking of translation symmetry, the particle suddenly reverses its momentum if it crosses the Brillouin zone boundary, and the scattering against a periodic potential is therefore also called 'Umklapp' (German for 'suddenly turn around') scattering. When the momentum increases further, the lattice becomes invisible again untill the next reciprocal lattice vector is approached, and the story repeats itself over and over again as function of increasing energy.

$\Longrightarrow$ Exercise 3.11.

What happens if the magnitude of the periodic potential increases? U_K/ε_K is no longer a small number and perturbation theory breaks down. All one can do for an arbitrary potential is to diagonalize the problem, taking all states into account up to a rather large total momentum $\vec{k}+\vec{K}$. For a purely one dimensional problem (which never occurs in nature: atoms have a finite spatial extent), the result will typically look as shown in figure 3.6. The dispersion of the low lying states, which are most strongly influenced, becomes more symmetric and approaches $\varepsilon_k \sim \cos(k)$, instead of the weakly perturbed $\sim k^2$ of the nearly free electron case. In the next section, the origin of these cosine dispersions will become clear.

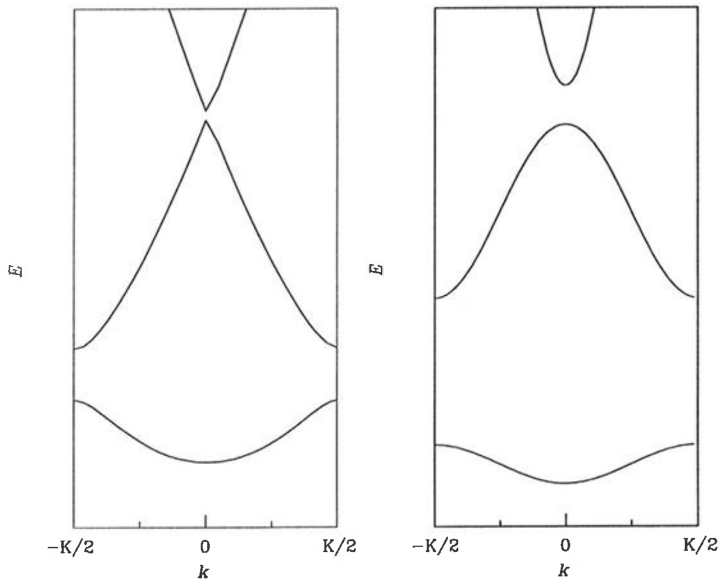

Figure 3.6: *Evolution of the one dimensional band structure from weak potential (left) - to strong potential (right) scattering, in the reduced zone scheme.*

Higher dimensions.

It all works the same in higher dimensions, except that it becomes harder to visualize how the free dispersions 'fold' in the Brillouin zone. For an impression of the four dimensional space in which the bands of a three dimensional crystal live, I refer to the extensive discussion in the book by Ashcroft and Mermin[4]. The notable differences from the one dimensional case can already be inferred from the simplest example of a higher dimensional system: the two dimensional square lattice. Folding the free electron bands in the Brillouin zone of figure 3.1 yields the result shown in figure 3.7. One would in fact like to present a three dimensional picture (k_x, k_y, E) but it is not easy to construct such a picture in a readable form, given that textbooks live in a two dimensional space. In the figure we therefore follow the general habit to only show the bands along the high symmetry directions in the zone - the extrema, band crossings, etcetera, are usually found along these directions and the mind does not

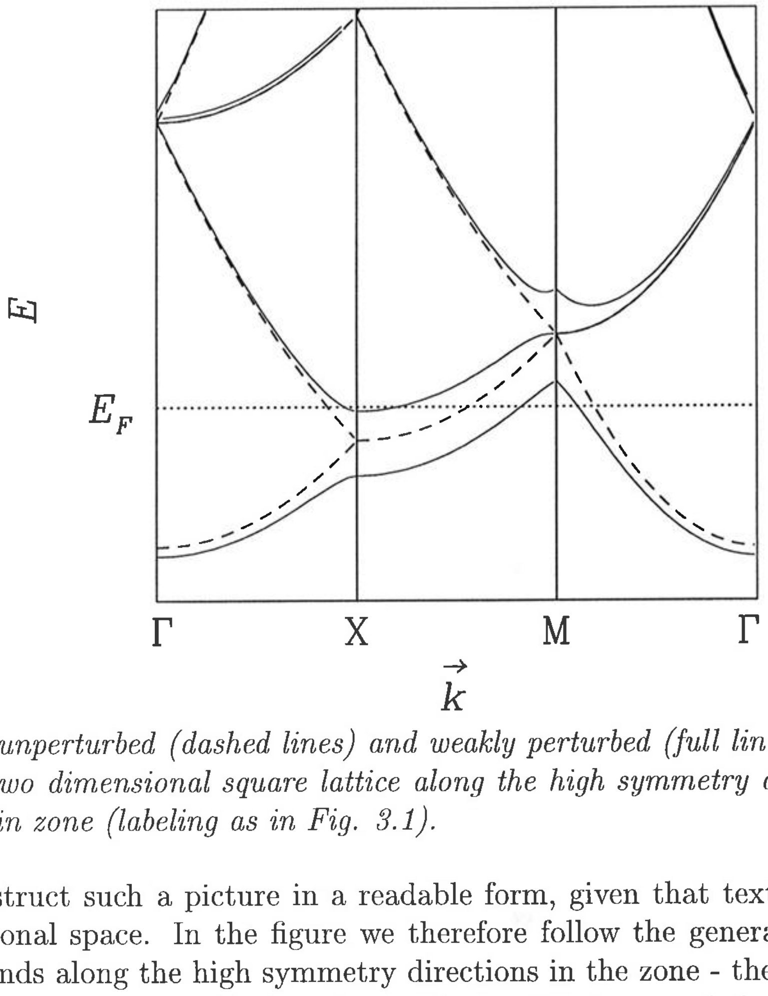

Figure 3.7: *unperturbed (dashed lines) and weakly perturbed (full lines) free-electron bands of a two dimensional square lattice along the high symmetry directions of the first Brillouin zone (labeling as in Fig. 3.1).*

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[4] N. W. Ashcroft and N. D. Mermin, 'Solid State Physics' (Saunders College Publ., 1976), pp. 152-283.

have difficulties interpolating the bands to the remainder of the zone.

$\Longrightarrow$ Exercise 3.12.

By construction, the free bands cross at the zone boundary and, as in the one dimensional case, it is along $X - M$ (and equivalent directions) that the gaps open up due to the potential scattering (figure 3.8).

Filling the bands: nesting.
In the independent electron picture, the only effect of a finite electron density comes from Fermi-Dirac statistics (section 2.3): fill up the bands with one electron per $\vec{k}$ state and spin direction. As a rule of thumb, one electron per unit cell fills up precisely one band. Including the spin degeneracy, this means that a density of one electron/unit cell gives rise to a *half-filled* band if there is only a single band accessible (with E_F roughly in the middle of the band). A single, spin degenerate band is precisely filled up with two electrons. The problem is that usually more bands are around and then one has to put effort in constructing the shape of the fermi-surface.

$\Longrightarrow$ Exercise 3.13.

In the one dimensional case, this becomes very simple. For every energy there is only a single, four-fold degenerate ($k, -k$ and spin) band state (fig. 3.6). Hence, for an even number of electrons the Fermi-'surface' (consisting of two points, k_F and $-k_F$) lies *exactly* on the Brillouin zone boundary ($k_F = K$). Since any potential, regardless its magnitude, causes band gaps at the zone boundary, an even number of electrons corresponds with a complete filling of the highest lying band. Therefore, even an infinitesimal small periodic potential will cause a one dimensional electron system to become a band insulator, if the electron density corresponds with an even number of electrons/unit cell. This property is called 'nesting' and we will see that it plays an important role in the weak-coupling theory of classical condensation (chapters V, VI).

Nesting is rather special to one dimension, and it never occurs in a precise sense in higher dimensions. For instance, in the two dimensional band structure of figure 3.8 the energies where the unperturbed bands cross (midpoint of the gap) vary considerably as function of momentum along the zone boundary ($X - M$ direction). For two electrons/unit cell, the Fermi-energy will be as indicated in the figure. If the potential is infinitesimal, the Fermi-surface will only hit the gap in the neighbourhood of the point $(\frac{\pi}{a}, \frac{\pi}{2a})$ and equivalent points. Only if $U_{(0,2\pi/a)}$ exceeds $\frac{(\pi\hbar)^2}{2ma}$, this system will turn into a band insulator since E_F lies in a gapped spectrum for all values of the momentum.

$\Longrightarrow$ Exercise 3.14.

What happens in the higher dimensional cases if the potential becomes stronger and stronger? Since the low energy states eventually have to end up as atomic states, one expects the band structure to acquire atomic-like features. It is obviously rather hard to recognize anything atomic-like in the nearly-free electron bands. Starting with atomic states, it is easier to imagine how to eventually reach the plane wave limit. This is the subject of the next section.

3.3 Tight-binding electrons.

The nearly free electron picture of the previous section is rather impractical if one is interested in typical valence electrons. Except for some special cases ('free electron metals', like $Li, Na, \cdots$), the structure of the valence bands looks completely different from the figures of the previous section. Usually, one gets much closer expressing the problem in a basis of atomic states, and this is called 'tight-binding'.

One can define this in a very precise and quantitative way: the 'linear combination of atomic orbital' (LCAO) method. This is the standard technique used by chemists to calculate the electronic structure of molecules - physicists find this inefficient and prefer to use the smarter methods summarized in the next section. Let us nevertheless consider how this works, to get a better feel for the approximations introduced later on. One starts defining a basis describing the atomic states of all atoms in the solid, $|\vec{R}, j, \eta, \sigma\rangle$ ($\eta \sim n, l, m_l$), describing the m_l'th component of a state with angular momentum l, radial quantum number n and spin σ, centered on the j-th atom in the unit cell, located at point $\vec{R}$ of the reciprocal lattice. Although the states on one atom are orthogonal, the states centered on different atoms are non-orthogonal. We assume that the above states are already orthogonalized in the remainder of the discussion. This basis forms a complete set

$$\sum_{\vec{R},j,\eta,\sigma} |\vec{R}, j, \eta, \sigma\rangle\langle\vec{R}, j, \eta, \sigma| = 1 \tag{3.33}$$

and one can resolve the Hamiltonian (3.1) in this basis,

$$\hat{H} = \sum_{\vec{R},j,\eta;\vec{R}',j',\eta';\sigma} |\vec{R}, j, \eta, \sigma\rangle\langle\vec{R}, j, \eta, \sigma| \left[-\frac{\hbar^2}{2m}\Delta + U(\vec{r})\right] |\vec{R}', j', \eta', \sigma\rangle\langle\vec{R}', j', \eta', \sigma| \tag{3.34}$$

Because the atomic wave functions are known explicitly, one can evaluate the matrix elements appearing in (3.34).The outcome will have the following structure,

$$\begin{aligned} \hat{H} &= \sum_{\vec{R},j,\eta,\sigma} |\vec{R}, j, \eta, \sigma\rangle\varepsilon(\vec{R}, j, \eta)\langle\vec{R}, j, \eta, \sigma| \\ &+ \sum_{\vec{R},j,\eta;\vec{R}',j',\eta';\sigma} |\vec{R}, j, \eta, \sigma\rangle t(\vec{R}, j, \eta; \vec{R}', j', \eta')\langle\vec{R}', j', \eta', \sigma| \end{aligned} \tag{3.35}$$

where the matrix elements ε and t can be calculated numerically. The 'on-site' energies ε amount to a modified energy for the atomic states - they will be similar to the atomic energies, except that they will also contain some effect of the lattice. For instance, the degeneracy of the states with the same l quantum number will be lifted because the atoms are no longer in a spherical symmetric environment. The 'hopping integrals' or 'transfer matrix elements' t parametrize the fact that electrons can delocalize in the solid: electrons can tunnel from a state on one atom to a state on another atom, (compare with the H_2^+ model, section 2.1).

Finally, one can profit from the periodicity of the potential to further simplify the problem. Using Bloch's theorem,

$$|\vec{R}, j, \eta, \sigma\rangle = \frac{1}{\sqrt{\Omega}} \sum_{\vec{k}} |\vec{k}, j, \eta, \sigma\rangle e^{i\vec{k}\cdot\vec{R}} \tag{3.36}$$

one obtains a Hamiltonian which is diagonal in momentum space

$$\begin{aligned} \hat{H} &= \sum_{\vec{k}\sigma} [\sum_{j,\eta} |\vec{k}, j, \eta, \sigma\rangle \varepsilon(j,\eta) \langle \vec{k}, j, \eta, \sigma| \\ &+ \sum_{j,\eta;j',\eta'} |\vec{k}, j, \eta, \sigma\rangle t(\vec{k}; j, \eta; j', \eta') \langle \vec{k}, j', \eta', \sigma|] \end{aligned} \tag{3.37}$$

Assuming a periodic lattice, the on-site energies are the same in all unit cells, and we may as well drop the $\vec{R}$ (or $\vec{k}$) label. The kinetic energy, associated with the motion through the lattice, is entirely contained in the hopping terms t, and for this reason all the momentum dependence is in (compare 3.20),

$$t(\vec{k}, j, \eta; j', \eta') = \frac{1}{\Omega} \sum_{\vec{R}} t(\vec{R}_0, j, \eta; \vec{R}, j', \eta') e^{-i\vec{R}\cdot\vec{k}} \tag{3.38}$$

where $\vec{R}$ runs over all points of the Bravais lattice ($\vec{R}_0$ is the origin).

As (3.30), (3.37) would become exact if all atomic states could be used. The issue is again *practicality*: can we get away with only a small number of states? In addition, we would like the hopping to fall off quickly with distance so that we only have to know very few terms in (3.38). This becomes a real problem if one tries to use tight-binding to understand the band structure qualitatively. For every state one adds, one needs to know one more diagonal matrix element ε and a couple of hopping parameters t. Since one wants to avoid a large calculation, one likes to consider these parameters to be undetermined within certain bounds. When too many states have to be taken into account, one looses track in no time because parameter space grows too large.

Under which circumstances do we expect to get away with few states and short range (nearest-neighbour) hoppings? This is obviously the case in the low energy region of figure 3.4. One can first form bound states which lie deep in the potential wells, which are very close to purely atomic states. Since the potential barrier is finite, electrons can tunnel from atom to atom with a small amplitude (the t's). The tunneling probability drops off exponentially with distance and this causes the hopping to be short ranged. This picture applies only to the atomic core states (energies less than ~ -10 eV below E_F) and it is not at all realistic for valence band states.

Nevertheless, it turns out that one can obtain a quite accurate description of the valence bands, with a minimal basis consisting of only the atomic states which lie directly at E_F: typically one s state and one set of p states, augmented with the valence d states for transition metal atoms, and the f states for the rare earth- and actinides. Exploiting in addition point group symmetry and some general empirical rules regarding the magnitude of the matrix elements, this means that one can calculate realistic band structures for many crystals nearly by hand[5]. This has its special reasons. It appears possible to transform the sophisticated basis sets of the next section in a way that the Hamiltonian acquires a 'hopping' structure, like (3.37)[6]. Subsequently one can show that the hopping elements between the valence states (s, p) and the higher lying states can be forced to be quite small while the hopping matrix elements between the valence states are of a reasonable range at the same time. Keep in mind that these 'first principle' tight-binding states are quite different from atomic states. They leak out considerably in the interstitial regions, and instead of the exponential decay, the hopping matrix elements depend algebraically on the interatomic separation (typically $t \sim 1/d^\eta$, where d is the bond-length, while η depends on the angular momenta: see Harrison).

Let us consider how tight-binding works in practice, aiming at an understanding of the bandstructure of La_2CuO_4.

Single band models on cubic lattices.

The simplest tight-binding model is the *single band* model, which is nothing else than the two-level model of chapter II, extended to the lattice. It is assumed that only one electronic state $|\vec{i}\sigma\rangle$ is present in the unit cell at $\vec{R}_i$ and the hopping is restricted to nearest-neighbours. The vectors $\vec{\delta}$ point along the nearest-neighbour bonds, such that $\vec{i} + \vec{\delta}$ are the positions of the nearest-neighbours of site $\vec{i}$. The single band Hamiltonian is[7],

$$\hat{H} = \sum_{\vec{i},\sigma} |\vec{i}\sigma\rangle \varepsilon \langle \vec{i}\sigma| + \sum_{\vec{i},\vec{\delta},\sigma} |\vec{i}\sigma\rangle t \langle \vec{i} + \vec{\delta}\sigma| \tag{3.39}$$

Because only one state is present per unit cell, the problem is diagonalized by the Fourier transformation (3.36),

$$\hat{H} = \sum_{\vec{k},\sigma} |\vec{k}\sigma\rangle \left(\varepsilon + zt\gamma_{\vec{k}}\right) \langle \vec{k}\sigma| \tag{3.40}$$

where z is the coordination number (the number of nearest-neighbours) and

$$\gamma_{\vec{k}} = \frac{1}{z} \sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}} \tag{3.41}$$

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[5] See the book by W. A. Harrison 'Electronic structure and the properties of solids' (Freeman, San Francisco, 1980).

[6] see O. K. Andersen and O. Jepsen, Phys. Rev. Lett. 53, 2571 (1984).

[7] Notice that the restriction to nearest-neighbours is often indicated by $\sum_{<ij>} |i\rangle\langle j|$.

The function $\gamma_{\vec{k}}$ contains the information regarding the lattice structure. Notice that we set the lattice constant $a = 1$, such that the Brillouin zone is measured in units of π. For a hypercube (d is dimensionality),

$$\gamma_{\vec{k}} = 2\sum_{i=1}^{d} \cos(k_i) \quad , \quad \vec{k} = (k_1, \cdots, k_d) \tag{3.42}$$

$\Longrightarrow$ Exercise 3.15.

In the one dimensional case, the dispersion becomes $\omega_k = \varepsilon + 2t\cos(k)$: we recover the cosine band of figure (3.7)! In higher dimensions, the bands remain 'cosine like'. For instance, on a $d = 2$ square lattice

$$\hat{H} = \sum_{\vec{k},\sigma} |\vec{k}\sigma\rangle \; (\; \varepsilon + 2t(\cos(k_x) + \cos(k_y)) \;) \; \langle\vec{k}\sigma| \tag{3.43}$$

and so on. Notice that the total band width $W = 4zt$ ($z = 2d$) - this total bandwidth is the best measure of the kinetic energy in interacting problems, as we will see later on.

$\Longrightarrow$ Exercise 3.16.

$\Longrightarrow$ Exercise 3.17.

With a minimum effort we find bands which look quite realistic for a regime characterized by strong potential scattering. In the $d = 1$ case, it is not hard to see how to interpolate between the tight-binding bands and the picture obtained from the plane waves (figure 3.6). In higher dimensions this interpolation is not easy, although it is clear that the tight-binding limit should make sense if a single atomic-like state would become isolated (separated by large gaps) from all other states. In reality, there are always more states in the neighbourhood, although their total number tends to be small. To approach reality, we have to consider 'few band' models.

Two band models on cubic lattices.

Let us now consider the simplest extension of the single band model: a cubic crystal containing two different states per unit cell. These occur in different varieties and to keep the focus on La_2CuO_4, we will specialize on perovskite-like lattices in the text, leaving some other possibilities to the exercises. Let us first consider a $d = 1$ 'perovskite' lattice, consisting of alternating Cu and O atoms: $Cu-O-Cu-O-\cdots$. We assume that we only have to consider one orbital for Cu and one orbital for O which are relatively close in energy. Anticipating on real CuO, we denote the Cu orbital in the i-th unit cell with $|d; i\sigma\rangle$ (from the atomic $3d$ state) and the O state with $|p; i\sigma\rangle$ (from $2p$). The Hamiltonian is ($h.c.$ is hermitian conjugate),

$$\begin{aligned} \hat{H} \;=\; & \sum_{i,\sigma} (|d; i\sigma\rangle\varepsilon_d\langle d; i\sigma| \;+\; |p; i\sigma\rangle\varepsilon_p\langle p; i\sigma| \;+\; (|d; i\sigma\rangle t_{pd}\langle p; i\sigma| \;+\; h.c.)) \\ & + \sum_{i\sigma} (|p; i-1\sigma\rangle t_{pd}\langle d; i\sigma| \;+\; |d; i+1\sigma\rangle t_{pd}\langle p; i\sigma|) \end{aligned} \tag{3.44}$$

i counts here the $Cu - O$ unit cells, while $\varepsilon_{p,d}$ are the on-site energies and t_{pd} the hopping parameter from Cu to O. Notice the arrangement of the hopping matrix elements: in the first line the hops occurring within the unit cell are counted, and in the second line the hops connecting cell i with the neighbouring cells to the left and to the right. (3.36) becomes (N is number of unit cells),

$$\begin{aligned} |d; j\sigma\rangle &= \frac{1}{\sqrt{N}} \sum_k |d; k\sigma e^{ikj}\rangle \\ |p; j\sigma\rangle &= \frac{1}{\sqrt{N}} \sum_k |p; k\sigma e^{ikj}\rangle \end{aligned} \tag{3.45}$$

and the Hamiltonian in momentum space becomes,

$$\begin{aligned} \hat{H} &= \sum_{k,\sigma} [|d; k\sigma\rangle \varepsilon_d \langle d; k\sigma| \; + \; |p; k\sigma\rangle \varepsilon_p \langle p; k\sigma| \\ &+ \; (|d; k\sigma\rangle t_{pd} (1 + e^{ik}) \langle p; k\sigma| + h.c.)] \end{aligned} \tag{3.46}$$

because we started with two orbitals/unit cell, we find that the Fourier transformation does not diagonalize the problem entirely: we are left again with a 2×2 ('two level') problem in k-space. This is easy to diagonalize (chapter II), and the eigenvalues are,

$$\omega_{\pm,\vec{k}} = \frac{\varepsilon_d + \varepsilon_p}{2} \pm \frac{1}{2} \sqrt{(\varepsilon_d - \varepsilon_p)^2 + 16 t_{pd}^2 \cos^2(\frac{k}{2})} \tag{3.47}$$

We find two bands: a 'bonding' band ($\omega_{-,k}$) and an 'antibonding' ($\omega_{+,k}$) band. To understand the nature of these bands, let us consider the limits. When the splitting

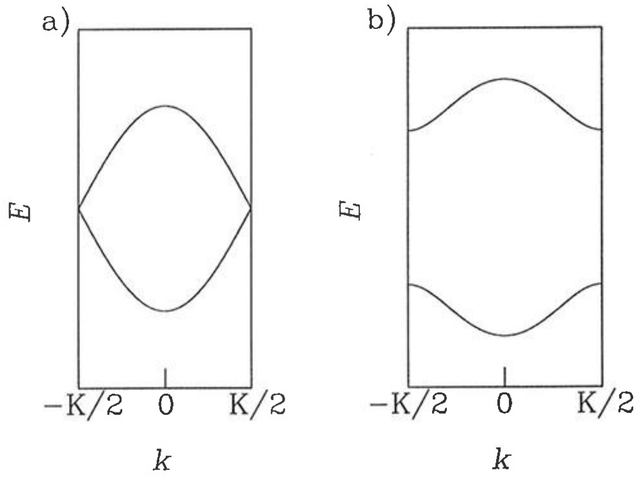

Figure 3.8: *Band structure of 'Cu − O' chain. (a) The 'covalent/metallic' limit:* $\varepsilon_d = \varepsilon_p$. *(b) The 'ionic' limit:* $\varepsilon_d - \varepsilon_p >> t_{pd}$.

of the atomic levels vanishes ($\varepsilon_p = \varepsilon_d$), the band structure reduces to that of the single band model. Because we doubled the unit cell, the Brillouin zone became half as large and $\pm 2|t_{pd} cos(k/2)|$ is the folded version of the cosine band of the single band model (Fig. 3.8a). On the other hand, if the splitting becomes much larger than the bandwidth ($W = 4t_{pd}$), the bands are well separated and the bandwidth of both p- and d like bands can be estimated to be $\sim 4t_{pd}^2/|\varepsilon_d - \varepsilon_p|$ (Fig. 3.8b).

$\Longrightarrow$ Exercise 3.18.

This minimal one dimensional problem reveals the basic principles and everything else is a variation on this theme, except that the bands are harder and harder to calculate if dimensionality and/or number of basis states increases.

$\Longrightarrow$ Exercise 3.19.

Eleven bands: La_2CuO_4.

To illustrate this, let us focus on the bandstructure of La_2CuO_4. As a typical example of the versatility of the tight-binding method, it turns out that all the bands shown in figure (3.2) can already be quite well understood if one only considers the $Cu3d$ orbitals and the $O2p$ orbitals of the planar Cu and O atoms. The crystal structure consists of a square Bravais lattice, with a CuO_2 unit cell (see Fig. 3.3). This amounts still to a rather large problem: there are 5 $3d$-orbitals associated with Cu and 6 $2p$ orbitals coming from the two O atoms: a 11 × 11 Hamiltonian has to be solved for every $\vec{k}$ point. The 'crystal' is tetragonal, in the sense that the x and y directions in the square lattice are equivalent, while the z-direction is inequivalent. In this case, it makes sense to use the cubic harmonics: $2p_x, 2p_y, 2p_z$ on the two oxygens and $3d_{x^2-y^2}, 3d_{3r^2-1}, 3d_{xy}, 3d_{xz}, 3d_{yz}$ on the copper. Indeed, counting the total number of bands in figure 3.2, we find a total of 11 (omitting the free electron bands at the very top of the figure).

$\Longrightarrow$ Exercise 3.20.

It is clear that one needs many tight-binding parameters to describe such a complex band structure. Such a set was extracted from a full band structure calculation. Taking only nearest-neighbour hoppings, the outcome of the tight-binding calculation looks as follows,

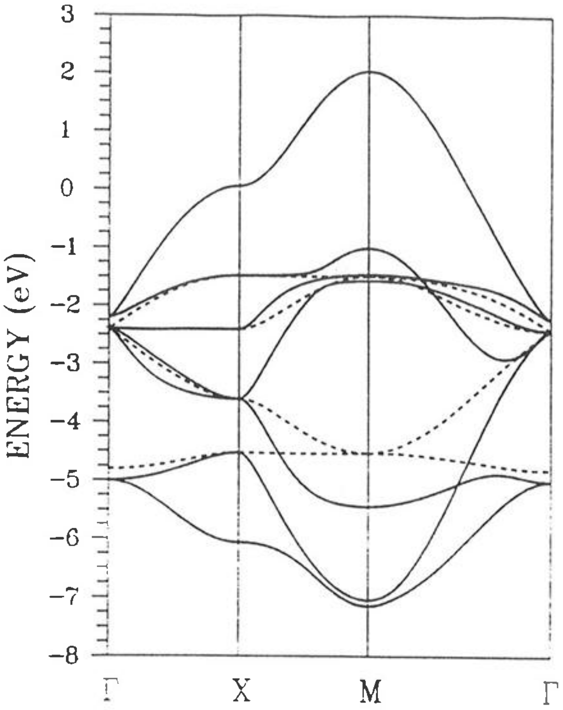

Figure 3.9: *Tight-binding band structure of the perovskite planes of La_2CuO_4 in the valence band region. Only the oxygen 2p and the copper 3d states have been used (after: H. Eskes, thesis, Groningen University, 1992). The labeling of the Brillouin zone is indicated in figure 3.1.*

Comparing this with the 'exact' band structure (figure 3.2), one finds that the correspondence is not perfect, but good enough to get some qualitative ideas about the nature of the electronic states. The interest is in first instance in the states close (within 1-2 eV) to the Fermi-energy. The $Cu - O$ band structure is nearly filled: for the 22 bands (including spin), there are 21 electrons available ($2 \times O^{2-} = 12$ plus $Cu^{2+} = 3d^9$). According to figures (3.2) and (3.9), the uppermost part of the valence band is dominated by a single band, which shows such a strong dispersing that it 'outclimbs' all other bands. As can be seen from the figures, the Fermi-energy lies in a region where there are no other bands, except for the strongly dispersive one. Since the density is one hole/unit cell, this band becomes half-filled and the states near E_F have something to do with the character of this particular band. All other states are fully occupied and are therefore of secondary interest.

One observes that the tight-binding calculation reproduces the strongly dispersive band particularly well. Because of the simple structure of tight-binding, it becomes easy to get a clear answer to the urgent question: what is the character of the states close to E_F? Recalling the simple $Cu - O$ chain example, we found that large bandwidths are caused by (a) a large $p - d$ hopping matrix element, and (b) a rather covalent character, in the sense that the Cu and O levels are close to being degenerate. The second condition is fulfilled for all states. It was already known for a long time that cuprates are rather covalent materials. Hence, to identify the nature of the states near E_F one only has to look for the largest t_{pd}. The magnitude of the hoppings depend on the cubic-harmonic quantum numbers of both orbitals involved in the hopping process (see 3.35). In the present case it is easy to estimate the relative magnitude of the different hoppings. Consider a pair of orbitals, centered on neighbouring lattice sites. Some examples are shown in figure 3.10. One can

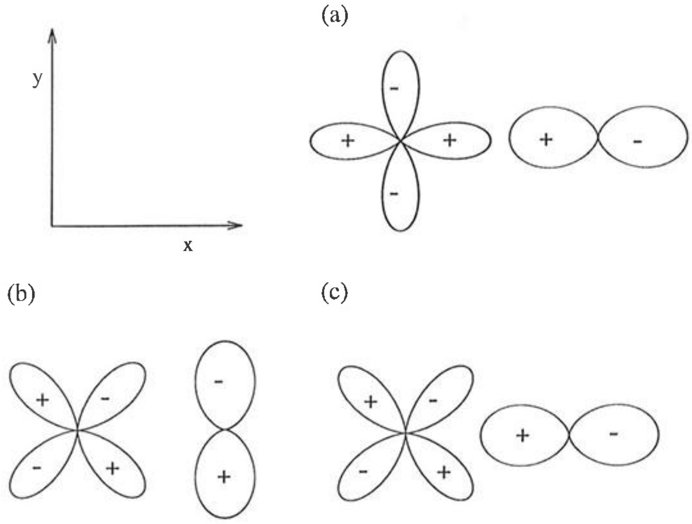

Figure 3.10: *Cubic harmonics of* 3*d and* 2*p orbitals on neighbouring* Cu *and* O_1 *lattice sites: (a)* $3d_{x^2-y^2}$ *and* p_x*. (b)* $3d_{xy}$ *and* p_y*. (c)* $3d_{xy}$ *and* p_x*.*

estimate the overlaps from these pictures. As a first rule, the more orbitals point *towards* each other, the larger the overlaps are, and thereby the hoppings. Both the $3d_{x^2-y^2}$ and the p_x orbitals have their lobes pointing precisely along the bond and this will optimize the hopping (figure (3.10a): this is called a σ bond). On the other hand, the $3d_{xy}$ and p_y states are both oriented perpendicular to the bond direction, and this will yield a finite hopping which is, however, much smaller than the σ hopping (fig. 3.10b: π bond, t_π is typically half t_σ). Also the phases of the different lobes of the cubic harmonics play an important role: if a plus lobe overlapping with a plus lobe gives rise to a net positive hopping, a plus lobe overlapping with a minus lobe will give rise to a negative value of the hopping matrix element. If both overlaps are equally large, the hopping will interfere away completely. For instance, an electron cannot hop from a $3d_{xy}$ orbital to a neighbouring p_x orbital (figure 3.10c).

$\Longrightarrow$ Exercise 3.21.

$\Longrightarrow$ Exercise 3.22.

From the preceding discussion, it is clear that the prime candidate for the strongly dispersing band in the cuprate is the one derived from Cu $3d_{x^2-y^2}$ and the σ-like oxygen states, p_x on O_1 and p_y on O_2. We only consider the $p-d$ hoppings, and in the same parametrization as for the one dimensional CuO problem, the bands are given by

$$\begin{aligned}
\omega_{\pm,\vec{k}} &= \frac{\varepsilon_d+\varepsilon_p}{2} \pm \frac{1}{2}\sqrt{(\varepsilon_d-\varepsilon_p)^2 + 16t_{pd}^2(\sin^2(\frac{k_x}{2})+\sin^2(\frac{k_y}{2}))} \\
\omega_{0,\vec{k}} &= \varepsilon_p
\end{aligned} \tag{3.48}$$

consisting of a (for accidental reasons) 'non-bonding' band ω_0 and a pair of bonding and anti-bonding bands $\omega_\pm$.

$\Longrightarrow$ Exercise 3.23.

The bands of this 'three-band' model are shown in figure 3.11. The strongly dispersive anti-bonding band is already accurately reproduced by this very simple model! It turns out that this simple model reproduces the correct physics - also the full-size calculations indicate that the states near E_F are nearly exclusively of $x^2-y^2, p_{x,y}$ character. Stronger, although band structure theory has not much to say about the electronic structure of high T_c superconductors in general, it gets this orbital aspect right. The extension of the three band model, including the electron-electron interactions, is nowadays the standard starting point for the study of the problem of high T_c superconductivity.

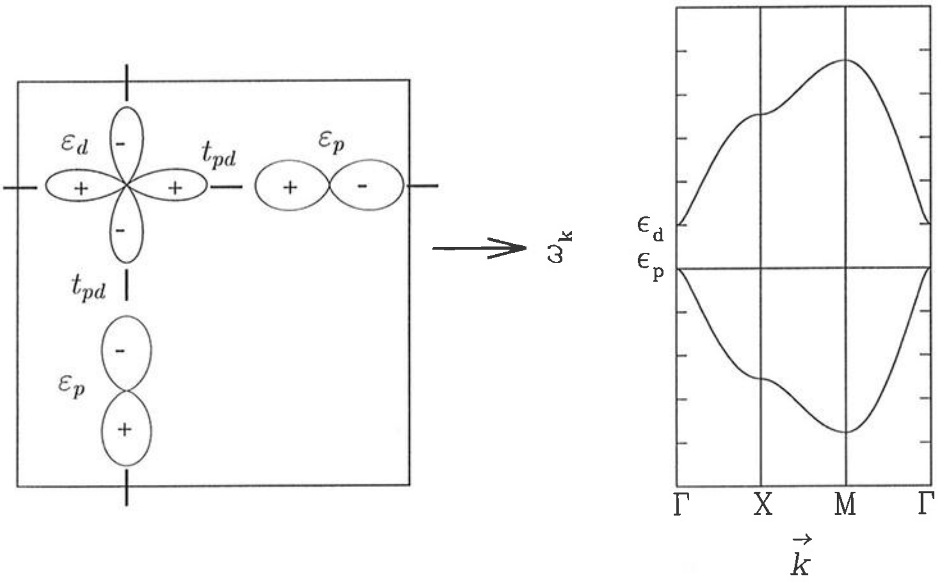

Figure 3.11: *definition of the three band model, and its band structure* (t_{pd} = 1.5 eV, *and* $\varepsilon_d - \varepsilon_p$ = 1 eV).

3.4 High-tech band structure methods.

Let me finish this chapter by a very brief description of the popular band structure methods. I will do this from a strict consumers perspective: except for the first, they all rely on rather sophisticated tricks and a full discussion of any of them would take up many pages. I refer the interested student to the literature[8]. Instead, I will only hint at the underlying formalisms, and point out which method performs best, given a specific problem.

1 *Semi-empirical tight-binding.* This is nothing else than the tight-binding method of the previous section, augmented with tables for the tight-binding parameters (established by fitting experiment and first principle calculations) so that one can attempt quantitative calculations. This is the cheapest-, but also the most unreliable of all methods. It is typically used to calculate very big problems (like extended defects, screw dislocations etcetera) involving simple atoms (typically silicon).

2 *Pseudo-potentials.* This is in spirit very close to the weak potential problem of section 3.2. I argued that the plane wave expansion becomes problematic because of the the strong variation of the atomic potential. In fact, this 'bare' atomic potential is not quite the potential which is seen by the valence electrons. The reason is that the wave-functions of the valence electrons have to be orthogonal to the wave-functions of the atomic core-electrons. This orthogonality condition tends to keep the valence electrons away from the atomic-cores. It turns out to be possible to derive recipies for effective potentials, seen by the valence electrons, which take into account this orthogonality effect. These 'pseudopotentials' are much smoother than the bare atomic potentials. As a consequence, the plane wave expansion converges much more rapidly than would be the case if the bare atomic potentials would be used. This method works of course best if the pseudopotentials are indeed very weak, as is the case in the nearly free electron metals. It turns out, however, that it is the most efficient method in other cases as well, as long as one is not dealing with the (atomic like) $3d, 4d, 4f$ and $5f$-derived valence electrons. In these latter cases, the problem is more than mere efficiency. When the pseudo-potential is not shallow, it is actually no longer possible to define it in an unambiguous way.

3 *The muffin-tin methods: LAPW, KKR and LMTO.* The truly hard cases are the ones where neither the atomic-like basis sets, nor the plane waves are of much use because the valence electrons scatter against an effective potential which is of an intermediate strength. This is typically the case for d- and f like valence electrons. The starting point is to divide up space in 'atomic spheres' where the potential is atomic like and 'interstitial regions' where the potential is rather flat (see figure 3.4): the 'muffin-tin potential'. Inside the

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[8] The most extensive discussion is probably by J. Kuebler and V. Eyert, in: Materials Science and Technology (Eds. R. W. Cahn, P. Haasen and E. J. Kramer, VCH, Weinheim, 1991). A reasonable introductory discussion is found in the second edition of Callaway's 'Quantum theory of solids'.

atomic spheres one expands in terms of atomic-like states and in the interstitial regions the wavefunction is described in a plane-wave like basis. In the spirit of the Kronig-Penney model (exercise 3.10), one has now to match both basis sets at the atomic sphere boundary. In the 'Linearized Augmented Plane Wave' (LAPW) method one chooses atomic states inside the sphere which have to be matched to plane waves in the interstitial regions. This yields a very robust and accurate method, which can deal with every type of potential. The downside is that it is very expensive: one typically needs 100 basis states per atom in the unit cell. Given the performance of the present supercomputers, this means that the largest unit cells which can be dealt with are like the ones of the high T_c cuprates. Alternatively, the matching problem can be dealt with in a Greens function formalism: the Korringa-Kohn-Rostoker (KKR) method. This is also a very expensive method. However, a special type of basis can be extracted from this formalism: the so-called muffin-tin orbitals, which are particularly suited to deal with the matching problem. Starting from this basis, the so-called 'Linearized Muffin Tin Orbital' (LMTO) method has been developed, which exists both in a cheap and less accurate version (the so-called LMTO-ASA method, typically 9 states/atom) and a very accurate and highly efficient, so called 'full potential LMTO', version. When pseudo-potentials do not work, the latter seems the best choice on the market, with the added advantage that it allows for a 'first principle' mapping onto an effective tight binding model (see the discussion in the previous section).

3.5 Exercises

3.1 Show that there are exactly $N_1N_2N_3 = N$ allowed values of k within a unit cell of the reciprocal lattice.

3.2 Prove the equivalence of (3.10) and (3.19).

3.3 Also in the many body context one can exploit the periodicity of the lattice, although the symmetry property is of much less help in this context than in single particle theory. We consider a Hamiltonian of the form

$$\mathcal{H} = \sum_i \mathcal{H}_1(\vec{r}_i) + \sum_{ij} \mathcal{H}_2(\vec{r}_i, \vec{r}_j) + \ldots$$

a) Under what kind of translation is this Hamiltonian invariant?

b) To which conserved quantity is this invariance related?

c) Introduce an operator which generates this translation and express it in terms of the single-particle translation operators $\hat{T}_{\vec{r}_i}$. Write down a Bloch theorem of the form (3.19) for the many-particle case.

3.4 In order to count states in k-space, it is convenient to apply periodic boundary conditions. The wave functions have to fulfill $\Psi(\vec{r}_i) = \Psi(\vec{r}_i + N_i\vec{a}_i)$ $(i = 1, 2, 3)$. The allowed wave vectors now live on a fine mesh in k-space (see pp 42-43).

Show that, regardless the crystal structure, the volume per allowed $\vec{k}$-state is given by

$$\Delta\vec{k} = \frac{(2\pi)^d}{\Omega},$$

where d is the dimension of the crystal and Ω its real space volume.

3.5 a) Show that the Hamiltonian $\mathcal{H}_{\vec{k}}$ (3.20) is hermitian.

b) Check the normalization and orthogonality of the Bloch functions.

3.6 a) Check (3.24).

b) Show that, for a free particle, the eigenstates of $\mathcal{H}$ are also eigenstates of the momentum operator $\vec{p}$, with eigenvalues $\vec{p} = \hbar\vec{k}$. This implies that a particle with wave function $e^{\imath\vec{k}\cdot\vec{r}}$ has momentum $\vec{p} = \hbar\vec{k}$.

c) What is the wavelength of a free electron with energy 1 eV? What kind of energy must electrons in an electron microscope at least have, in order to resolve structures on a length scale of one Angstrom?

3.7 Consider a three-dimensional cubic lattice with length L in each direction and periodic boundary conditions.

a) Prove (3.25)

b) Show that in the (continuum) limit $L \to \infty$

$$\prod_i^d \sum_{k_i=2\pi n_i/L} \to \left(\frac{L}{2\pi}\right)^d \int d\vec{k}$$

c) Show that the inner product of two states is given by

$$< \vec{k}\sigma|\vec{k}'\sigma' >= \frac{(2\pi)^d}{\Omega}\delta_{\sigma\sigma'}\delta(\vec{k}-\vec{k}').$$

for L going to infinity.

3.8 a) Show that, for the case of periodic boundary conditions, the density of states $\rho_p(E)$ of a spinless free particle in a cube of volume L^3 is given by

$$\rho_p(E) = \frac{mkL^3}{2\pi^2\hbar^2} = \frac{m\sqrt{2mE}}{2\pi^2\hbar^3}L^3$$

b) We now consider a particle inside the same volume but with the boundary condition that $\psi = 0$ at the boundaries. We assume the wave function to be of the form

$$\psi_{\vec{k}} = A\sin k_1x \sin k_2y \sin k_3z.$$

What are the allowed values of k_1, k_2 and k_3? Why should one only consider positive values?

c) Normalize the wave function.

d) The following general formula for the density of states ρ_0 for a spinless particle with boundary condition $\psi = 0$ was derived by Weyl

$$\rho_0(E) = \rho_p(E) - \frac{mS}{8\pi\hbar^2} + \mathcal{O}(L).$$

S is the surface of the box in which the particle is confined. Since $\rho_p(E) \sim L^3$, the difference between the two boundary conditions vanishes for L going to infinity. Verify this formula for the particle which we analyzed under b).

3.9 a) In the previous exercise, we derived the density of states for a 3D spinless non-interacting jellium using periodic boundary conditions. Adding spin introduces an extra factor 2 in the density of states. Use this result to show that the zero temperature total energy for a 3D non-interacting jellium with spin is given by $E_0 = \frac{3}{5} N \varepsilon_\mathrm{F} \sim n^{2/3}$, where n is the density of electrons and ε_F the Fermi energy.

b) The specific heat as a function of temperature is given by

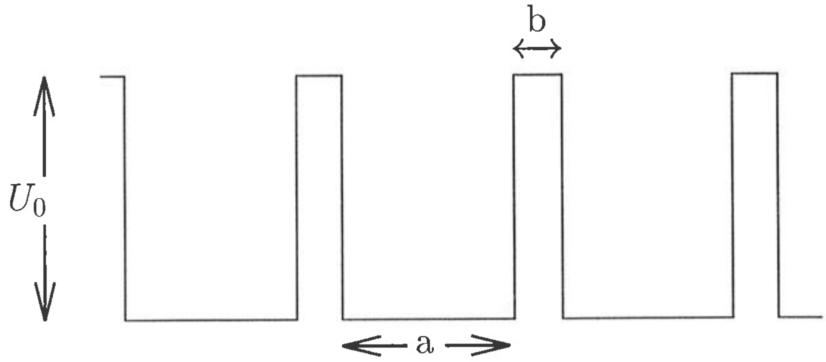
$$c_V = \left(\frac{\partial \mu}{\partial T}\right)_V = \frac{\pi^2}{3} k_\mathrm{B}^2 T \rho(\varepsilon_\mathrm{F}),$$

where $\rho(\varepsilon_\mathrm{F}) = m k_\mathrm{F}/(\hbar\pi)^2$ is the density of states at the Fermi energy. Prove this. Hint: use $n = \int \mathrm{d}\varepsilon \rho(\varepsilon) n_\mathrm{F}(\varepsilon) = \text{constant}$, to derive the temperature-dependence of the chemical potential μ. The standard integral

$$\int_{-\infty}^{\infty} \mathrm{d}x x^2 \frac{\partial}{\partial x} \frac{1}{\mathrm{e}^x + 1} = -\frac{\pi^2}{3}$$

may be usefull.

3.10 We consider the Kronig-Penney-model. This is a strongly simplified, one dimensional lattice-model, for which the bandstructure can be calculated exactly. Let $U(x)$ be the potential which is defined by the following figure:



We consider this model in the limit where $b \to 0$ and $U_0 \to \infty$, while $P \equiv \left(\frac{ma}{\hbar^2}\right) bU_0$ remains fixed. In this limit, $U(x)$ consists of delta-functions with strength P, spaced at an interval a: $U(x) = \sum_{i=-\infty}^{\infty} P\delta(x - ia)$.

a) Solve the Schrödinger equation in this limit

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+U(x)\right)\psi(x)=E\psi(x). \tag{3.49}$$

Show that the dispersion relation is determined by the equation

$$\cos k\alpha = \cos a\alpha + P\frac{\sin a\alpha}{a\alpha}, \tag{3.50}$$

where $\alpha=\sqrt{2mE/\hbar^2}$.

b) Plot the righthand side of this equation as a function of $a\alpha$ for different values of P. Note that all curves intersect at $a\alpha = n\pi$, where n is a positive integer number.

c) The equation determining the dispersion relation only has solutions for those values of α for which the absolute value of its righthand side is not larger than one. Since α is a measure of the energy, these values of α determine the energy bands. Use the result from b) to show that the energy bands become broader as P becomes smaller. In other words, if we increase the strength of the potential and thereby more strongly confine the electrons in each interval, the width of the energy bands reduces.

d) Draw the low-lying energy bands both for small and for large P.

3.11 a) The velocity operator is given by

$$\vec{v}=\frac{\mathrm{d}\vec{r}}{\mathrm{d}t}=\frac{1}{\imath\hbar}[\vec{r},\mathcal{H}]=\frac{\vec{p}}{m}=-\frac{\imath\hbar}{m}\vec{\nabla}.$$

Prove that the velocity of Bloch electrons in the state $\psi_{n\vec{k}}$ (n is the bandindex) can be expressed directly in terms of the dispersion relation by

$$\vec{v}_n(\vec{k})=\frac{1}{\hbar}\frac{\partial\varepsilon_n(\vec{k})}{\partial\vec{k}}.$$

b) What happens at the zone boundary if the crystal potential is finite?

c) Use $\varepsilon(\vec{k})=\varepsilon(-\vec{k})$ to show that a completely filled band does not contribute to the conductance.

3.12 Check fig. 3.8 for yourself. Construct the bands for the following directions as well: $(-\pi/4,0)\rightarrow(\pi/4,3\pi/4)\rightarrow(\pi/4,0)\rightarrow(\pi/2,\pi/4)$ (see fig. 3.1).

3.13 The density of states of non-interacting jellium electrons in two dimensions is given by

$$\rho(e)=\frac{mA}{2\pi\hbar^2}\qquad\text{per spin direction,} \tag{3.51}$$

where A is the surface in which the electrons are confined.

a) Derive this using periodic boundary conditions.

b) Express the Fermi energy in terms of the total number of electrons.

c) Calculate the total band energy for a filling of n electrons per unit cell.

3.14 a) Indicate the Fermi energy in the band structure in figure 3.7 for a filling of $n = 1, 2$ and 4 electrons per unit cell.

b) Fold the spherical Fermi surface for the different band fillings into the first Brillouin zone, using the unperturbed bands.

c) Switch on the potential and show how the Fermi surface evolves as a function of the potential strength at the filling $n = 2$.

3.15 Derive (3.40)-(3.42).

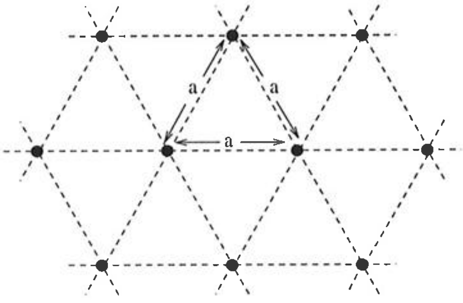
3.16 Consider the two-dimensional case (3.43).

a) Sketch the band structure along the usual high symmetry directions (e.g. fig. 3.8).

b) Include a next-nearest neighbor hopping matrix element t' (along the diagonals of the elementary plaquette) and show how the bands evolve along the high symmetry directions as a function of t/t'.

3.17 a) Assume a single state to live on every site of the Bravias lattice of an orthorhombic crystal: this is like a cubic crystal, except that the lattice constants in the x, y and z directions are different. Derive the dispersion relation in terms of the three different nearest-neighbor hoppings.

b) Consider a triangular lattice in $d = 2$ with a single orbital per site and nearest neighbor hoppings. Derive the dispersion relation and plot the



bands along high symmetry directions.

3.18 The simple '$Cu-O$' chain model can be used to illustrate the chemists' concepts of 'covalent' versus 'ionic' binding. If the system is half-filled, $(\varepsilon_d - \varepsilon_p)/t_{pd} \gg 1$ is the ionic case.

a) Rederive (3.47) and determine the wave functions as well for all k.

b) Take 2 electrons per unit cell and calculate the total energy as well as the charge distribution within the unit cell as a function of $(\varepsilon_d - \varepsilon_p)/t_{pd}$. In the covalent case, the cohesive energy is coming mainly from the kinetic (band) energy. Which interaction (not included in the model) stabilizes the ionic solids?

3.19 Consider the following lattice:

$$\begin{array}{ccccc} A & B & A & B & A \\ B & A & B & A & B \\ A & B & A & B & A \\ B & A & B & A & B \\ A & B & A & B & A \end{array}$$

It is a square lattice, except that the potentials are staggered. Assume one orbital per site, nearest-neighbor hopping and on-site energies $\varepsilon_A \neq \varepsilon_B$.

a) Establish the Bravais lattice and the basis and deduce the shape of the Brillouin zone.

b) Set up the Hamiltonian. Transform the states to k-space and diagonalize. Plot the bands along high-symmetry directions for $\varepsilon_A = \varepsilon_B$ and for $\varepsilon_{A/B} = \varepsilon \pm \delta\varepsilon$, with $\delta\varepsilon$ small.

c) What is the relation with the single band model on a square lattice (3.43)? Consider the case of two electrons per unit cell. Sketch the Fermi surface for $\varepsilon_A = \varepsilon_B$ and $\varepsilon_{A/B} = \varepsilon \pm \delta\varepsilon$. Is this Fermi-surface nested?

(d) Is the Fermi-surface nested if t' is finite (excercise 3.16)?

3.20 a) Sketch all 3d and 2p cubic harmonics on the CuO_2 pervoskite planes.

b) Consider the reflections, rotations etc. with regard to points centered on either the Cu or the O atoms. Which orbitals are equivalent under these symmetry operations (= point group)?

3.21 Consider all possible hops between the eleven states in the unit cell. Estimate which hops are likely the largest and which are the smallest.

3.22 Consider a square lattice with one s and one $d_{x^2-y^2}$ orbital at each site. Parametrize the nearest-neighbor hoppings with $< d_{x^2-y^2}, i|\mathcal{H}|s, i+\ \delta >\sim t_{ds}$, $< d_{x^2-y^2}, i|\mathcal{H}|d_{x^2-y^2}, i+\ \delta >\sim t_{dd}$ and $< s, i|\mathcal{H}|s, i+\ \delta >\sim t_{ss}$. The on-site energies are denoted by $< s, i|\mathcal{H}|s >= \varepsilon_s$ and $< d_{x^2-y^2}, i|\mathcal{H}|d_{x^2-y^2}, i >= \varepsilon_d$. Derive the bands along the usual high symmetry directions. Be aware of signs! Why do the d and the s states not hybridize along $\Gamma - M$?

3.23 Derive (3.48) (be aware of signs). Include a nearest-neighbor hopping t_{pp} between $|p_x(O_1) >$ and $|p_y(O2) >$. Derive the Hamiltonian in k-space. This cannot be easily diagonalized. What do you expect to happen with the non-bonding band?

4 The crystalline condensate.

The crystalline state of atoms in normal solids is the most familiar of all classical condensates: most of the rigid objects appearing in the daily world are of this kind, and the human senses are optimized to deal with them. Despite this familiarity, these condensates are on the fundamental level as interesting as all other (less obvious) condensates discussed later on. Crystals do not provoke the mind to question the validity of the classical state. Atoms are heavy, and large masses surpress quantum-fluctuations. With few exceptions (hydrogen, helium) semi-classics works too well, because classicalness is already closely approached in the ultraviolet of this problem. At the moment we start to deal with electrons this will change radically. In electron problems, one is constantly bothered with a need to convince oneself that classicalness makes sense at all.

In this chapter, we will use the crystalline state to put flesh on the bare bones of section 1.2, in a scenery which is maximally intuitive. In addition, because of the smallness of the quantum fluctuations, the qualitative aspects of the theory are rather straightforward to understand, and this chapter is meant as a template for the more complicated condensates of the next chapters.

In fact, it is quite difficult to formulate a rigorous *quantitative* theory of the crystalline state, mainly because the interactions between the atoms are very complicated: with few exceptions (van der Waals solids), they are not of the pair-interaction kind. The problem is that the glue, keeping crystalline solids together, is made out of valence electrons. The electronic structure of the valence electrons has something to do with the bands of the previous chapter: the glue is of a quantum nature. Although it starts out with pair-wise Coulomb interactions, after 'integrating out' the electrons (see next section) the effective atom-atom interactions are of a multi-particle kind[1]. This is the reason, that the classical level (in the sense of the definition of section 1.2) will only be treated in a rather sketchy way (section 4.1). The remainder of this chapter is devoted to an exposition of the perturbation theory, which lifts the classical state to the semi-classical level (section 1.2). The main actors are the collective modes, in this case the (acoustic) phonons. In section 4.2 these will be discussed on the classical level and in section 4.3 it will be shown how these classical modes can be directly used to develop the quantum perturbation theory around the classical state. The next two sections are devoted to higher order corrections: the phonon-phonon (section 4.4) and electron-phonon (section 4.5) interactions. This yields and interesting, quantum-electrodynamics like world living on top of the classical state. At the same time, however, it will become clear that these additional effects cannot threaten the condensate, with as a possible exception the small polaron physics explained in section 4.5.

Personally, I find the story of section 4.6 the most interesting one. Using the 'Gaus-

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[1] This is still a subject of active research. It turns out that even in seemingly simple crystals like silicon, one needs at least 10-point interactions or so to obtain a reasonable description of dislocations.

sian' theory of the previous sections, it is not hard to prove that the crystalline condensate *cannot exist in one dimension.* Without much effort, it is possible to deduce the nature of the non-classical state which is realized instead: the floating solid. In addition, the reason will be discussed why Helium is not a crystal at zero temperature.

4.1 On the wave function of a crystal.

Let us start out with writing down the starting point of all of condensed matter physics: for energies less than a MeV or so, the world consists of nuclei and electrons, which are subject to Coulomb interactions, The Hamiltonian is known,

$$
\begin{aligned}
\hat{H} &= \hat{H}_N + \hat{H}_e + \hat{H}_{eN} \\
\hat{H}_N &= \sum_i \frac{\vec{P}_i^2}{2M} + \sum_{i<j} \frac{(Ze)^2}{|\vec{R}_i - \vec{R}_j|} \\
\hat{H}_e &= \sum_i \frac{\vec{p}_i^2}{2m} + \sum_{i<j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \\
\hat{H}_{eN} &= \sum_{i<j} \frac{Ze^2}{|\vec{R}_i - \vec{r}_j|}
\end{aligned}
\tag{4.1}
$$

a single species of nuclei is assumed with charge Ze, mass M, momenta $\vec{P}_i$ and positions $\vec{R}_i$, and the electron momenta and positions are indicated with $\vec{p}_i$ and $\vec{r}_i$. This is a rather unpractical expression and a first simplification arises from the smallness of the ratio of the electronic- to the nuclear mass: we can attempt a perturbation expansion with m/M being the small parameter. What is the zero-th order? Consider the limit that $M \to \infty$ (the so-called adiabatic limit). Because the kinetic energy of the nuclei vanishes we can simply fix their positions and the electrons move in the static potential coming from the localized nuclei. The electronic problem can now be solved (in many cases one comes close to the exact answer with LDA) and the total energy can in principle be determined as function of all choices for the atomic positions $\{\vec{R}_i\}$. This defines a potential energy V, describing the effective *interactions* between the atoms. Considering now a nuclear mass which is still very large but finite, the effective Hamiltonian describing the system of nuclei becomes,

$$
\hat{H}_{lat} = \sum_i \frac{\vec{P}_i^2}{2M} + \sum_{i<j<k<\cdots} V(\vec{R}_i, \vec{R}_j, \vec{R}_k, \cdots) \tag{4.2}
$$

where the interaction term is of a complicated form because it originates partly in the system of electrons. One should subsequently consider correction terms $O(m/M)$ - because the electron system is in many cases characterized by very slow excitations, these 'non-adiabatic corrections' become quite important at large length scales. This perturbation theory is most easily formulated 'around' the crystalline condensate and it will be discussed in more detail in section 4.5.

As for all Hamiltonians describing large ensembles of interacting particles, (4.2) cannot be solved exactly. Actually, only in the limit that the interactions vanish ($V \to 0$), we know the exact answers: $|0 >\sim \Pi_{k=0}^{k_F} c_k^\dagger |vac\rangle$ or $|0 >\sim \Pi_{i=1}^{N} c_{k=0}^\dagger |vac\rangle$ for fermions and bosons, respectively, where $c_k^\dagger$ creates an atom in a plane wave state. Although we will see that the fermionic wave-function does carry significance for the Fermi-liquid state of ^3He (chapter VII), these have obviously nothing to do with the crystalline state.

Let us turn instead to the general recipy of section 1.2. As I argued there, the central step is the identification of the ('coherent state') single particle operator $Y^\dagger(\{\eta_i\})$ which 'hard-wires' the nature of the macroscopic state in the total wave function. We now use our knowledge about the answer: we know that we can identify the locations of individual atoms in real space if they form a crystal (either by diffraction, or directly using a scanning tunneling microscope). The simplest way to incorporate this fact in the wavefunction is by taking a Gaussian wave-packet, centered around an average 'classical' position $\vec{R}_i$ with width σ_i

$$\psi_{\vec{R}_i,\sigma_i}(\vec{R}) = \left(\frac{1}{2\pi\sigma_i^2}\right)^{\frac{1}{4}} e^{-\frac{1}{4}\left(\frac{\vec{R}_i-\vec{R}}{\sigma_i}\right)^2} \tag{4.3}$$

where $\vec{R}_i, \sigma_i$ take the role of classical variables $\{\eta_i\}$. We define a set of second quantized operators $\{Y_{\vec{R}_i,\sigma_i}^\dagger, Y_{\vec{R}_j,\sigma_j}\}$, creating (annihilating) particles in the wavepackets (4.3). These can be either fermions or bosons, depending on the atom under consideration. As long as the 'coherence length' σ is much less than the typical interatomic spacing $\vec{R}_i - \vec{R}_{i+\delta}$, quantum statistics has no effect - in a moment we will see that this condition holds in nearly all crystals[2]. We now write the 'classical' part of the wavefunction of the crystal (section 1.2, Eq.'s 1.1, 1.3) as a single determinant wavefunction, constructed from the single particle states (4.3)

$$|\Phi_{Cl}^0(\{\vec{R},\sigma\})\rangle \; = \; \Pi_{i=1}^N Y_{\vec{R}_i,\sigma_i}^\dagger |vac\rangle \tag{4.4}$$

As a next step, one should calculate the expectation value of the energy

$$E_{Cl}(\{\vec{R},\sigma\}) \; = \; \langle\Phi_{Cl}^0(\{\vec{R},\sigma\})|\hat{H}_{lat}|\Phi_{Cl}^0(\{\vec{R},\sigma\})\rangle \tag{4.5}$$

for all possible choices of $\{\vec{R},\sigma\}$, compare Eq. (1.6), section 1.2. Because of the complicated form of the potential V, this is a very difficult task and I am not aware that this ever has been done explicitely. It is in fact in most cases not necessary either. The width of the wavepackets σ_i is controlled by the ratio of the kinetic to the potential energy, and this is controlled by the atomic mass M which we know is quite large. We can again first consider the 'truely' classical limit $M \rightarrow \infty$ to decide what happens if M is large but finite. In the infinite mass limit, only the interactions

---

[2] Helium crystals are the exception. For instance, the fermionic nature of ^3He is responsible for the phenomenon of ring exchanges.

are left, and we at least know the nature of the ground state in this case: the atoms form a structure characterized by long range order in physical space - the crystal.

We might as well try to quantify the magnitude of the long range order by introducing the order parameter,

$$O = \frac{1}{N} \langle \Phi_0 | \sum_{i, \vec{R}_0} \delta(\vec{R}_i - \vec{R}_0) | \Phi_0 \rangle \tag{4.6}$$

where $|\Phi_0\rangle$ is the ground state wave-function $\vec{R}_i$ the coordinate of atom i and $\vec{R}_0$ runs over all sites of the Bravais lattice (assuming a single component system, with one atom per unit cell). When the atoms would be exactly localized on every lattice site, O would be equal to one. Assume that the state (4.4) has something to do with the ground state if the $\vec{R}$'s would lie on the Bravais lattice $\vec{R}_0$. Since all atoms are equivalent because of the long range order, they have to be described by wave packets with the same width σ_0. If this width is non-zero, the order parameter will have a magnitude $O = 1/\sqrt{2\pi}\sigma_0$, a number which is smaller than one (the completely localized case), but still finite.

How to calculate the classical ground state? One can use the knowledge about the long range order of the ground state, by writing an ansatz for the wave function

$$|\Phi^0_{Cl}(\{a'_i, \sigma_0)\rangle = \Pi^N_{i=1} Y^\dagger_{\vec{R}'_0, \sigma_0} |vac\rangle \tag{4.7}$$

in terms of one width σ_0 and a set of lattice constants a'_i giving the dimensions of the Bravais lattice. It is assumed here that the symmetry of the crystal is already known - this can also be determined from (4.5), but we save us the effort. The classical energy is now only a function of σ_0 and the lattice constants, and it is minimized by

$$\begin{aligned} \frac{\delta E_{Cl}(\{a'_i\}, \sigma_0)}{\delta \sigma_0} &= 0 \\ \frac{\delta E_{Cl}(\{a'_i\}, \sigma_0)}{\delta a'_i} &= 0, \quad \forall i \end{aligned} \tag{4.8}$$

Since the potential V is not known, (4.8) cannot be solved explicitely. It turns out, however, that quite generally 'saddle point equations' like (4.8) give rise to *self-consistency* conditions for the classical variables $\{\eta\}$. Although these conditions cannot be derived in an explicit form, the principle can be vividly illustrated in the present context. Let us start, assuming that $M \to \infty$ so that $\sigma_0 = 0$. We adjust the a_i's untill we have found the minimum of the potential energy. We consider now all atoms fixed except for a single atom which we displace a little from its equilibrium position. If this displacement is small enough, the well will be harmonic: $E_{pot} \sim \frac{1}{2} K^{(0)} (\vec{R}_i - \vec{R}'_{0,i})^2$. We now switch on the kinetic energy of this atom and if its mass is large enough, the atom will only probe the bottom of the well. This amounts to an harmonic oscillator problem for the single particle wavepacket (4.3) (we only consider the radial motion)

$$\left[\frac{\hbar^2}{2M} \frac{d^2}{dR_i^2} + \frac{1}{2} K^{(0)} (R'_{0,i} - R_i)^2) \right] \psi_{R'_{0,i}, \sigma_i}(R_i) \;=\; E \psi_{R'_{0,i}, \sigma_i}(R_i) \tag{4.9}$$

This oscillator vibrates at $\omega_0 = \sqrt{K^{(0)}/M}$ and this will always be small compared to the magnitude of the potential if M is sufficiently large, validating the harmonic approximation. In addition, the ground state wave function will be of the Gaussian form (4.3), with a width $(\sigma_i^{(0)})^2 = \hbar/(2\sqrt{MK^{(0)}})$. This width will again be very small if M is large.

We are not quite finished because all atoms in the solid have a tendency to delocalize slightly, including the atoms neighbouring the atom we just considered which are in turn responsible for the shape of the potential well from which we determined the wave packet. There is no reason for the other atoms to behave differently from the one we just considered, and all we have to do is to recalculate the potential well of the 'central' atom, including the effects of the slight delocalization of the neighbouring atoms. This will increase the lattice constants slightly and it will tend to make the potential smoother, with the effect that the potential well becomes less deep,

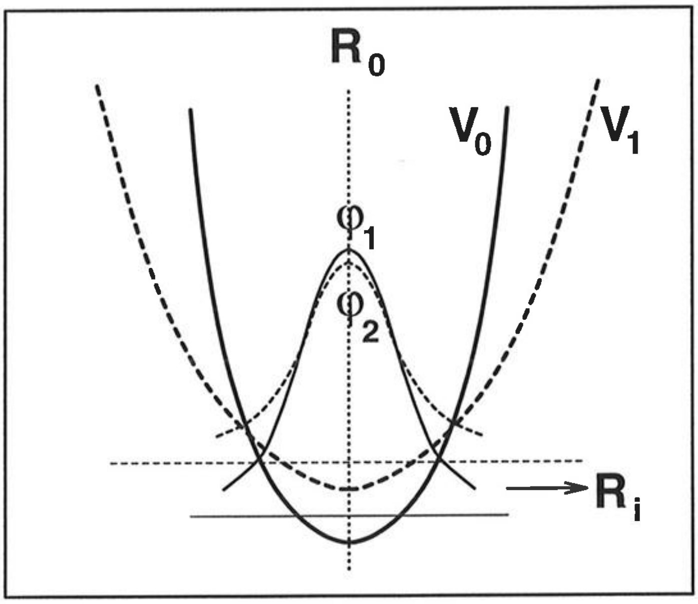

Figure 4.1: *Illustration of the mean-field problem, implied by the wavefunction (4.7). The potential well is indicated, seen by an individual atom, coming from the crystal as a whole* (V_0)*. The atom can delocalize slightly in this well* (ϕ_1)*, and because its neighbours also delocalize a little, the potential well becomes less steep* (V_1)*, and the atom delocalizes a little more* (ϕ_2)*, by an amount which is much less than in the first iteration. After a couple of iterations, the width of the wavepacket converges to a fixed value.*

Because the well is less deep, the new force constant $K^{(1)} < K^{(0)}$ and the wave-packet of the atom under consideration spreads out more. However, as long as the crystal exists, this spread is less than what is found the first time and if one continuous to 'iterate' one will find that both σ, the a_i's and K converge to a fixed value. This is called the self-consistent solution: using σ_0 and the a_i's to calculate the potential yields a K which on its turn yields the same σ_0 and a_i's. From the above, it is clear that there is only one consistent way to construct the crystal if the σ's and a's are allowed to vary, under the constraint that they are everywhere the same, and one concludes that the self-consistent state has to correspond with the classical ground state. In the context of electron problems, it will be explicitely shown that the above iteration procedure indeed amounts to the minimization of the energy.

If one is familiar with the Weiss molecular-field theory of statistical mechanics, one should now recognize why this procedure is called 'mean-field theory': a wave-function of the type (4.3, 4.4) (or in general, (1.2), (1.3)) maps the full problem on one of a single constituent moving in the average 'field' of all other constituents.

In the self-consistent solution, the wave packets will all be centered on the sites of the Bravais lattice $\vec{R}_0$ and the only difference with the purely classical ($M \rightarrow \infty$) crystal is in the reduction of the order parameter (4.6) by a factor $1/\sqrt{2\pi}\sigma_0$. This seems to be a credible interpretation for the wavefunction of the crystal. A fundamental problem is that this ground state wave function is *not an eigenstate of the Hamiltonian*! This is very simple to see. The original Hamiltonian (4.2) was defined with regard to homogeneous space. Therefore, total momentum is conserved. In other words, the operator

$$\vec{P}_{tot} = \sum_i \vec{P}_i \tag{4.10}$$

commutes with the Hamiltonian,

$$\left[\vec{P}_{tot}, \hat{H}\right] = 0 \tag{4.11}$$

and all eigenstates should be labelled with a total momentum quantum number K,

$$\vec{P}_{tot}|\Phi_{ex}; \vec{K}\rangle \;=\; \vec{K}|\Phi_{ex}; \vec{K}\rangle \tag{4.12}$$

Obviously, because all single particle states in the classical state are localized in space, each atom is characterized by a momentum uncertainty,

$$\langle vac|Y_{\vec{R}_0,\sigma_0}\; \vec{P}^2\; Y^\dagger_{\vec{R}_0,\sigma_0}|vac\rangle - \left(\langle vac|Y_{\vec{R}_0,\sigma_0}\; \vec{P}\; Y^\dagger_{\vec{R}_0,\sigma_0}|vac\rangle\right)^2 \;=\; (\Delta k)^2 \neq 0 \tag{4.13}$$

Because the classical state (4.7) is of the single determinant form, the momentum fluctuations of the individual particles are uncorrelated, and the total momentum is therefore also a fluctuating quantity,

$$\langle\Phi^0_{Cl}(\{\})|\; \vec{P}^2\; |\Phi^0_{Cl}(\{\})\rangle - \left(\langle\Phi^0_{Cl}(\{\}|\; \vec{P}\; |\Phi^0_{Cl}(\{\})\rangle\right)^2 \;=\; N(\Delta k)^2 \tag{4.14}$$

The classical state is not satisfying (4.12) and is therefore not an eigenstate of the Hamiltonian. One in fact expects that the classical state becomes precisely orthogonal to all eigenstates in the limit that $N \rightarrow \infty$. The reason that the classical state is the right one, despite its apparent violation of quantum mechanics, is a subtle one and this will be further discussed in the context of spin-ordering (chapter V).

$\Longrightarrow$ Excercise 4.1

4.2 The classical modes of vibration.

In the previous section we only explored a very small portion of the classical phase space: only motions were considered where the crystal changed uniformly. The global energy minimum occurs, however, in the phase space spanned by the degrees of freedom of all atoms, and therefore we should consider collective motions as well. The most important ones are those where all atoms are displaced simultaneously by an infinitisimal amount: the collective modes. These dominate the low energy part of the excitation spectrum. In this section, we will focus on the classical theory and in the next sections these results will be used to construct and investigate the quantum theory.

For simplicity we restrict ourselves for the time being to crystals characterized by one atom per unit cell. In addition, we neglect the effects of the spreading of the wavepackets ($\sigma_0 \neq 0$) alltogether - in most crystals this gives rise to insignificant corrections. In this limit, the ground state of the crystal follows from a minimization of the potential energy

$$\left.\frac{\partial \mathcal{V}}{\partial R_{n\alpha}}\right|_{\{\vec{R}_n^0\}} = 0 \qquad \text{for all } n = 1, \cdots, N, \quad \alpha = 1, 2, 3 \quad . \tag{4.15}$$

We now consider small displacements $\vec{u}_n$ of all atoms around their equilibrium positions: $\vec{R}_n \equiv \vec{R}_n^0 + \vec{u}_n$, with components (in $d = 3$) $\vec{R}_n = (R_{n1}, R_{n2}, R_{n3})$ and $\vec{u}_n = (u_{n1}, u_{n2}, u_{n3})$.

Because the displacements are small, the total energy can be expanded in a Taylor series. Because of the linear stability criterium (4.15) the first order vanishes and up to second order, ($\alpha = 1, 2, 3$)

$$\begin{aligned} V(\vec{R}_1, \cdots, \vec{R}_N) &= V(\vec{R}_1^0, \cdots, \vec{R}_N^0) \\ &\quad + \frac{1}{2} \sum_{n,n'} \sum_{\alpha,\beta} u_{n\alpha} u_{n'\beta} \left.\left(\frac{\partial^2 V}{\partial R_{n\alpha} \partial R_{n'\beta}} \right)\right|_{\{\vec{R}_n^0\}} + \cdots \\ &= V(\vec{R}_n^0, \cdots, \vec{R}_N^0) + \frac{1}{2} \sum_{n,n'} \sum_{\alpha,\beta} u_{n\alpha} u_{n'\beta} V_{n\alpha n'\beta} + \cdots \end{aligned} \tag{4.16}$$

In the second line, the matrix of derivatives $V_{n\alpha n'\beta}$ is defined. In the remainder, the ground state energy $\mathcal{V}(\vec{R}_1^0, \vec{R}_2^0, \cdots, \vec{R}_N^0)$ will be left implicit.

This amounts to a harmonic or 'Gaussian' approximation: V is quadratic in the displacements, because terms $\sim u^3$ and higher orders are not considered. This is a good approximation as long as the thermal and/or quantum fluctuations are small, such that the displacements u are much smaller than the average interatomic distance a,

$$|u_{n\alpha}| \ll a \quad . \tag{4.17}$$

The effects of the higher order (anharmonic) corrections will be considered in section 4.4.

$\Longrightarrow$ Excercise 4.2

Classical equations of motion.

In order to describe the classical dynamics 'around' the crystalline state, we simply have to add the kinetic term to obtain the effective Hamiltonian,

$$\begin{aligned} \mathcal{H} &= \sum_n \frac{\vec{P}_n^2}{2M} + V(\vec{R}_1, \cdots, \vec{R}_N) \quad , \\ &= \sum_n \frac{\vec{P}_n^2}{2M} + \frac{1}{2}\sum_{n,n'}\sum_{\alpha\beta} V_{\alpha\beta}(\vec{R}_n^0 - \vec{R}_{n'}^0) u_{n\alpha} u_{n'\beta} + \mathcal{O}(u^3) \quad , \end{aligned} \tag{4.18}$$

where the ground state energy is omitted. The classical dynamics is derived from the Hamilton equations,

$$\begin{aligned} \dot{u}_{m\gamma} &= \frac{\partial \mathcal{H}}{\partial P_{m\gamma}} = \frac{P_{m\gamma}}{M} \quad , \\ \dot{P}_{m\gamma} &= -\frac{\partial \mathcal{H}}{\partial u_{m\gamma}} = -\frac{1}{2}\sum_{n'\beta} V_{\gamma\beta}(\vec{R}_m^0 - \vec{R}_{n'}^0) u_{n'\beta} - \frac{1}{2}\sum_{n\alpha} V_{\alpha\gamma}(\vec{R}_n^0 - \vec{R}_m^0) u_{n\alpha} \quad , \\ &= -\sum_{n'\beta} V_{\gamma\beta}(\vec{R}_m^0 - \vec{R}_{n'}^0) u_{n'\beta} \quad . \end{aligned} \tag{4.19}$$

Combining the two equations yields the classical equations of motion,

$$\ddot{u}_{n\alpha} = \frac{\dot{P}_{n\alpha}}{M} = -\frac{1}{M}\sum_{n'\beta} V_{\alpha\beta}(\vec{R}_n^0 - \vec{R}_{n'}^0) u_{n'\beta} \quad . \tag{4.20}$$

Diagonalizing the classical Hamiltonian: normal modes.

In the harmonic approximation, the equations of motion are linear while V is real and symmetric, and therefore they can be diagonalized. The eigenfunctions are the modes while the eigenvalues define the mode spectrum. Let us first consider the simple example of a one dimensional chain of atoms characterized by only nearest-neighbour force constants K, We label the atomic positions $\vec{R}_0$ and associated displacements u by an integer j. In the harmonic approximation with only nearest-neighbour coupling, the Hamiltonian is that of a chain of balls, where every ball is connected to its nearest-neighbours by perfect springs with spring constants K,

$$H = \sum_j \left[\frac{P_j^2}{2M} + \frac{1}{2} K (u_j - u_{j+1})^2 \right] \tag{4.21}$$

and the equations of motions become, using (4.19,4.20),

$$M\ddot{u}_j = K\left[2u_j - u_{j-1} - u_{j+1}\right] \tag{4.22}$$

Substituting (a is lattice constant),

$$u_j(t) \;=\; u_0 e^{i(kja-\omega_k t)} \tag{4.23}$$

into (4.22) yields the diagonal form

$$-M\omega_k^2 u_0 = -2K(1-cos(ka))u_0 \tag{4.24}$$

and the dispersion takes the familiar form,

$$\omega_k = 2\sqrt{\frac{K}{M}}|sin(\frac{1}{2}ka)| \tag{4.25}$$

while the actual displacements are given by the real an imaginairy parts of (4.23). For large wavelengths (small k) the mode-frequency goes linearly to zero $\omega_k = c|k|, |k| \to 0$ with the sound velocity $c = a\sqrt{K/M}$ - this is a very general behavior as we will see later, and modes showing this behavior are called 'acoustic modes', 'zero-modes' or 'Goldstone modes'.

Let us now consider the general case. We look for solutions of (4.20) of the form,

$$u_{n\alpha}(t) \;=\; v_{n\alpha}e^{i\omega t} \quad . \tag{4.26}$$

Inserting (4.26) into (4.20) yields

$$\omega^2 v_{n\alpha} \;=\; \frac{1}{M}\sum_{n'\beta} V_{\alpha\beta}(\vec{R}^0_n - \vec{R}^0_{n'})v_{n'\beta} \quad . \tag{4.27}$$

which amounts to an eigenvalue problem for the matrix V/M. The eigenvalues are ω^2 en the eigenvectors the $v_{n\alpha}$'s. Because of the translation invariance, we can look for plane wave solutions,

$$v_{n\alpha} \;=\; v_\alpha(\vec{k})e^{i\vec{k}\cdot\vec{R}^0_n} \quad , \tag{4.28}$$

inserting this in (4.27)

$$\begin{aligned} \omega^2 v_\alpha(\vec{k}) \;&=\; \sum_\beta\sum_{n'} M^{-1}V_{\alpha\beta}(\vec{R}^0_n - \vec{R}^0_{n'})e^{i\vec{k}\cdot(\vec{R}^0_{n'}-\vec{R}^0_n)}v_\beta(\vec{k}) \quad , \\ &=\; \sum_\beta D_{\alpha\beta}(\vec{k})v_\beta(\vec{k}) \quad . \end{aligned} \tag{4.29}$$

with the so-called *dynamical matrix* D defined as

$$D_{\alpha\beta}(\vec{k}) \;=\; \sum_{\vec{T}_n} M^{-1}V_{\alpha\beta}(\vec{T}_n)e^{-i\vec{k}\cdot\vec{T}_n} \quad , \tag{4.30}$$

and the eigenvalue equation takes the simple form in terms of the matrix D,

$$\omega^2 v_\alpha(\vec{k}) \;=\; \sum_\beta D_{\alpha\beta}(\vec{k})v_\beta(\vec{k}) \tag{4.31}$$

Hence, for every $\vec{k}$ one has to solve this problem to obtain the mode spectrum - it is the lattice vibration equivalent of the matrices giving rise to band structure of the previous chapter. An important difference with the quantum case is that the basis is finite, and in fact rather small: the dimension of D is $d \times d$ (d is the space dimension). From the definition of D it follows immediately that,

$$\begin{aligned} D(\vec{k}) &= D^{\dagger}(\vec{k}) \quad (D \text{ is hermitian}) \quad , & (4.32a)\\ D(\vec{k}) &= D^{*}(-\vec{k}) \quad , & (4.32b)\\ D(\vec{k}) &= D(\vec{k}+\vec{K}) \quad \text{with } \vec{K} \text{ a reciprocal lattice vector} \quad . & (4.32c) \end{aligned}$$

$\Longrightarrow$ Excercise 4.3

$D(\vec{k})$ has for every $\vec{k}$ d eigenvalues which are labelled by λ

$$\text{eigenvalues: } \omega_{\lambda}^{2}(\vec{k}) \ , \qquad \text{eigenvectors: } v_{\alpha}^{\lambda}(\vec{k}) \ , \qquad \lambda = 1, 2, \cdots d \quad . \tag{4.33}$$

Because D is hermitian (the eigenvalues are real), while also $v_{\alpha}(\vec{k}) = v_{\alpha}^{*}(-\vec{k})$,

$$\begin{aligned} \omega_{\lambda}^{2}(\vec{k}) &= \omega_{\lambda}^{2}(-\vec{k}) \quad , \\ v_{\alpha s}^{\lambda}(\vec{k}) &= v_{\alpha s}^{\lambda}(-\vec{k}) \quad , \end{aligned} \tag{4.34}$$

and the eigenvectors can be choosen to be orthonormal [3]

$$\sum_{\alpha=1}^{3} v_{\alpha}^{\lambda'}(\vec{k})^{*} v_{\alpha}^{\lambda}(\vec{k}) = \delta_{\lambda'\lambda} \quad . \tag{4.35}$$

The eigenvectors of the dynamical matrix are called the normal modes.

We might as well write the Hamiltonian itself directly in a diagonal form. Knowing the eigenvectors, we can define a canonical transformation, starting from $u_{n\alpha}$ and $P_{n\alpha}$,

$$\begin{aligned} u_{n\alpha} &= \frac{1}{\sqrt{N}} \sum_{\vec{k}\in 1^{e}BZ} e^{i\vec{k}\cdot\vec{R}_{n}^{0}} \sum_{\lambda} v_{\alpha}^{\lambda}(\vec{k}) Q_{\lambda}(\vec{k}) \quad , \\ P_{n\alpha} &= \frac{1}{\sqrt{N}} \sum_{\vec{k}\in 1^{e}BZ} e^{i\vec{k}\cdot\vec{R}_{n}^{0}} \sum_{\lambda} v_{\alpha}^{\lambda}(\vec{k}) P_{\lambda}(\vec{k}) \quad . \end{aligned} \tag{4.36}$$

to the new variables $Q_{\lambda}(\vec{k})$ and $P_{\lambda}(\vec{k})$. Because $u_{n\alpha}$'s and $P_{n\alpha}$'s are real,

$$Q_{\lambda}(-\vec{k}) = Q_{\lambda}^{*}(\vec{k}) \quad , \qquad P_{\lambda}(-\vec{k}) = P_{\lambda}^{*}(\vec{k}) \quad . \tag{4.37}$$

Inserting (4.36) in the Hamiltonian (4.18) yields

$$H = \frac{1}{2M} \sum_{\vec{k},\lambda} P_{\lambda}(\vec{k}) P_{\lambda}(-\vec{k}) + \frac{1}{2} M \sum_{\vec{k},\lambda} \omega_{\lambda}^{2}(\vec{k}) Q_{\lambda}(\vec{k}) Q_{\lambda}(-\vec{k}) \quad . \tag{4.38}$$

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[3] The wavenumber $\vec{k}$ enters as a parameter and two eigenvectors with different $\vec{k}$ are therefore not orthogonal!

H is brought in a diagonal form by using the 'normal coordinates' P and Q.

$\Longrightarrow$ Excercises 4.4, 4.5

This derivation is straightforwardly generalized to the case with more than one atom per unit cell. The number of atoms per unit cell is n_s and the position of atom s with mass M_s is indicated by $\vec{R}_{n,s} = \vec{R}^0_{n,s} + \vec{u}_{ns}$. (4.31) now becomes,

$$\omega^2 v_{\alpha,s}(\vec{k}) = \sum_{\beta,s'} D_{\alpha s \beta s'}(\vec{k}) v_{\beta s'}(\vec{k}) \tag{4.39}$$

and the dynamical matrix becomes

$$D_{\alpha s \beta s'}(\vec{k}) = \sum_{\vec{T}_n} M_s^{-1} V_{\alpha s \beta s'}(\vec{T}_n) e^{-i\vec{k}\cdot\vec{T}_n} \quad , \tag{4.40}$$

where the force constants are given by

$$V_{n\alpha s n'\beta s'} = \left(\frac{\partial^2 V}{\partial R_{ns\alpha} \partial R_{n's'\beta}} \right) \Bigg|_{\{\vec{R}^0_{ns}\}} \tag{4.41}$$

The dimension of the dynamical matrix is now $dn_s \times dn_s$ and we expect therefore to find dn_s modes.

$\Longrightarrow$ Excercises 4.6, 4.7

The Goldstone modes of the crystal.

Let us now consider the physics behind these mathematical manipulations. The important step is the assertion that the Taylor expansion (4.16) exists. The existence of this expansion[4] is itself implied by the existence of the order parameter - the presence of the order parameter required the existence of a well defined global minimum of energy, and with 'well defined' we really mean that the expansion exists. In addition, we introduced the additional assumption that the cubic and higher order anharmonic terms in the expansion could in first instance be neglected. This is also an important assumption, because the anharmonic terms cause the modes to interact with each other (see also section 4.4). As a first effect of these mode couplings, individual modes will start to decay in other modes and they will acquire a finite lifetime. If the inverse of this lifetime becomes larger than the mode-frequency, the very notion of propagating excitations looses its sense (the so-called overdamped regime). As long as the mode frequency is the larger number one can still think perturbatively, taking the harmonic system as zero-th order and treating the anharmonic terms to cause corrections which do not change the physics fundamentally (the 'underdamped regime').

The vast majority of the modes as they occur in nature belong to this approximate, underdamped regime. They show up in a variety of experiments (such as inelastic neutron scattering and Raman scattering) as sharp peaks in spectra which are

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[4] The precise statement is that the total energy is analytic in the small displacements u around the classical ground state - see also chapter VII

measured as function of frequency for a given $\vec{k}$. However, these peaks have a finite intrinsic width and are in fact resonances: after a time inversely proportional to this frequency width they have decayed into something else. Only in one limit the modes become true in a rigorous sense: the limit of large wavelength and low frequency. The modes occurring in this regime are called the Goldstone modes or zero modes, and in the specific case of crystalline order, they are called acoustic phonons (or 'sound waves in crystals').

The exactness of the modes in this limit is a direct consequence of the existence of the order parameter, and they are always found regardless the precise nature of the long range order. In fact, it is very simple to understand why the acoustical modes become exact at low frequencies and long wavelengths. Let us first consider the infinite wavelength limit: the displacements of all atoms are the same $\vec{u}_n = \vec{u}^*$. This corresponds with an uniform displacement of the whole crystal and this does not cost energy, because the crystal as a whole is still subject to the full translational invariance. In addition, this motion is also undamped for the same reason: the mode with $\vec{k} = 0$ has frequency $\omega_{\vec{k}} = 0$ and is exact[5]. One can directly count the number of these modes: in $d = 3$ there are three modes, because the crystal can be moved in three independent directions and in d dimensions there are d modes of this type (more generally, the number of Goldstone modes is equal to the number of components of the continuous symmetry group which have been subjected to symmetry breaking).

Let us now consider a finite, but large wavelength. We want to find out first why the anharmonicities disappear in this regime. In the crystal, the interactions are short ranged and it is easy to see why the harmonic approximation becomes better and better if the wavelength of the acoustic modes increases. It is not so much the absolute displacements which matter but instead the displacement of a particular atom relative to that of its neighbours. The relative displacement behaves like $\delta u \sim 1/\lambda$ for large λ. For instance, consider the simple example (4.21-4.25). As can be seen from figure (4.2), the mode becomes a weaker and weaker perturbation if its wavevector decreases and the harmonic approximation becomes increasingly better - for $\vec{k} \to 0$ it 'merges' with the zero-frequency mode which did not perturb the ground state at all. In section 4.4 an explicit expression will be derived for the damping in the quantized version of the theory.

For the same reasons, the frequency of the Goldstone modes approaches zero linearly in k. This is proved as follows. To avoid indices, let us consider a mono-atomic Bravais lattice in three dimensions. Because $\omega_\lambda(\vec{k} = 0) = 0$

$$0 = \sum_\beta D_{\alpha\beta}(0) v^\lambda_\beta(0) \quad . \tag{4.42}$$

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[5] One has to be careful. According to (4.30), $D_{\alpha\beta}(\vec{k} = 0)$ is a sum over the contributions of all sites and it only exists if the potential falls off sufficiently fast as function of the distance R. In three dimensions, it turns out that the potential has to fall off faster than $1/R$. In crystals this is always the case. This is not the case in for instance the charged Fermi-liquid (Coulomb interactions !) In chapter VII we will see that in these cases the Goldstone modes acquire a finite frequency $\omega_{\vec{k} \to 0} \neq 0$. However, the lifetime approaches still infinity and this so-called plasmon is as well defined as the phonons in this chapter.

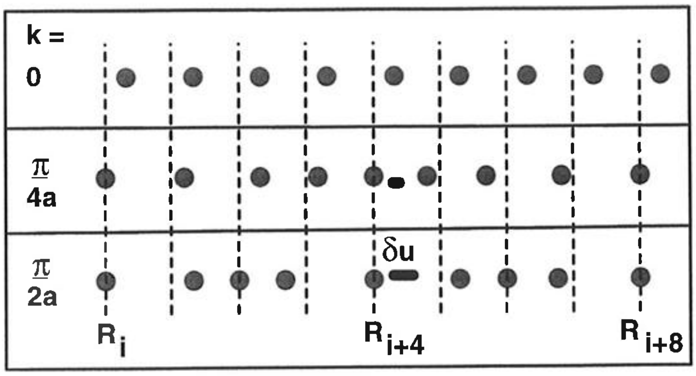

Figure 4.2: *Indicated are the displacement patterns associated with the (longitudinal) acoustic mode of a one dimensional chain for different wave vectors. One infers that the differences in the relative displacement of nearest neighbour atoms (δu) becomes smaller with increasing wavelength, to vanish at k = 0.*

and therefore

$$D_{\alpha\beta}(\vec{k}=0) \;=\; 0 \quad . \tag{4.43}$$

Consider now the limit $\vec{k} \to 0$

$$\begin{aligned}
\omega_\lambda^2(\vec{k}) v_\alpha^\lambda(\vec{k}) &= \sum_\beta D_{\alpha\beta}(\vec{k}) v_\beta^\lambda(\vec{k}) \quad , \qquad\qquad \lambda = 1,2,3 \quad , \\
&= \sum_{\vec{T}_n} \sum_\beta M^{-1} V_{\alpha\beta}(\vec{T}_n) e^{-i\vec{k}\cdot\vec{T}_n} v_\beta^\lambda(\vec{k}) \quad , \\
&= \frac{1}{2} \sum_{\vec{T}_n} \sum_\beta M^{-1} V_{\alpha\beta}(\vec{T}_n) \left[e^{-i\vec{k}\cdot\vec{T}_n} + e^{i\vec{k}\cdot\vec{T}_n} - 2 \right] v_\beta^\lambda(\vec{k}) \quad , \\
&= \frac{1}{2} \sum_{\vec{T}_n} \sum_\beta M^{-1} V_{\alpha\beta}(\vec{T}_n) \left[2\cos\left(\vec{k}\cdot\vec{T}_n\right) - 2 \right] v_\beta^\lambda(\vec{k}) \quad , \\
&= \frac{1}{2} \sum_{\vec{T}_n} \sum_\beta M^{-1} V_{\alpha\beta}(\vec{T}_n) \left[-\left(\vec{k}\cdot\vec{T}_n\right)^2 + \mathcal{O}(\vec{k}\cdot\vec{T})^4 \right] v_\beta^\lambda(\vec{k}) \quad .
\end{aligned} \tag{4.44}$$

$\vec{k}$ is written as $k\hat{\Omega}_k$, where $\hat{\Omega}_k$ is a unit vector pointing in the direction of $\vec{k}$, and we define

$$C_{\alpha\beta}(\hat{k}) \;=\; \sum_{\vec{T}_n} -\frac{1}{2M} V_{\alpha\beta}(\vec{T}_n) \left(\hat{\Omega}_k \cdot \vec{T}_n\right)^2 \tag{4.45}$$

It follows that for small k

$$\omega_\lambda^2(\vec{k}) \;=\; c_\lambda^2(\hat{\Omega}_k) k^2 \quad , \qquad (k \ll 2\pi/a) \quad , \tag{4.46}$$

$$\omega_\lambda(\vec{k}) \;=\; k c_\lambda(\hat{\Omega}_k) \quad , \qquad \lambda = 1,2,3 \quad . \tag{4.47}$$

The three $c_\lambda^2(\hat{\Omega}_k)$ are the eigenvalues of the matrix $C(\hat{\Omega}_k)$ which only depend on the direction of $\vec{k}$. The c's itself are the sound velocities and the sound velocity is an anisotropic quantity in a crystal.

In crystals with one atom per unit cell, the three acoustic branches are all. The acoustic branches become flat at large momenta and the dispersions tend to look similar to the $|sin(k/2)|$ dispersion of the simple monoatomic chain. In crystals with larger unit cells, we already found that the total number of modes amounts to $n_s d$ (n_s number of atoms per unit cell, d dimensionality). The above discussion shows that there are only d acoustic modes. There are therefore $n_s(d-1)$ modes with a finite frequency at zero wavenumber. These are called optical modes and correspond with out-of-phase motions of the atoms within the unit cell (at least at $\vec{k}=0$) (see excercise 4.7). As we already stated, the full mode spectrum can be accurately measured, especially by inelastic neutron scattering. In addition, rather accurate methods have been developed to calculate the mode spectrum, with as a latest development that dynamical matrices are determined using the full machinery of LDA band structure theory[6].

4.3 Quantizing lattice vibrations: Phonons.

The essence of the previous section is, that in the harmonic approximation the low frequency dynamics of the crystal is described completely in terms of an *ensemble of independent harmonic oscillators.* For every $\vec{k}$ and λ the collective vibration can be described by a pendulum with force constant $\sim M(\omega_\lambda(\vec{k}))^2$. One should recall that in the beginning of the previous section we have boldly switched off quantum-mechanics - we should treat all motions of the atoms quantum-mechanically, including their collective motions. A priory, there is no reason for the classical story of the previous section to make sense.

As a lucky circumstance, the classical nature of the whole crystal (as opposed to its collective vibrations) imposes the existence of the Taylor expansion for the potential, including the theorem that the expansion gets better if the wavelength of the displacement pattern gets larger. Hence, the Taylor expansion is also the proper starting point for the quantum theory, at least as long as the long range order itself survives. The quantum theory is also about harmonic potentials, and therefore about quantum harmonic oscillators. It is a specialty of the harmonic oscillator that it is very easy to quantize: the energetics can be directly taken from the classical problem. As we will see, at the very last moment quantum-mechanics can be incorporated.

Although the mode spectrum (the ω_k^λ's) does not change, the physics does if the lattice waves are treated quantum-mechanically. The modes are no longer just vibrations, but become particles as well, which are called phonons. These phonons have an intruiging resemblence with the force-carrying particles of field theory - the word phonon should be understood as 'sound like photon'. This analogy goes further. The

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[6] See S. Yu. Savrasov, Physical Review Letters **69**, 2819 (1992), and references therein.

non-adiabatic corrections give rise to couplings between phonons and electrons which look very similar to the minimal couplings of field-theory. Different from quantum-elecrodynamics, the phonons also *self-interact*: the anharmonic corrections give rise to phonon-phonon interaction terms.

Quantization of the lattice modes does more: it 'changes the vacuum', it is in fact the leading order of the perturbation theory of section 1.2, which is a necessary step to bring the classical ground state (the crystal of section 4.1) to the true, semiclassical groundstate. The general structure of the theory as presented in the remainder of this chapter is in fact tied to the existence of the classical ground state itself, and is rather insensitive to the specifics of the state. The underlying, general scheme is called 'Gaussian fluctuations' - Gaussian, because the modes are treated as being independent. We will see it return a couple of times when the other condensates are discussed.

Finding the normal coordinates.

The derivation of the quantum equations of motions from the harmonic Hamiltonian (4.18) is quite easy. We again consider the monoatomic crystal. Momentum and position become operators with the usual commutators,

$$[P_{n\alpha}, P_{n'\beta}] = 0 \quad , \qquad [u_{n\alpha}, u_{n'\beta}] = 0 \quad , \qquad [P_{n\alpha}, u_{n'\beta}] = \frac{\hbar}{i}\delta_{nn'}\delta_{\alpha\beta} \quad . \tag{4.48}$$

The quantum-equations of motion become (compare eq. (2.125)),

$$\begin{aligned} \dot{u}_{n\alpha} &= \frac{1}{i\hbar}[u_{n\alpha}, \mathcal{H}] &= \frac{P_{n\alpha}}{M} \quad , \\ \dot{P}_{n\alpha} &= \frac{1}{i\hbar}[P_{n\alpha}, \mathcal{H}] &= -\sum_{n'\beta} V_{\alpha\beta}(\vec{R}^0_m - \vec{R}^0_{n'})u_{n'\beta} \quad . \end{aligned} \tag{4.49}$$

and these equations are identical to the classical equations (4.19), except that they describe the time evolution of operators. We learned how to handle these equations in section 2.4: it amounts to diagonalizing the Hamiltonian. We first do the transformation to the normal coordinates and this is identical to the transformation used in the classical case (4.36), because of the similarities of the equations of motions - this is a specialty of the harmonic problem. The only difference is that the new $P_\lambda(\vec{k})$'s and $Q_\lambda(\vec{k})$'s are still operators, obeying the commutation relations,

$$\begin{aligned} \left[P_\lambda(\vec{k}), P_{\lambda'}(\vec{k}')\right] &= \left[Q_\lambda(\vec{k}), Q_{\lambda'}(\vec{k}')\right] = 0 \quad , \\ \left[P_\lambda(\vec{k}), Q_{\lambda'}(\vec{k}')\right] &= \frac{\hbar}{i}\delta_{\lambda\lambda'}\delta_{\vec{k}\vec{k}'} \quad . \end{aligned} \tag{4.50}$$

The new operators are equally good momentum and position operators as the old ones - transformations like (4.36) do not change the algebra (section 2.4). The quantum Hamiltonian becomes (4.38), with the P's and Q's obeying (4.50): this describes now an ensemble of non-interacting quantum oscillators, each having an effective force constant $M\omega_\lambda^2(\vec{k})$.

Phonon creation- and annihilation operators

To diagonalize the Hamiltonian (4.38) we simply have to diagonalize each of the oscillators independently and we learned to do this in section (2.2). In direct correspondence with Eq.'s (2.42), (2.44) we define creation- and annihilation operators,

$$\begin{aligned} b_{\vec{k}\lambda} &= \sqrt{\frac{M\omega_\lambda(\vec{k})}{2\hbar}} Q_\lambda(\vec{k}) + i\sqrt{\frac{1}{2M\hbar\omega_\lambda(\vec{k})}} P_\lambda(-\vec{k}) \quad , \\ b^\dagger_{\vec{k}\lambda} &= \sqrt{\frac{M\omega_\lambda(\vec{k})}{2\hbar}} Q_\lambda(-\vec{k}) - i\sqrt{\frac{1}{2M\hbar\omega_\lambda(\vec{k})}} P_\lambda(\vec{k}) \quad . \end{aligned} \tag{4.51}$$

The commutation relations become,

$$\left[b_{\vec{k}\lambda}, b_{\vec{k}'\lambda'}\right] = 0, \quad , \quad \left[b^\dagger_{\vec{k}\lambda}, b^\dagger_{\vec{k}'\lambda'}\right] = 0, \quad , \quad \left[b_{\vec{k}\lambda}, b^\dagger_{\vec{k}'\lambda'}\right] = \delta_{\vec{k}\vec{k}'}\delta_{\lambda\lambda'} \quad . \tag{4.52}$$

and the Hamiltonian is,

$$\mathcal{H} = \sum_{\vec{k},\lambda} \hbar\omega_{\vec{k}\lambda}(b^\dagger_{\vec{k}\lambda} b_{\vec{k}\lambda} + \frac{1}{2}) \quad , \qquad \omega_{\vec{k}\lambda} \equiv \omega_\lambda(\vec{k}) \quad . \tag{4.53}$$

$\Longrightarrow$ Excercise 4.8

As in the case of the $M \to \infty$ crystal, there are d (or dn_s in the general case) different vibration modes with frequencies $\omega_\lambda(\vec{k})$. The difference is that the amplitudes of the vibrations are now quantized in bosons carrying each an energy $\hbar\omega_\lambda(\vec{k})$. These bosons are the phonons. The ground state of the crystal has changed as well by the simple manipulations (4.51-4.53). Although the phonon states are all unoccupied, we have build a zero-point motion of the atoms into the ground state which is driven by the collective vibrations. For instance, the energy is increased by the zero-point contribution $\Delta E_{Gaussian} = \frac{1}{2}\sum_{k,\lambda} \hbar\omega_\lambda(\vec{k})$. Because the energy has changed, the ground state wavefunction should also be different. We will take up this theme again in section 4.6.

The Debye model.

Dealing with quantum-mechanical excitations, one likes to know the density of states. The phonon density of states can be calculated in the usual way (units $\hbar = 1$),

$$g(\omega) = \sum_\lambda \int_\omega \frac{dS}{(2\pi)^3} \frac{1}{|\vec{\nabla}_k\omega_\lambda(\vec{k})|} \quad . \tag{4.54}$$

$1/|\vec{\nabla}_k\omega_s(\vec{k})|$ is the distance between the surfaces in $\vec{k}$ space following from the conditions $\omega_s(\vec{k}) = \omega$ and $\omega_s(\vec{k}) = \omega + d\omega$ and the integral over the surface area (dS) yields the volume enclosed by the two surfaces. In addition one has to sum over the different modes (λ). A number of finite temperature properties are related to the density of states, weighted by the Bose factor: $\sim \int d\omega g(\omega) n_B(\omega)$, where

$$n_B(\omega) \;=\; \frac{1}{e^{\omega/k_BT}-1} \quad , \tag{4.55}$$

$\Longrightarrow$ Excercise 4.9

Real phonon dispersions and densities of states tend to be rather complicated. At least in the limits of high- and low temperature one is not interested in all this information and instead one can come quite far with very simple models. In the high temperature limit, all the details are washed away by the Bose factor and many properties are only sensitive to the first moment of the phonon density of state $\omega_E \sim \int d\omega \omega g(\omega)$. To good approximation, one can assume that the lattice vibrates at a single frequency (ω_E): this is the Einstein model.

In the low temperature limit, only the acoustic phonons matter and this allows for considerable simplifications as well. Next to neglecting the optical modes alltogether, in the Debye model the assumption is made that the sound velocity is isotropic in space. As long as one is not explicitely interested in measurable effects of spatial anisotropy in he crystal, this is a very reasonable thing to do - the sound velocity in the Debye model is just the angle average of the real velocities (4.47). The dispersion relations are approximated by

$$\omega_\lambda(\vec{k}) \;=\; c|k| \quad , \qquad \lambda = 1, \cdots, d \quad . \tag{4.56}$$

To normalize, one assumes that the allowed wavevectors $\vec{k}$ lie within a sphere of radius k_D, containing N $\vec{k}$ points. In three dimensions,

$$\frac{4}{3}\pi k_D^3 \left(\frac{L}{2\pi}\right)^3 \;=\; N \quad . \tag{4.57}$$

Because $N/L^3 = n_i$ (the density of atoms),

$$k_D \;=\; (6\pi^2 n_i)^{1/3} \quad . \tag{4.58}$$

k_D has the meaning of an 'ultraviolet' cut-off momentum: the largest momentum carried by a phonon is of order k_D, given an ion density n_i. This also defines the cut-off frequency (the 'Debye frequency') and the associated Debye temperature,

$$\begin{aligned} \omega_D &= c k_D \quad , \\ \Theta_D &= \hbar\omega_D / k_B \quad . \end{aligned} \tag{4.59}$$

Under the rule of the Goldstone theorem, the low energy asymptote of the excitation spectrum has to be dominated by the zero-modes, in this case the acoustical phonons. For this reason, the low temperature properties in so far they are caused by the lattice show an *universal* behaviour, because the zero-modes are universal, and the Debye model is good enough to catch this universality. For instance, the specific heat of a d-dimensional crystal behaves like $c_v = AT^d$ - although the prefactor (A) depends on k_D, the exponent depends only on the dimension of the space in which the crystal lives.

$\Longrightarrow$ Excercises 4.10 and 4.11

4.4 Anharmonicity: phonon-phonon interactions.

I have stressed several times that the assumption of harmonicity (the necessary condition for the existence of modes) becomes rigorously correct only in the limit $\omega, k \to 0$. At finite frequencies, the anharmonicities always play a role. As long as their strength is small, their effect can be treated using perturbation theory: this is nothing else than doing the next orders of the perturbation expansion 'around' the classical state. The main effect will be that one particular mode can decay in other modes, giving it a finite lifetime τ. As in the classical case, the phonons are no longer precisely defined objects: they are more like resonances in the continuum of true many atom states. All you know for sure is, that after an infinite time the system will have relaxed into a state which is again completely specified: infinitely many, infinitely low frequency zero-modes. Nevertheless, as long their inverse lifetime (the width of the resonance) is small, these decaying phonons are still quite usefull to get an accurate picture of reality. In essence, their 'non existence' is irrelevant for the questions which really matter, like the question after the existence of the crystalline condensate.

There is one lifetime issue which really matters: does the zero-mode become infinitely long lived if its wavelength approaches infinity? If not, there could have been something really wrong with our assumption that the crystalline state exists: perturbation theory knows about wrong ground states. More precisely, the limit $k \to \infty$ has to be well behaved, in the sense that the energy of the excitation $\omega \sim ck$ should go to zero slower than the inverse lifetime $\delta\omega \sim 1/\tau$ (all in units of $\hbar$). We will actually find that $\delta\omega \sim k^{d+2}$ (d is dimension) and because the $d+2$'th power of a very small number is of course much smaller than the number itself, the zero modes are 'well behaved'. What follows is a first example of testing condensates by perturbation theory.

Phonon-phonon interactions.

Let us consider the structure of the perturbation theory beyond the Gaussian (harmonic) order. The existence of the crystalline ground state implies that the potential can be written as the Taylor series (4.16),

$$\hat{H} = \hat{H}_{harm} + \hat{H}_3 + \hat{H}_4 + \cdots \quad , \tag{4.60}$$

where $\hat{H}_{harm}$ is given by (4.53) and the leading order correction is given by the cubic term,

$$\begin{aligned} \hat{H}_3 &= \frac{1}{3!}\sum_{n\alpha}\sum_{n'\beta}\sum_{n''\gamma} u_{n\alpha}u_{n'\beta}u_{n''\gamma}V_{\alpha,\beta,\gamma}(\vec{R}^0_n, \vec{R}^0_{n'}, \vec{R}^0_{n''}) \\ V_{\alpha,\beta,\gamma}(\vec{R}^0_n, \vec{R}^0_{n'}, \vec{R}^0_{n''}) &= \left(\frac{\partial^3 \mathcal{V}}{\partial R_{n\alpha}\partial R_{n'\beta}\partial R_{n''\gamma}}\right)_{\{\vec{R}^0_n\}} \quad . \end{aligned} \tag{4.61}$$

As long as the displacements are small, one expects the effects coming from $\hat{H}_3$ to dominate over the higher orders in the expansion (4.60)[7]. In the spirit of perturbation

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[7] One has to be careful: (i) For $u \to \infty$ $E^3_{pot} \to -\infty$ and the neglect of the higher order terms only makes sense if the u's are small enough. (ii) Sometimes it happens that the kinematics (conservation of energy and momentum) limits the number of allowed third order scattering processes to such an extent that the fourth order terms yield a larger net correction.

theory, one now expresses the correction term $\hat{H}_3$ in the eigenstates of the zero-th order Gaussian problem H_{harm}. The Hilbert space is therefore spanned by the complete set of oscillator states, in occupation number representation,

$$|\left\{n_{\vec{k}\lambda}\right\}> \quad , \qquad n_{\vec{k}\lambda} = 0, 1, 2, \cdots \tag{4.62}$$

$\Longrightarrow$ Excercise 4.12

According to (4.36), the displacements u are written in terms of the normal coordinates as

$$u_{n\alpha} = \frac{1}{\sqrt{N}} \sum_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{R}_n^0} v_\alpha^\lambda Q_\lambda(\vec{k}) \quad . \tag{4.63}$$

To quantize the Q's, we have simply to invert (4.51),

$$Q_\lambda(\vec{k}) = \sqrt{\frac{\hbar}{2M\omega_\lambda(\vec{k})}} \left(b_{\vec{k}\lambda} + b^\dagger_{-\vec{k}\lambda}\right) \quad , \tag{4.64}$$

and it follows that the displacements are expressed in terms of the boson Heisenberg algebra as,

$$u_{n\alpha} = \frac{1}{\sqrt{N}} \sum_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{R}_n^0} v_\alpha^\lambda \sqrt{\frac{\hbar}{2M\omega_\lambda(\vec{k})}} \left(b_{k\lambda} + b^\dagger_{-k\lambda}\right) \tag{4.65}$$

Substituting (4.65) into (4.61) yields an expression of the anharmonic term, in terms of the phonon creation and annihilation operators,

$$\begin{aligned} \hat{H}_3 = & \sum_{\vec{k}_1\lambda_1\vec{k}_2\lambda_2\vec{k}_3\lambda_3} V'_{\lambda_1\lambda_2\lambda_3}(\vec{k}_1\vec{k}_2\vec{k}_3)\ [\ b^\dagger_{-\vec{k}_3\lambda_3} b^\dagger_{-\vec{k}_2\lambda_2} b^\dagger_{-\vec{k}_1\lambda_1} + b^\dagger_{-\vec{k}_3\lambda_3} b^\dagger_{-\vec{k}_2\lambda_2} b_{\vec{k}_1\lambda_1} \\ & + b^\dagger_{-\vec{k}_1\lambda_1} b_{\vec{k}_2\lambda_2} b_{\vec{k}_3\lambda_3} + b_{\vec{k}_1\lambda_1} b_{\vec{k}_2\lambda_2} b_{\vec{k}_3\lambda_3}\ ] \quad . \end{aligned} \tag{4.66}$$

Because of translational invariance, $V_{\alpha,\beta,\gamma}(\vec{R}_n^0, \vec{R}_{n'}^0, \vec{R}_{n''}^0) = V_{\alpha,\beta,\gamma}(\vec{R}_n^0 - \vec{R}_{n''}^0, \vec{R}_{n'}^0 - \vec{R}_{n''}^0)$ and it follows that crystal momentum is conserved,

$$\hat{H}_3 = \sum_{\vec{k},\vec{q},\vec{K};\lambda_1,\lambda_2,\lambda_3} V_{\lambda_1\lambda_2\lambda_3}(\vec{k},\vec{q},\vec{K}) \left[\ b^\dagger_{\vec{k}-\vec{q}\lambda_3} b^\dagger_{\vec{q}+\vec{K}\lambda_2} b_{\vec{k}\lambda_1} + b^\dagger_{\vec{k}\lambda_1} b_{\vec{q}+\vec{K}\lambda_2} b_{\vec{k}-\vec{q}\lambda_3}\right] \tag{4.67}$$

where we neglected the terms $\sim b^\dagger b^\dagger b^\dagger$ and bbb because they play no role in the lowest order perturbation theory we will consider next. The matrix elements are given by the rather formidable expression,

$$\begin{aligned} V_{\lambda_1\lambda_2\lambda_3}(\vec{k},\vec{q},\vec{K}) = & \frac{\hbar^{3/2}}{3!(2MN)^{3/2}} \sum_{n\alpha n'\beta n''\gamma} \\ & \times \frac{v_\alpha^{\lambda_1} v_\beta^{\lambda_2} v_\gamma^{\lambda_3} V_{\alpha,\beta,\gamma}(\vec{R}_n^0, \vec{R}_{n'}^0, \vec{R}_{n''}^0) e^{i((\vec{k}-\vec{q})\cdot\vec{R}_n^0 + (\vec{q}+\vec{K})\cdot\vec{R}_{n'}^0 + \vec{k}\cdot\vec{R}_{n''}^0)}}{\sqrt{\omega_{\lambda_1}(\vec{k}-\vec{q})\omega_{\lambda_2}(\vec{q}+\vec{K})\omega_{\lambda_3}(\vec{k})}} \end{aligned} \tag{4.68}$$

$\Longrightarrow$ Excercise 4.13

The lifetime of the zero-mode.

What does (4.67) physically? Take the term $\sim b^\dagger b^\dagger b$: it means that initially the phonon with wave number $\vec{k}$ is annihilated, while two new phonons are created. In other words, the $\vec{k}$ phonon decays into a pair of phonons with momenta $\vec{k} - \vec{q}$ and $\vec{q}$, modulo the umklapp $\vec{K}$. We can draw a diagram for this process,

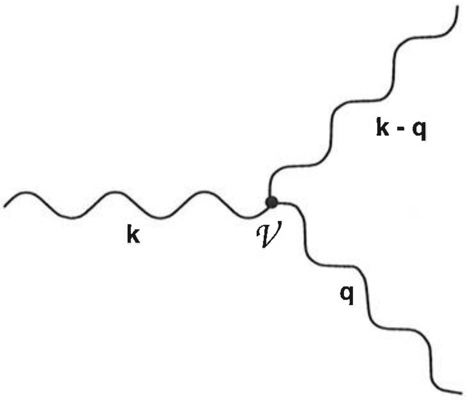

Figure 4.3: *'Nursery school diagram' of the decay of a phonon in other phonons, due to the anharmonicity of the crystal potential.*

In order to pursue the perturbation theory systematically, one needs the Greens functions and diagrams which are introduced in chapter VII. However, as long as we do not want to know more than the decay rate of the phonon up to second order in $\hat{H}_3$, we might as well use Fermi's golden rule. A decay rate (or energy spread) is according to the golden rule given by

$$\delta\omega_{(i)} \sim \sum_f |\langle i|H_{pert}|f\rangle|^2 \delta(E_f - E_i) \tag{4.69}$$

The initial state $|i\rangle$ is the state with a single phonon occupied with momentum $\vec{k}$ and energy $E_i = \omega_{\lambda_1}(\vec{k})$ and the final states $|f\rangle$ are the *two* phonon states, with one phonon at $\vec{k} - \vec{q}$ and the other at $\vec{q}$, and energy $E_f = \omega_{\lambda_2}(\vec{k} - \vec{q}) + \omega_{\lambda_3}(\vec{q})$. In addition, the two emitted phonons have to be real, and therefore the total energy of the final state has to be equal or less than the energy of the initial state $E_i \leq E_F$. For an arbitrary phonon, (4.69) is rather hard to evaluate because one needs detailed knowledge about the matrix elements (4.68), as well as the full phonon spectrum, and these are not easy to calculate. This is different for the decay rates of the zero-modes. The qualitative behaviour of their decay rate is again universal.

Since spatial anisotropies are irrelevant, as are the optical modes, we adopt the Debye model. In addition, to keep the calculation as transparent as possible we omit all prefactors - these do not matter either and can be determined by experiment. In the isotropic case we can drop the λ and $\alpha \cdots$ labels in (4.68) and Umklapp does not play a role in the $\vec{k} \to 0$ limit. In addition, we can expand $e^{i\vec{k}\cdot\vec{R}} \to 1 + ik\hat{\Omega}_k \cdot \vec{R}$ (k is the radial component of $\vec{k}$ and Ω_k the directional unit vector) and because the matrix elements (4.68) are only non-zero if all space components $\vec{R}^0_n, \vec{R}^0_{n'}, \vec{R}^0_{n''}$ appear in the sum, (4.68) simplifies in the long wavelength limit to,

$$\begin{aligned} V_{\lambda_1\lambda_2\lambda_3}(\vec{k},\vec{q}) &\to \frac{V(\hat{\Omega}_k,\hat{\Omega}_q)k|\vec{k}-\vec{q}|q}{(\omega_k\omega_{|\vec{k}-\vec{q}|}\omega_q)^{1/2}} \\ &\to V(\hat{\Omega}_k,\hat{\Omega}_q)\sqrt{k|\vec{k}-\vec{q}|q} \end{aligned} \qquad (4.70)$$

where we used the Debye dispersion $\omega_{\vec{k}} = ck$. In addition, the energies of the initial and final states are $E_i = ck$ and $E_f = c|\vec{k}-\vec{q}| + cq$ and it follows from (4.69) that the decay rate of an acoustic phonon with momentum $\vec{k}$ in d dimensions is proportional to,

$$\delta\omega_{\vec{k}} \sim \int_0^k d^d\vec{q}\; |V(\hat{\Omega}_k,\hat{\Omega}_q)|^2\; k|\vec{k}-\vec{q}|q\; \delta(q + |\vec{q}-\vec{k}| - k) \qquad (4.71)$$

This is a simple example of the type of integrals one frequently encounters in perturbation theory. Since the interest is in the radial part, it is easy to handle by 'power counting'. One splits all momenta in a radial and angular part $\vec{q} = q\hat{\Omega}_q$ and $d^d\vec{q} = q^{d-1}dqd\hat{\Omega}_q$, one scales out q by $q = \tilde{q}k$ and because $\delta(ax) = (1/a)\delta(x)$, (4.71) becomes

$$\begin{aligned} \delta\omega_{\vec{k}} &\sim A(\hat{\Omega}_k)k^{d+2} \\ A(\hat{\Omega}_k) &\sim \int_0^1 d\tilde{q} \int d\hat{\Omega}_q\tilde{q}^d\; V(\hat{\Omega}_k,\hat{\Omega}_q)\; |\hat{\Omega}_k - \hat{\Omega}_q\tilde{q}|\delta(1-\tilde{q}-|\hat{\Omega}_k-\hat{\Omega}_q\tilde{q}|) \end{aligned} \qquad (4.72)$$

Hence, the decay rate goes to zero as k^{d+2} in the long wavelength limit and the acoustic phonon gets better and better defined if its wavelength increases, to become 'exact' if its energy is infinitisimal. One could now argue that the above is only a rather naive second order calculation and that one cannot be certain that some high order contribution behaves in a more harmfull way. It turns out, however, to be possible to *proof* that the higher orders only contribute terms in the decay rate which fall off more quickly than k^{d+2}, and these are therefore always less dangerous than the second order contribution. Although one needs the full machinery of field-theoretic perturbation theory to deliver these proofs[8], with the simple machinery we use here one already sees the principle at work. From (4.71) it is clear that the theory becomes 'less well' behaved if one lowers the dimensionality. However, on the second order level there is even in one dimension no reason to worry about the stability of the condensate. As will be demonstrated in section 4.6, we actually overlook here the fact that the one dimensional crystal has already been blown into pieces by the *Gaussian* fluctuations!

$\Longrightarrow$ Excercise 4.14

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[8] I am actually not aware of such a proof in the context of crystalline order - it has been delivered in a more complicated context, see chapter VII.

4.5 Non-adiabatic corrections: the electron-phonon coupling.

We started out assuming that the lattice dynamics could be decoupled from the electron dynamics because the typical electron moves much faster than the typical ion. Although this is definitely true for the vast majority of the electrons, it is not true for a small fraction of electrons which are very close to E_F. For these electrons, non-adiabatic effects become quite important and one is faced with a 'mixed' dynamics. Although in many cases one can still get away with perturbation theory, I will highlight a simple case where this is not true: the polaron.

The electron-phonon interaction.

Let us write the electron-lattice coupling in terms of the phonons. This follows the same pattern as in the previous section. The fundamental electron-ion coupling can again be expanded around the crystalline state. In the spirit of the pseudopotentials (chapter III), one can first fill up the atomic cores, ending up with an effective electron-ion interaction,

$$V_{ie}(\{\vec{R}_n, \vec{r}_i\}) = \sum_i \sum_N V(\vec{r}_i - \vec{R}_n) \quad . \tag{4.73}$$

and this is expanded, as usually, in terms of the displacements u_n,

$$\begin{aligned} V_{ie}(\{\vec{R}_n, \vec{r}_i\}) &= \sum_i \sum_n V(\vec{r}_i - \vec{R}^0_n) - \sum_i \sum_n \vec{u}_n \cdot \vec{\nabla}_{\vec{R}} V(\vec{r}_i - \vec{R}^0_n) + \cdots \\ &\equiv \sum_i U_0(\vec{r}_i) \quad + \quad \hat{H}_{e-ph} \quad . \end{aligned} \tag{4.74}$$

The first term is the static lattice potential which gives rise to the band structure, and the second term describes the lowest order contribution to the dynamical coupling between the lattice and the electrons. With the exception of the polarons, this lowest order term is far more important than the higher order terms, much in the spirit of the previous section. Also in this case, the subset of phonon-like motions of the lattice are the most important ones. To profit fully from the periodicity of the lattice, it is convenient to span up the Fock space of the electrons in terms of single particle Bloch states $\{c^\dagger_{\vec{k}\sigma}, c_{\vec{k}'\sigma'}\}$. The total Hilbert space becomes the product space of the electronic Fock space $|\{n_{\vec{k}\sigma}\}\rangle$ and the phonon Fock space $|\{n_{\vec{q}\lambda}\}\rangle$. In order to evaluate the first order term in (4.74), one needs an electronic part

$$\vec{\nabla}_{\vec{R}} V(\vec{r}_i - \vec{R}^0_n) = \sum_{\vec{k}\vec{k}'\sigma} \langle \vec{k}'\sigma | \vec{\nabla}_{\vec{R}} V(\vec{r}_i - \vec{R}^0_n) | \vec{k}\sigma \rangle c^\dagger_{\vec{k}'\sigma} c_{\vec{k}\sigma} \tag{4.75}$$

Using (4.65), the first order electron-phonon coupling is written as,

$$\hat{H}_{e-ph} = \sum_{\vec{K},\vec{k},\vec{q},\lambda} M_\lambda(\vec{K}, \vec{k}, \vec{q}) \; c^\dagger_{\vec{k}+\vec{q}+\vec{K},\sigma} c_{\vec{k}\sigma} \; (b^\dagger_{-\vec{q}\lambda} + b_{\vec{q}\lambda}) \tag{4.76}$$

$\Longrightarrow$ Excercise 4.15

One can draw the following 'diagram',

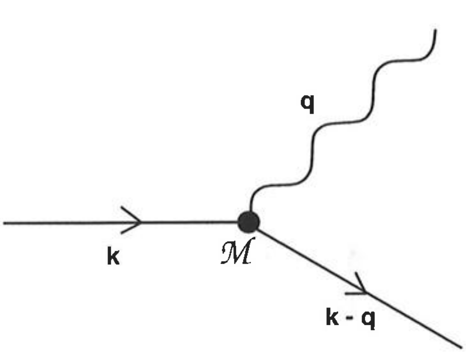

Figure 4.4: *'Nursery school diagram' of the electron ('full line') emitting or absorping a phonon ('wiggly line').*

This looks similar to the minimal coupling between fermions and gauge particles which is one of the axioms of elementary particle theory. According to field theory, the interactions between the fermions are caused by virtual exchange of photons, etcetera. Our 'wiggly lines' (which can also be other modes) also mediate interactions between the electrons in the solids, with the specialty that they can cause *attractive* interactions, as will be discussed in Chapter VI.

Model interactions.

It is usually very hard to calculate the electron-phonon matrix-elements. As always, to study qualitative effects one can get away with simple models. One extreme is that perturbation theory works well in terms of the Bloch states: this is usually the case in metals and semiconductors. In these cases, one is interested in electrons very close to E_F behaving as nearly free electrons and the following model works very well

$$\hat{H}_{e-ph} = M \sum_{\vec{q}\lambda} \rho_{\vec{q}} (b^{\dagger}_{-\vec{q}\lambda} + b_{\vec{q}\lambda}) \tag{4.77}$$

where

$$\rho_{\vec{q}} = \sum_{\vec{k}\sigma} c^{\dagger}_{\vec{k}+\vec{q}\sigma} c_{\vec{k}\sigma} \tag{4.78}$$

measures a density wave in a jellium with a wavevector $\vec{q}$. Except for momentum conservation, further momentum dependences of the electron-phonon coupling are neglected.

$\Longrightarrow$ Excercise 4.16

Non-perturbative effects are often associated with rather tightly bound electrons (strong lattice potentials !) and these effects are usually adressed starting from the tight-binding like Peierls- and Holstein models. In the Peierls model it is assumed that the electrons couple to the phonons, because the latter modulate the bondlengths and thereby the hopping matrix elements. We learned that the hopping elements behave like $t \sim 1/d^{\alpha}$ (section 3.3). Expanding the length of the bond between the sites

$\vec{i}$ and $\vec{i}+\vec{\delta}$ as $d_{\vec{i}\vec{\delta}} = d^{(0)}_{\vec{i}\vec{\delta}} - u_{\vec{i}\vec{\delta}}$ and defining the equilibrium hopping as $t^{(0)}_{\vec{i}\vec{\delta}} \sim 1/(d^{(0)})^{\alpha}_{\vec{i}\vec{\delta}}$, the hopping part of the Hamiltonian can be written as,

$$\hat{H}_t = \sum_{\vec{i}\vec{\delta}\sigma} t^{(0)}_{\vec{i}\vec{\delta}} (1 + \alpha u_{\vec{i}\vec{\delta}}) c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} \tag{4.79}$$

and the displacements $u_{\vec{i}\vec{\delta}}$ are 'phononized' as usually. The Holstein model is even simpler. It is assumed that the *diagonal* energies are modulated by the lattice vibrations,

$$\hat{H} = \sum_{\vec{i}\sigma} \varepsilon_{\vec{i}} (1 + \alpha u_{\vec{i}}) \hat{n}_{\vec{i}\sigma} + \sum_{\vec{i}\vec{\delta}\sigma} t_{\vec{i}\vec{\delta}} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} \tag{4.80}$$

How can this happen? One should imagine a system with more than one atomic orbital per unit cell, and $|i>$ is some linear combination of orbitals on different atoms within the unit cell, which ends up having an energy close to E_F. If one now modulates the structure *within* the unit cell, the level position of the hybrid orbital will also change. For this to happen one needs optical phonons (out-of-phase vibrations within the unit cell), and optical phonons usually disperse little. Hence, one can take as well a (Einstein) phonon which is localized within the unit cell ($b^{\dagger}_{\vec{i}}$). Including this phonon,

$$\hat{H} = \sum_{\vec{i}\sigma} \left[\varepsilon \hat{n}_{\vec{i}\sigma} + \mathcal{M} \hat{n}_{\vec{i}\sigma} (b^{\dagger}_{\vec{i}} + b_{\vec{i}}) + \omega b^{\dagger}_{\vec{i}} b_{\vec{i}} \right] + t \sum_{\vec{i},\vec{\delta},\sigma} (c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} + h.c.) \tag{4.81}$$

where $\mathcal{M} = \alpha\varepsilon\sqrt{\hbar/M\omega}$. Notice that in the case of the Peierls model one needs more realistic phonons for the model to make sense.

$\Longrightarrow$ Excercise 4.17

Strong coupling: small polarons.

It is actually not at all true that the adiabatic approximation is a good one under all circumstances. In fact, it is because of non-adiabatic 'corrections' that practical electronic insulators exist. Perfect crystals can be band insulators. However, practical insulators are usually littered with defects, and defects cause free charge carriers. Why are these free carriers deemed to be immobile in practical insulators? It turns out that such a carrier dresses itself up with a lattice distortion, and this bound state of hole or electron and its lattice 'polarization cloud' is called 'polaron'. In order to move, the carrier has to drag around pieces of the lattice and this makes the polaron very heavy. The bandwidth associated with the polaron motion becomes small and even weak static- or thermal disorder causes a complete localization. Even for the case of a single carrier, the theory of polaron formation is not completely known. However, the story becomes simple in some limits, and especially the limit where the lattice is strongly deformed is quite informative. In this limit, the object is called the 'small polaron' and the Holstein model (4.81) is taylored to clarify its physics.

If one expects that the interactions dominate, it is always a good idea to first consider the classical limit, which is reached by neglecting the kinetic terms in the Hamiltonian.

Therefore, we put $t = 0$ and the atom mass $M \to \infty$ in (4.81). The classical energy is then given by (the force constant $K = M\omega^2$),

$$E_{Cl} = \sum_{\vec{i}} \left[\varepsilon(1 + \alpha u_{\vec{i}})\bar{n}_{\vec{i}} + \frac{K}{2} u_{\vec{i}}^2 \right] \tag{4.82}$$

where $\bar{n}_{\vec{i}}$ is now either 0 (singly unoccupied), 1 (occupied) or 2 (doubly occupied), because the electronic problem is diagonal in the site basis. We consider one electron which is localized at a particular site $\vec{j}$. The energy becomes,

$$E_{Cl} = \varepsilon(1 + \alpha u_{\vec{j}}) + \frac{K}{2} u_{\vec{j}}^2 + \frac{K}{2} \sum_{\vec{i} \neq \vec{j}} u_{\vec{i}}^2 \tag{4.83}$$

This energy is minimized to all u's and we find all displacements to be zero except for $u_{\vec{j}}^0 = -\alpha\varepsilon/K$. We substitute this back in (4.83) to find that the ground state energy becomes $E_{Cl} = \varepsilon(1 - \frac{\alpha^2 \varepsilon}{2K})$. Hence, *the localized electron has deformed the lattice* ($u_{\vec{j}} \neq 0$) *and thereby gained a 'polaron binding energy'* $E_{pol} = \varepsilon^2\alpha^2/2K$, for the simple reason that the electron-phonon energy decreases linearly in u while the restoring force grows only quadratically.

This simple story is the essence of the polaron idea. The problems start if one tries to treat this problem quantum-mechanically. As long as one can stick to the gaussian order (somewhat questionable in this context, because the local displacements tend to be large), the lattice kinetic energy does not pose much of a problem. In first instance, we are interested in the low electron density limit, and the classical polaron is characterized by a length scale: it is localized within the unit cell. It is expected that the quantum polaron will also be characterized by a length scale: only a small part of the lattice in the direct vicinity of the electron is altered, and the crystal as a whole will stay intact. Hence, at least in the low density limit, polarons cannot destroy the crystalline condensate. In addition, the phonons exhibit again their pleasant habit of not alterning their energetics under quantization, and taking a finite atomic mass yields the same answer as in the classical case.

$\Longrightarrow$ Excercise 4.18

The problems start if the quantum mechanics of the electron is reinstored - finite t. This will tend to spread out the electron. In the case that the hopping $t >> E_{pol}$ it is clearly not a good idea to completely localize the electron, and if the electron is not localizable, it is no longer possible to gain the polaron energy. Hence, eventually the electron will loose its polarization cloud alltogether. One expects that in this limit the electron-phonon effects can be taken into account perturbatively, to find small shifts and broadenings of the bare electron Bloch states. Although the strong coupling (classical) and weak coupling (nearly non-interacting) limits are easy, it turns out that the regime in between is very difficult and despite a very large effort which started already in the fifties this problem is still unsolved. To get some feeling, it is interesting to approach this difficult intermediate coupling regime from the strong coupling side: consider the electron hopping as the small parameter in the problem. What follows is an example of the technique of 'strong coupling perturbation theory', which we will encounter more often in the course of these lectures. We start out taking the problem (4.81) with $t = 0$ as a zeroth order, to subsequently consider the hopping as a small perturbation. We consider (4.81), omitting the hopping term, and we try to find a transformation e^S, with $S^\dagger = -S$, which brings this Hamiltonian in a diagonal form in terms of new localized electron-like objects $\bar{c}^\dagger$ and modified phonons $\bar{b}$,

$$\begin{aligned} H_0 &= \sum_{\vec{i}} \left[\varepsilon \hat{n}_{\vec{i}} + \mathcal{M} \hat{n}_{\vec{i}} (b^\dagger_{\vec{i}} + b_{\vec{i}}) + \omega b^\dagger_{\vec{i}} b_{\vec{i}} \right] \\ \bar{H}_0 &= e^S H_0 e^{-S} \\ &= \sum_{\vec{i}} \left[\sum_\sigma \varepsilon' \bar{c}^\dagger_{\vec{i}\sigma} \bar{c}_{\vec{i}\sigma} \; + \; \omega' \bar{b}^\dagger_{\vec{i}} \bar{b}_{\vec{i}} \right] \end{aligned} \tag{4.84}$$

Notice that this 'canonical transformation' lives entirely in operator 'space' - it is actually not so easy to imagine how to execute this transformation directly in Hilbert space. We need three useful properties of this transformation:

1 The transform of a product of operators is the same as the product of transformed operators,

$$e^S ABC \cdots e^{-S} = \bar{A}\bar{B}\bar{C} \cdots \tag{4.85}$$

We need this for the next theorem:

2 Transforming an operator function which can be expanded as a power series in terms of the operators yields the same function in terms of the transformed operators,

$$e^S f(A) e^{-S} = f(\bar{A}) \tag{4.86}$$

This is useful, because the new Hamiltonian will be the old one with the new operators.

3 The transformation can be written in terms of commutators as,

$$\bar{A} \; = \; e^S \, A \, e^{-S} \; = \; A \; + \; [S, A] \; + \; \frac{1}{2!} [S, [S, A]] \; + \; \cdots \tag{4.87}$$

$\Longrightarrow$ Excercise 4.19

In the next chapter it will be shown how to determine S from the requirement that it should diagonalize the Hamiltonian. We save us the effort here, and we conjecture that

$$S \; = \; - \sum_{\vec{i}\sigma} c^\dagger_{\vec{i}\sigma} c_{\vec{i}\sigma} \frac{\mathcal{M}}{\omega} (b^\dagger_{\vec{i}} - b_{\vec{i}}) \tag{4.88}$$

will do the job. According to theorem (4.86) we can first transform the fermion- and boson operators. Using (4.87),

$$\begin{aligned}
\bar{c}^{\dagger}_{\vec{i}\sigma} &= c^{\dagger}_{\vec{i}\sigma} B^{\dagger}_{\vec{i}} \\
\bar{c}_{\vec{i}\sigma} &= c_{\vec{i}\sigma} B_{\vec{i}} \\
\bar{b}^{\dagger}_{\vec{i}} &= b^{\dagger}_{\vec{i}} + \frac{\mathcal{M}}{\omega} \sum_{\sigma} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}\sigma} \\
\bar{b}_{\vec{i}} &= b_{\vec{i}} + \frac{\mathcal{M}}{\omega} \sum_{\sigma} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}\sigma} \qquad (4.89)
\end{aligned}$$

introducing the operator

$$B_{\vec{i}} = e^{-\frac{\mathcal{M}}{\omega}(b^{\dagger}_{\vec{i}} - b_{\vec{i}})} \qquad (4.90)$$

We leave it to the reader to show that the Holstein Hamiltonian without the hopping term becomes in the new operators,

$$\hat{H} = \sum_{\vec{i}} \left[(\varepsilon - E_{pol}) \sum_{\sigma} \bar{c}^{\dagger}_{\vec{i}\sigma} \bar{c}_{\vec{i}\sigma} + \omega \bar{b}^{\dagger}_{\vec{i}} \bar{b}_{\vec{i}} \right] \qquad (4.91)$$

Although (4.88) does *not* diagonalize the electron hopping term of the full Hamiltonian, we are of course allowed to express the hopping in the new fermions,

$$\begin{aligned}
\hat{H}_t &= t \sum_{\vec{i}\vec{\delta}\sigma} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} \\
\bar{H}_t &= t \sum_{\vec{i}\vec{\delta}\sigma} B_{\vec{i}} \bar{c}^{\dagger}_{\vec{i}\sigma} \bar{c}_{\vec{i}+\vec{\delta}\sigma} B^{\dagger}_{\vec{i}+\vec{\delta}} \qquad (4.92)
\end{aligned}$$

$\Longrightarrow$ Excercise 4.20

What is the physics behind the above manipulations? The transformation (4.88-4.91) is the phonon equivalent of the simple classical procedure (4.82-4.83). As long as the electron is classical (localized on a site) there is virtually no difference in outcome - as said before, this is related to the peculiarity of harmonic oscillators to not change the energetics under quantization (excercise 4.18). In terms of the algebra, the phonon is simply 'shifted' $b \rightarrow b + constant$. All the effort (4.84-4.92) was needed to keep track of the electron: *the* $\bar{c}^{\dagger}$ *creates an electron together with its classical-like lattice polarization cloud.* $\bar{c}^{\dagger}$'s are therefore the lattice-quantized version of the simple classical polarons, (4.83). This lattice polarization cloud is created by the operator $B^{\dagger}$ (4.90). The 'bare' boson operators appear exponentiated in this expression. The reason is that every phonon represent an infinitisimal displacement of an atom, and an infinity of phonons has to be excited to create the classical-like finite *local* displacement[9]. $B^{\dagger}$ can be written as a power series,

$$B^{\dagger}_{\vec{i}} = 1 + \frac{\mathcal{M}}{\omega}(b^{\dagger}_{\vec{i}} - b_{\vec{i}}) + \frac{1}{2!}(\frac{\mathcal{M}}{\omega})^2 (b^{\dagger}_{\vec{i}} - b_{\vec{i}})^2 + \cdots \qquad (4.93)$$

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[9] If one lets such an operator act on the QED vacuum one creates states corresponding with the coherent states as they were originally introduced in quantum optics.

The n-th power of this series will contribute terms like $(b^\dagger_{\vec{i}})^n$, and one infers that $B^\dagger$ excites large numbers of phonons if the coupling constant $\mathcal{M}/\omega$ becomes large.

These infinities start to play a role if the electron becomes quantum-mechanical ($t \neq 0$). By inserting (4.93) in the expression (4.92), one immediately sees that every hopping event of the polaron is accompanied by excitation and deexcitation of large numbers of phonons on both sites. Only one limit is easy. When t is very small compared to the polaron binding energy the hopping cannot change much in the phononic part of the polaron which is centered either on the $\vec{i}$'th or on the $\vec{i}+\vec{\delta}$'th site. One can now consider the phonon clouds to be rigid and it is easy to deduce an effective tunneling rate for the polaron as a whole. According to (4.92) this should correspond with t multiplied by the overlap of the phonon clouds, which is easily calculated to be,

$$\begin{aligned} \bar{H}_{t/E_P \to 0} &\simeq t \sum_{\vec{i}\vec{\delta}\sigma} \langle 0 | B_{\vec{i}+\vec{\delta}} B^\dagger_{\vec{i}} | 0 \rangle \bar{c}^\dagger_{\vec{i}+\vec{\delta}\sigma} \bar{c}_{\vec{i}\sigma} \\ &= t e^{-(\frac{\mathcal{M}}{\omega})^2} \sum_{\vec{i}\vec{\delta}\sigma} \bar{c}^\dagger_{\vec{i}+\vec{\delta}\sigma} \bar{c}_{\vec{i}\sigma} \end{aligned} \tag{4.94}$$

The vacuum $|0\rangle >$ is the vacuum on which the barred operators are defined ($\bar{b}_i|0\rangle = 0, \bar{c}_i|0\rangle = 0$). The polaron hops with a rate which is reduced by a factor $\exp(-(\mathcal{M}/\omega)^2)$ compared to the bare electron, and this rate gets very small if the electron-phonon coupling is large - the electron has to drag round a piece of the crystal when it hops and this tends to localize the polaron.

$\Longrightarrow$ Excercise 4.21

When t becomes of order of the classical polaron energy, the above picture breaks down because of the avalanches of multi-phonon excitations. I repeat: if $t >> E_{pol}$ the classical localization ends because it costs an energy $\sim t$ to localize a particle on one site. Starting from the large t limit, it is much better to use the propagating electron states as the zero-th order, using the electron-phonon coupling as the small perturbation. As said, the outcomes are unremarkable.

Electron-phonon coupling in metals.

It is a prerequisite for the understanding of the workings of the electron-phonon coupling in the metallic state to understand the metallic state itself, which is the subject of chapter VII. In addition, one needs the convenience of diagrammatic perturbation theory (also explained in chapter VII) to appreciate the subtleties of the problem. Let me here only comment on the obvious question: why is the polaron mechanism usually not active if the system is characterized by a high density of electrons? Clearly, if the above polaron mechanism would be active always, one could wonder why the metallic state exists at all. The answer is actually rather straightforward: it is the Pauli-principle. Electrons in metals are characterized by an enormous energy scale for their zero point motion, the Fermi-energy. In order to localize all the electrons, the polaron binding energy has to exceed the Fermi energy and in a typical metal this will never happen. The Fermi energy is like 5 eV while the (classical) polaron energy is typically $O(0.1)$ eV. In addition, a second time scale plays a role: the typical (Debye/Einstein) phonon frequency ω_p. This is again much smaller than the typical Fermi energy (≤ 0.1 eV). As will be further discussed in the context of superconductivity (chapter VI), one should compare this with the energy of the electrons relative to the Fermi energy. Only the electrons in a small shell with width ω_p around the Fermi energy are moving slower than the lattice. The vast majority of electrons therefore moves much faster than the lattice, and this guarantees that the lattice can be considered to be static. Only the electrons very close to E_f are subject to non-adiabatic effects. The most important of these effects is the attractive interactions between the low lying electrons, caused by the virtual exchange of (fast) phonons, which is the driving force behind conventional superconductivity - see chapter VI. The crystal itself, on the other hand, is not affected: one can calculate again the decay rate of the zero-modes due to the creation of electronic excitations, to find that this vanishes sufficiently rapidly approaching the long wavelength limit.

What happens if $E_F \simeq E_{pol}$? This is actually a subject of active research. Starting from the classical side, polarons would occur at a relative high density. Recently, evidence has started to accumulate that the physics is much richer than either the single polaron- or the metallic limit. Apparently, the electrons (accompanied by their polarization clouds) have the tendency to form intricate patterns which themselves are strongly fluctuating, and it is believed that this kind of physics could be responsible for the anomalous behaviour of for instance the high T_c superconductors[10]. In this regime, it is even not clear if the atoms are in a true crystalline state. The atoms seem to fluctuate in a way which cannot be explained in terms of simple Gaussian theory[11].

4.6 The stability of the crystalline condensate: quantum melting.

What has happened up to now in this chapter? The argument started with the *assumption* that the crystalline condensate exists. This we found quite reasonable, because nature is doing it all the time. The existence of crystalline order tells us immediately how to construct the wavefunction: the 'ansatz' (4.7) should have a finite overlap with the true wavefunction of the crystal. In the process of constructing this ansatz we became aware that the way we intuitively handle the crystalline state is not unproblematic. By its very nature (localized atoms), it is violating the basic principles of quantum mechanics. Subsequently we found out that the mere existence of crystalline order allowed us to make non trivial statements regarding the long-wave length properties: if the crystal exists, a global minimum of energy exists, implying that the Taylor expansion exists, implying that zero-modes exist. We investigated whether this construction is at least internally consistent. Perturbation theory is a

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[10] See, e.g., J. Zaanen and P. B. Littlewood, Phys. Rev. B **50**, 7222(1994); J. Zaanen, M. Horbach and W. van Saarloos. Phys. Rev. B **53**, 8671 (1996).

[11] T. Egami and S. L. J. Billinge, in 'Physical Properties of High temperature Superconductors', D. M. Ginsberg (World Scientific, Singapore, in press).

way to investigate the stability of the (semi-classical) ground state and a divergent term in the expansion would signal a serious problem with the starting assumption of the existence of the minimum. Up to this point, this looked fine: it is a necessary condition for the classical state to exist that the zero-modes live infinitely long, and we found that neither the electron-phonon nor the phonon-phonon corrections could change this.

Actually we were a bit too hasty. Perturbation theory has the pleasant habit to diverge in the lowest order, if something is wrong. Calling the basic act of quantizing the modes a 'perturbation theory up to Gaussian order', the electron-phonon and phonon-phonon couplings represent a first- and second order correction to this order, respectively. However, already in Gaussian order we started to dress up the classical state with fluctuations (adding the $|\Phi_i\rangle$'s to the $|\Phi^0_{Cl}\rangle$'s), and we did not investigate yet whether the expansion in this lowest order is healthy. It turns out that the pathologies appear in this order. It will be shown that sufficiently strong microscopic quantum fluctuations will *always* destroy crystalline order and this will be illustrated in the context of the heliums. More beautifully, it turns out that *dimensionality* yields real control. It is easy to prove that the crystalline condensate *never* exists in one space dimension, while it can only exist in two dimensions at the absolute zero of temperature. As long as the microscopic fluctuations are weak enough, another state will take over: the floating solid. The one dimensional, zero temperature floating solid is the simplest of all non-classical states and it is the only non-classical state which will get some exposure in this text.

The argument which follows is originally due to Landau and has been further elaborated in the context of statistical mechanics (thermal fluctuations) by Mermin and Wagner, where it is known as the 'Mermin-Wagner theorem'. The essence is very simple: zero-modes are an inescapable byproduct of the order and by doing the simple quantization procedure of section 4.3, these zero-modes dress up the classical state. In doing so, they produce *infinities* in low dimensions which are caused by the longest wavelength (and therefore best defined) modes. We have not seen this yet because we did not ask the right question.

Melting criteria.

The question is after the mean square fluctuation of a particular atom around its equilibrium position. For the crystal to exist, this fluctuation should at least be finite, and even be small compared to the lattice constant. The mean-square fluctuation is,

$$\begin{aligned} \langle \delta \vec{R}_n^2 \rangle &= \sum_\alpha \langle | \mid u_{n\alpha}|^2 \mid \rangle \\ &= \frac{1}{N} \sum_{\vec{k},\vec{k}'} e^{i(\vec{k}-\vec{k}')\cdot \vec{R}^0_n} \sum_{\alpha,\lambda,\lambda'} v^\lambda_\alpha(\vec{k}) v^{\lambda' *}_\alpha(\vec{k}') \langle | Q_\lambda(\vec{k}) Q^*_{\lambda'}(\vec{k}') | \rangle \end{aligned} \tag{4.95}$$

We have to calculate the expectation value $\langle | Q_\lambda(\vec{k}) Q^*_{\lambda'}(\vec{k}') | \rangle$ and we have learned how to do this. We again use $Q \sim b^\dagger + b$ (4.64) and we have to evaluate expectation values of the form $\langle | (b_{\vec{k}\lambda} + b^\dagger_{-\vec{k}\lambda})(b_{-\vec{k}'\lambda'} + b^\dagger_{\vec{k}'\lambda'}) | \rangle$. In what follows, we really need the zero-modes and for those we can ignore mode-couplings alltogether. In the absence of phonon interactions, the problem is diagonal in the Fock space spanned by the single phonon states,

$$\cdots \Pi_{m=0}^{n_{\vec{k}_1}} b^\dagger_{\vec{k}_1} \cdots \Pi_{m'=0}^{n_{\vec{k}_2}} b^\dagger_{\vec{k}_2} \cdot\cdot |vac.\rangle = |\cdots, n_{\vec{k}_1}, \cdots, n_{\vec{k}_2}, \cdots\rangle \tag{4.96}$$

and this implies,

$$\begin{aligned} \langle|(b_{\vec{k}\lambda} + b^\dagger_{-\vec{k}\lambda})(b_{-\vec{k}'\lambda'} + b^\dagger_{\vec{k}'\lambda'})|\rangle &= \langle|b^\dagger_{-\vec{k}\lambda} b_{-\vec{k}\lambda} + b_{\vec{k}\lambda} b^\dagger_{\vec{k}\lambda}|\rangle \delta_{\vec{k},\vec{k}'} \delta_{\lambda,\lambda'} \\ &= (1 + 2n_B(\beta\omega_\lambda(\vec{k})))\ \delta_{\vec{k},\vec{k}'}\ \delta_{\lambda,\lambda'} \qquad (4.97) \end{aligned}$$

with the Bose-factor ($\beta = 1/k_B T$),

$$\langle|b^\dagger_{\vec{k}\lambda} b_{\vec{k}\lambda}|\rangle = \frac{1}{e^{\hbar\omega_\lambda(\vec{k})/k_B T} - 1} = n_B(\beta\omega_\lambda(\vec{k})) \tag{4.98}$$

$\Longrightarrow$ Excercise 4.22

From (4.64), (4.97) it follows,

$$< (\delta \vec{R}_n)^2 >= \frac{1}{N} \sum_{\vec{k},\lambda} \frac{\hbar}{M\omega_\lambda(\vec{k})} \left(n_B(\beta\omega_\lambda(\vec{k})) + \frac{1}{2} \right) \tag{4.99}$$

This is an important result. It tells us that the position uncertainty of a *particular* atom is caused by the quantum-mechanical admixing, or thermal occupation, of the *collective* excitations of the whole system. The sum in (4.99) is actually dominated by the *long wavelength zero-modes*, corresponding with the 'most' collective excitations of the system. Let us first focus on the one dimensional case at $T = 0$. We make the Debye assumptions (4.56-4.59) and we consider the relative fluctuation (a is the lattice constant),

$$\begin{aligned} \gamma &= \frac{\langle(\delta\vec{R}_n)^2\rangle}{a^2} \qquad (4.100) \\ &= \frac{L}{N} \frac{\hbar}{4\pi a^2 c M} \int_0^{k_D} \frac{dk}{k} \to \infty \qquad (4.101) \end{aligned}$$

The perturbation theory blows up because of the 'exact' long wavelength fluctuations, and the crystalline order can therefore not exist in $d = 1$!

What happens in higher dimensions? At $T = 0$, the integral (4.99) behaves as $\int_0^{k_D} k^{d-2}$ and this is convergent if $d \geq 2$. It is now a matter of numbers whether the crystal survives the quantum fluctuations. The fluctuation should be a fraction of the bond length, $\gamma < 1$, and we find that the magnitude of gamma is controlled by the prefactor,

$$\mu = \frac{\hbar}{4\pi a^2 c M} \tag{4.102}$$

which is called the 'dimensionless quantum of action' (or 'coupling constant'), $\hbar$ dressed up with the dimensionful parameters of the problem, to yield a dimensionless number. These numbers depend on the microscopy.

What happens at finite temperatures? Because zero modes extent all the way down to zero frequency, there will always be modes with an energy smaller than temperature, and we can therefore approximate $n_B(\hbar ck/k_BT) \simeq k_BT/\hbar ck$ if we are interested in the small k behaviour. The integral behaves therefore at finite temperature as $\int_0^{k_D} k^{d-3}dk$: *it seems as if the thermal fluctuation is one dimension more 'dangerous' than the quantum fluctuation*[12]. One concludes immediately that condensation at any finite temperature is not only impossible in $d = 1$, but in two dimensions as well: the Mermin-Wagner theorem. In addition, one expects that the two dimensional thermal fluid will bear some similarities with the one dimensional quantum fluid.

Although there is no theorem saying that crystals in $d = 3$ should melt always, we know from experience that eventually every solid will melt if the temperature becomes high enough. The details of this melting process are usually rather complicated. The above Gaussian picture definitely falls short - it is actually much better to think that the melting transition is driven by a proliferation of dislocations[13], instead of the above population of modes. However, dislocations are more easily created in crystals which are already subject to large uncorrelated thermal motions for which the modes are responsible. This rationalizes the success of the so-called *Lindemann criterion.* This is an empirical law saying that if the root mean square thermal fluctuation as calculated from (4.99) becomes of order of $\sim 0.1 - 0.15a$, the three dimensional crystal will melt. Doing the integral (4.99) in three dimensions in the Debye approximation, neglecting the zero-point contribution, yields

$$\gamma \simeq 1.6\ \frac{k_BT}{Mc^2} \tag{4.103}$$

When the thermal disorder, relevant to the melting process, is primarily due to the modes, a relationship between the sound velocity (which can be deduced from the Debye temperature) and the melting temperature T_m follows,

$$\gamma_m \simeq 1.6\ \frac{k_BT_m}{Mc^2} \tag{4.104}$$

with $\sqrt{\gamma_m} \sim 0.1 - 0.15$. It turns out that this relationship is quite well obeyed in many solids.

Let us now turn to the quantum fluctuations. (4.99) becomes in $d = 3$ at zero temperature (Θ_D is the Debye temperature),

$$\gamma \simeq 0.4\ \frac{k_B\Theta_D}{Mc^2} \tag{4.105}$$

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[12] This is not an accident. It turns out that a d-dimensional quantum problem can be reformulated as a statistical mechanics-like problem in one higher dimension, using the functional integral formalism (Feynman path integrals for many particle problems). The present 'free' quantum theory turns out to correspond precisely with the classical free theory in $d+1$ dimension, with an effective temperature in 'euclidian space-time' $\sim \mu$.

[13] More generally, 'topological defects' if one is dealing with other types of condensates.

From the comparison of (4.103) and (4.105), it follows directly that the thermal fluctuations start to dominate over the quantum fluctuations at temperatures larger than $\theta_D/4$. Since most solids melt at temperatures $T_M >> \theta_D$, quantum fluctuations are in most cases irrelevant for the melting process.

$\Longrightarrow$ Excercise 4.23

There are some exceptions, however. When the coupling constant μ (4.102), measuring the magnitude of the quantum fluctuations in the ultraviolet, becomes large enough, the three dimensional crystal might even be destroyed at zero temperature. This coupling constant is in first instance controlled by the atomic mass M and one would expect that a prime candidate for quantum melting would be the rather poorly (van der Waals) bonded, light mass Helium crystal. Since the thermal- and the quantum fluctuations act similarly on the harmonic level, one would expect that one can apply as well the Lindemann criterion to the zero temperature melting process. We leave it to the reader to show that the quantum-Lindemann criterium indeed predicts Helium to be a non-crystal at zero temperature.

$\Longrightarrow$ Excercise 4.24

At ambient pressures, He indeed prefers to be a non-crystal[14]. This does not mean that it does not fit any longer the classical 'paradigm' of section (1.2). Instead, it forms a different type of condensate which incorporates much more zero-point motion: the superfluids which are explained in chapter VI.

Floating solids.

It was found that the crystalline condensate cannot exist in one dimension even at zero temperature, and the question immediately arises what happens instead. It turns out, that the actual ground state no longer fits the definition of classical state as given in section 1.2. It is something else that one might want to call a 'quantum fluid', in the sense of 'quantum is everything else than classical'. It is a highly collective state, however, which has still many features in common with the classical crystal and for this reason I prefer to call it 'the floating solid' (solid in the sense of crystal, floating in the sense of floating in the swimming pool). Because of its closeness to the crystalline state, it is actually not hard to understand its nature.

The basic simplification comes from the observation that the crystal is eventually destroyed by rare, very long wavelength fluctuations. μ controls the fluctuation of every individual atom. When we keep this quantity small, we are assured that the displacements of individual atoms are quite small, so that there is nothing wrong with the harmonic approximation: although there is no classical ground state, the zero-modes are still well defined. In order to see what is going on we have to ask a question which is more sophisticated than (4.95): knowing the position of an atom at some particular position R_0, what is the uncertainty in the position of an atom L

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[14] It is actually a border line case: at moderate pressures it crystallizes again.

lattice sites away? Defining $l = La$, we have to calculate

$$\begin{aligned} \langle [u(l) - u(0)]^2 \rangle &= \langle (\Delta u(l))^2 \rangle \\ &= \int_{-\pi/a}^{\pi/a} dk (1 - \cos(kl)) \langle |Q(k)Q(-k)| \rangle \end{aligned} \tag{4.106}$$

The expectation value in the second line we have seen before, (4.95),

$$\langle (\Delta u(l))^2 \rangle = \frac{\hbar}{\pi M c} \int_0^{\pi/a} dk \frac{(1 - \cos(kl))}{k} (1 + 2n_B(\beta\omega_k)) \tag{4.107}$$

This looks similar to (4.95) except for the factor $1 - cos(kl)$, complicating the integral. What this does is to limit the allowed k values to those which are smaller than π/l - modes with a wavelength larger than l cannot contribute to the uncertainty (4.107). Hence, the cosine can be dropped, if one starts integrating at $k_{min} = \pi/l$,

$$\begin{aligned} \langle (\Delta u(l))^2 \rangle &= a^2 \mu \int_{\pi/l}^{\pi/a} \frac{dk}{k} \\ &= a^2 \mu \ln(\frac{l}{a}) \end{aligned} \tag{4.108}$$

This gives away the story: everytime the length scale is increased by an order of magnitude, the relative position uncertainty increases by a factor of two, as indicated in figure 4.5.

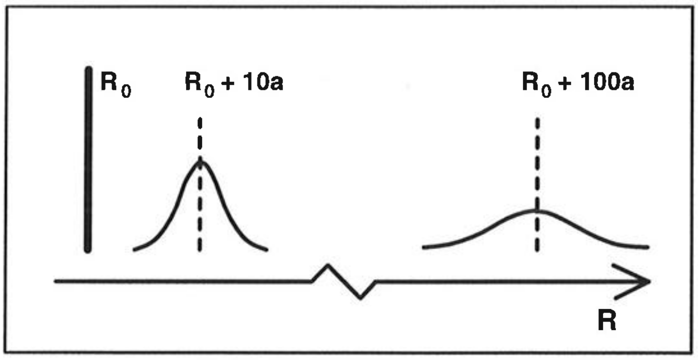

Figure 4.5: *in the floating solid, the uncertainty in the spatial position of atoms relative to some reference position doubles, everytime that the length scale is increased by an order of magnitude.*

In the higher dimensional worlds, we are used to the idea that quantum-fluctuations (think Heisenberg uncertainty relations) grow in magnitude if the spatial size of the system is *decreased*. In the one dimensional world it is opposite: starting with a fairly classical behavior on small length scales, the quantum fluctuations become more and more important if the size of the system *increases*! Hence, the quantum fluctuations dominate in the macroscopic realms. This is actually nothing else than the familiar phenomenon that rare fluctuations eventually dominate in one dimensional systems. Even cars on motorways are subject to this phenomenon. Imagine dense traffic on a one lane road. Clearly, the speed of all cars will be set by the speed of the slowest driver. By theorem, if the road is infinitely long, there will be always at least one car moving at a speed of 0 mph (the rare fluctuation), and therefore the whole system of cars comes to a standstill. Clearly, this will not happen on a motorway with an infinity of parallel lanes ($d = 2$), let alone it will happen with airplanes ($d = 3$).

It is not straightforward to observe these one dimensional crystalline floating solids. It is not an easy task to fabricate a line of atoms, which does not know about the rest of the world[15]. In addition, the (stronger divergent) thermal fluctuations tend to take over already at very low temperatures because of the largeness of the atomic mass. In fact, for these reasons the quantum mechanical floating crystal has never been observed experimentally. However, although the phenomenon is tied to classical condensation, it is not at all special to the crystalline state. As is everything in this chapter, this phenomenon is of a far greater generality. Floating quantum solids are formed (and observed) in one dimensional spin systems. They are especially important in one dimensional metals. The so-called Luttinger liquids, realized in the $d = 1$ electron systems, are best understood to correspond with quantum floating solids, build from the Fermi-liquid condensate - see chapter VII.

4.7 Excercises

4.1 It will be shown in chapter VI that the superfluid state of ^4He is characterized by a finite overlap with the free boson ground state $|0\rangle_B = \Pi_{i=1}^N b^\dagger_{\vec{k}=0}|vac\rangle$, where $b^\dagger_{\vec{k}}$ creates bosons in plane wave states. Expand the position states (4.3) in plane waves and derive the N (number of particles) dependence of the overlap of the free boson state with the classical part of the wavefunction of a ^4He crystal.

4.2 Show that the matrix of force constants has the following general properties:

(a) The matrix elements only dependent on the interatomic separations (translational symmetry):

$$V_{n\alpha n'\beta} = V_{\alpha\beta}(\vec{R}^0_n - \vec{R}^0_{n'}) \quad . \tag{4.109}$$

(b) The matrix is real and symmetric (order of taking derivatives !).

(c) The matrix V is non-negative.

(d) Given that the Bravais lattice is symmetric under inversion, $V_{\alpha\beta}(\vec{R}^0_n - \vec{R}^0_{n'}) = V_{\alpha\beta}(\vec{R}^0_{n'} - \vec{R}^0_n)$.

4.3 Proof (4.32a,4.32b,4.32c).

4.4 Proof (4.37).

4.5 Derive (4.38).

4.6 Derive (4.39).

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[15] For an ingenious example, and further theoretical analysis, see V. J. Emery and J. D. Axe, Phys. Rev. Lett. **40**, 1507 (1978).

4.7 Consider a linear chain of ions with alternating masses (M_1 and M_2) and alternating force constants K and G living on the bonds between the ions: $\cdots M_1 \; -(K)- \; M_2 \; -(G)- \; M_1 \; -(K)- \; M_2 \; -(G)-\cdots$. Apply periodic boundary conditions and calculate the normal modes and their spectrum. Discuss the following issues for the following cases: (i) $M_1 = M_2$ and $K = G$. (ii) $M_1 \neq M_2$ and $K = G$. (iii) $M_1 = M_2$ and $K \neq G$. (iv) $M_1 \neq M_2$ and $K \neq G$.

a The form of the dispersion relations.

b The nature of the modes at $k \to 0$.

c The nature of the modes at the zone boundary, $k \to \pi/a$ (a lattice constant).

4.8 Check the commutation relations (4.52), starting from (4.48).

4.9 a Sketch the phonon density of states (DOS) of the chain model of excercise 4.7 for $M_1 \neq M_2$ or $K \neq G$.

b The 'van Hove' singularities in the $d = 1$ densities of states are due the disappearance of the derivative of $\omega(\vec{k})$ at high symmetry points. Are these singularities also found in $d = 3$?

4.10 Calculate the specific heat of the lattice in the Debye model for $d = 1, 2, 3$. How does the dimensionality influence the temperature dependence in arbitrairy dimensions?

4.11 Show that the T^3 law for the specific heat, as found from the Debye model, holds as well for the general case (4.47) in the low temperature limit. Express the specific heat in the angle-average of the sound velocity.

4.12 It is instructive to consider the perturbative corrections coming from anharmonicity on the single oscillator level. The relevant perturbation theory can be found in "Inleiding in de Quantummechanica II" by R.H. Terwiel.

a Consider the perturbation $\lambda H_1 = \lambda q^4$ on a single oscillator $H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2$. Calculate the energy levels up to first order. Are they still equidistant?

b Why does a cubic term q^3 not alter the level splittings?

c Calculate the second order corrections to the energies both for a q^3 and q^4 potential.

d Calculate the states themselves up to first order in a αq^3. Determine the expectation value of the observable q in the n-th level. Hint: take only the terms which are linear in α. Use these findings to argue that the crystal will tend to expand if temperature increases.

4.13 Derive (4.67-4.68). Point out why $k, k', k'' \to k, q, K$. What is the reason that the terms containing only a single boson operator can be neglected?

4.14 Consider H_4 and derive the dependence of the decay rate on momentum in the long wavelength limit due to this term. Consider only the processes where the phonon decays in three other phonons.

4.15 Derive an expression for M in (4.76).

4.16 By definition, the electron-density operator in real space is given by $\rho(\vec{r}) = \sum_i \delta(\vec{r}-\vec{r}_i)$ ($\vec{r}_i$ is the position of electron i). Show that $\rho(\vec{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\vec{q}} \rho_{\vec{q}} \exp(i\vec{q}\cdot \vec{r})$ with $\rho_{\vec{q}}$ given by (4.78), with the fermion operators creating fermions in plane wave states.

4.17 Consider a chain of atoms with one electron orbital per site and nearest-neighbour hoppings. The system of atoms is described by the balls and springs of (4.21-4.25). The atoms and electrons are coupled by the Peierls coupling (refph85). Derive the Hamiltonian in terms of electronic Bloch states and phonons, including an explicit expression for the momentum and phonon-frequency dependent electron-phonon interaction 'vertex'. This is the so-called Su-Schrieffer-Heeger (or SSH) model, which plays a central role in polymer physics.

4.18 Consider the following 'displaced oscillator' problem (q and p are position and momentum, respectively): $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 + \alpha q$.

   a. Derive and solve the classical equation of motions. Explain the solution.

   b. Solve the quantum-problem. Hint: rewrite the Hamiltonian in terms of boson operators and try the 'shifted boson' transformation $\tilde{a}^\dagger = a^\dagger + constant$.

4.19 Proof (4.85-4.87).

4.20 Derive (4.91) and (4.92): use (4.87) to derive the new fermions and bosons (4.89) and use subsequently (4.86) to find the Hamiltonian in the new operators. Discuss the nature of the new boson/fermion Fock space.

4.21 Derive (4.94). Hint: use the relation $e^A e^B = e^{A+B+\frac{1}{2}[A,B]}$ and realize that $|0\rangle$ contains a fixed occupancy of phonons which does not change during the hop.

4.22 Check that (4.97) follows from (4.96): check the action of the different operators appearing on the left hand side of (4.97) on the states (4.96).

4.23 Derive (4.103) and (4.105) from (4.99,4.101). Hint: in the Debye model $N = k_D^3/(6\pi^2) = 3/(4\pi a^3)$ ($a =$ roosterconstante).

4.24 In this excercise the quantum-fluctuation (4.105) is estimated for noble gas crystals. The interaction between noble gas atoms is well described by the Lennard-Jones potential (van der Waals + hard core): $V(r) =$

$4\epsilon\left[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}\right]$. For He this potential is:

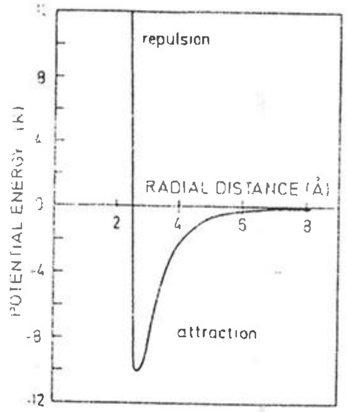

Figure 2.4 Interaction potential of two ^{4}He atoms as a function of separation.

a. The crystal potential is well approximated by a sum of pair potentials. Show that the sound velocity can be estimated by $c \simeq \sqrt{2U/M}$, where U is the minimum of the Lennard-Jones potential.

b. Show that $\gamma \simeq 1.1\hbar/(a\sqrt{MU})$. How large is $\sqrt{\gamma}$ for ^4He ?

c. Assume that the lattice constant does not change. Calculate the γ's for the other noble gasses using the Lennard-Jones parameters:

	Ne	Ar	Kr	Xe
ε (eV)	0.0031	0.0104	0.0140	0.0200
$\sigma(A)$	2.74	3.40	3.65	3.98

5 Strongly correlated electrons: Magnetism.

Electron systems, as they occur in crystals, form a more interesting environment to study quantum many body theory than the atomic systems of the previous chapter. The difference between atoms and electrons is in first instance quantitative. The mass of an electron is a factor 100000 or so smaller than the mass of a typical atom - as a consequence, the electrons are subject to severe quantum fluctuations on length scales of Angstroms. This prohibits the formation of electron crystals - there are examples of real space orderings of electrons but these are always accompanied by lattice deformations[1]. Instead, other condensates are found in electron systems. In this chapter we will focus on the *spin* systems. The reasons to start here are twofold: spin systems occur in nature in both the real space condensation and momentum space condensation varieties. The first one is conceptually close to the crystalline condensation of the previous chapter, while momentum space condensation (underlying superconductivity/superfluidity and the Fermi-liquids) is harder to grasp. A main purpose of this chapter will be to clarify how the first can be continued in the second (sections 2.5 and 2.6). A second reason to study spin systems first is that they form a relatively benign mathematical environment to study matters of principle. In the sections 2.3 and 2.4, dealing with the Néel (antiferromagnetic) state, we will do some deep probing into the dark corners of the classical state. Before we turn to the spin systems, we first have to learn how electrons can be forced to behave as spins. What is needed is strong repulsive interactions, high density and a crystal potential, as will be explained in the first two sections.

5.1 Electron correlations.

In the previous two chapters we have been confronted with two viewpoints which seem mutually exclusive. In the chapter on band structure, we boldly neglected the electron-electron interactions and let the static lattice potentials and the electron kinetic energy do their work. The outcome was the band picture, completely dominated by the effects of kinetic energy. In the study of the crystalline state, we found a complete domination of the *interactions*, while the quantum kinetic energy played a minor role. A focus point of modern condensed matter physics is the study of systems where neither of these two pictures apply. This discipline is called 'electron correlations' or 'correlated fermions'.

Correlation means in this context that a particle can only move if its motion is synchronized with the motions of other particles. This is naturally found in situations where the interactions dominate. The crystalline condensate is an extreme example: a single atom in the crystal can only freely move if all 10^{23} particles move with it in the same direction - the property of rigidity. These correlated motions are also common in classical fluids. Consider for instance liquid ^3He at a temperature of a view Kelvins. Quantum effects can be neglected and it can be looked at as a

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[1] A candidate for a proper electron crystal could be the Wigner crystal, conjectured to exist in two dimensional electron gasses. Research is still in progress.

simple, classical hard sphere fluid. Although the rigidity property got lost in the fluid, locally the fluid looks still quite similar to a close packed arrangement of hard spheres. Clearly, in order for a He-atom to move, a neighbour has to get out of its way which is only possible if this neighbour has found a place to go, etcetera. This represents a very complicated problem and even this simplests of classical fluids has escaped a rigorous treatment up to now: the understanding of the hard sphere fluid relies heavily on results of numerical simulations.

Quantum-mechanics should complicate matters further. What happens if ^3He is cooled down? Miraculously, a state is realized which is quite similar to that of electrons in a free electron metal: it seems as if the He atoms forgot about their hard cores and instead they only know from each other existence via the Pauli-principle. This low temperature Fermi-liquid state is in fact better understood than the classical liquid (chapter VII). The problem is, however, to understand what is happening in the regime in between the Fermi-liquid and the high temperature classical liquid at intermediate temperatures. Such a situation is quite commonly found also in other (mostly electron[2]) systems and the truth of the matter is that very little is understood - this is the problem of correlated fermions.

Turning to electron systems in crystals, the problem is further complicated by the loss of full translational invariance: the electrons also feel the periodic potential of the ions. In most cases this is a curse, but sometimes it is a blessing: under the special condition of charge commensuration one finds that at low energies only the spins of the electrons matter. Charge commensuration means that there is an integer number of valence electrons per unit cell of the lattice.

The interactions between electrons in the vacuum or in a weak potential are of the Coulomb type and, as will be explained in chapter VII, these favour the Fermi-liquid state at the electron densities found in most solids[3]. However, this changes drastically if the lattice potential becomes strong. One has now to calculate the matrix elements of the Coulomb interactions between electrons in atomic-like wave functions. Because the charge distributions of the valence electrons are rather localized in the vicinity of the atomic cores, the short range part of the effective interactions is strongly amplified, compared to the bare Coulomb potential. This can be easily seen by approaching the problem from the atomic side. We consider well-localized tight binding electrons, with a bandwidth $W = 2zt$ (section 3.3). Assume one orbital per atom and consider the charge commensurate case: the number of electrons per atom $n_e = N_e/N$ is an integer. As a reference, we take $t = 0$ (classical limit) and put n_e electrons on every atom. For finite t, the electrons want to delocalize. In the figure is indicated what happens if one electron hops to another atom,

After the hop (Fig. 5.1 b) a state is reached, where one atom has one electron more ($n_e + 1$) and one atom has one electron less ($n_e - 1$). Because of the atomic character

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[2] For instance, the heavy fermion- and mixed valence systems, high T_c superconductors and other doped Mott-Hubbard insulators, organic metals.

[3] The only well established exception is the fractional quantum Hall state found in the low density two dimensional electron gas in a magnetic field.

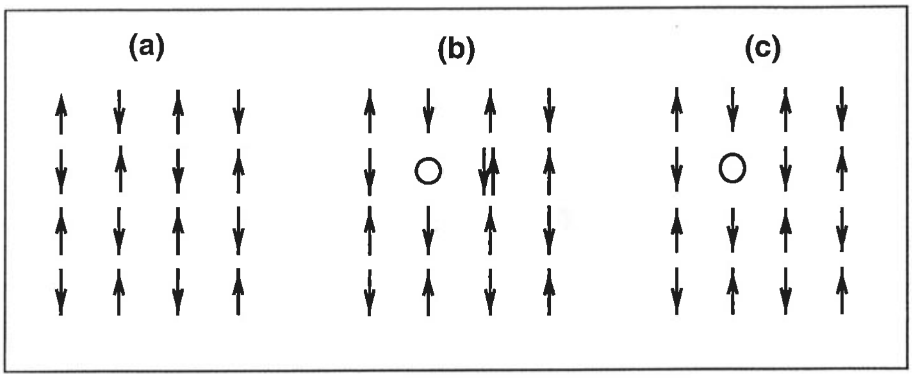

Figure 5.1: *(a) The classical state for $t = 0$ for a single band problem with one electron per site. (b) The hopping of an electron produces an unoccupied- and a doubly occupied site. This costs a large electrostatic energy (U) because the electrons on the doubly occupied site are close together. When $U > W$ this prohibits the delocalization of electrons. (c) Away from charge commensuration, hops occur which do not cause double occupancy. Indicated is a single hole which can move relatively freely.*

of the wave functions, the hopping process has caused a piling up of charge and this costs an electrostatic energy,

$$U = E_{\text{at}}^{n_e+1} + E_{\text{at}}^{n_e-1} - 2E_{\text{at}}^{n_e} \tag{5.1}$$

This quantity can be estimated from ionization- and electron affinity energies of isolated atoms. Especially for $d-$ and $f-$ electrons the atomic U's are quite large (15–30 eV). As long as $U >> W$ (bandwidth), *the kinetic energy cannot overcome the interaction energy, and the electrons are localized on the atoms.* Because the electrons cannot move, the whole system is an electronic insulator: the 'Mott-Hubbard' insulator. What is the difference with the band insulators of chapter III? A necessary condition to find an insulating state in a non-interacting system is the presence of an *even* number of electrons per unit cell. The Mott-Hubbard insulators occur for an *integer* number of electrons, also in the case that the number of electrons is *uneven.* When independent electron theory would indicate a band insulator, the effects of the interactions are in first instance quantitative: the neglect of the U's will lead to an underestimation of the gap[4]. However, if independent electron theory would indicate a metal because the number of electrons per unit cell is uneven, the interactions would cause an insulating state which is qualitatively different from the band insulator. In this case, one ends up with a *spin system* at low energies. For instance, in figure (5.1) we consider a single band system with $n_e = 1$. Every electron has to stay 'at home' on its particular site and therefore it cannot pair up its spin with the spins of the other electrons, as would happen in the metal. In the classical limit ($t = 0$), we would deal with a system of non-interacting spins - although the charge of the

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[4] This is a well known flaw of LDA-band structure theory. Even in weakly correlated systems like silicon, the band gap is underestimated by a factor of two. Although the qualitative origin of this effect can be understood from the simple Mott-Hubbard perspective, one needs at least the GW method as explained in chapter VII to arrive at reliable quantitatie estimates for the gap magnitudes.

electron is localized, its spin is still free to point in all possible directions. It will be shown in the next section that for finite t the spins start to interact because of virtual fluctuations, involving states like the one in Fig. 5.1b. This is the simplest way to undress the electron from its charge such that only its spin remains.

In the above we have considered a limiting case, which is realistic only if the atoms are very far apart. How does this work in real solids? When the atoms are brought closer together, we learned that the t's and thereby the bandwidth increases. At the same time, the system becomes a better dielectric and this leads to a reduction (screening) of the bare atomic Coulomb interactions. Hence, W is increasing and U is decreasing. To give some feeling, in real magnetic insulators the screened U's are typically of order 5-10 eV, while the bandwidths are in the range $1 - 5$ eV. Typical examples are the 3d and 4f salts like NiO and Ce_2O_3. When $W \simeq U$, the above arguments no longer apply and a transition occurs to a metallic state. A typical example is V_2O_3 which is a Mott-Hubbard insulator at ambient pressure, undergoing a transition into a metallic state under pressure: pressure decreases the lattice constant.

Next to the U/W ratio, one can also try to control the electron density. For instance, the Mott-Hubbard insulator can be doped in the same way as normal semiconductors are doped. Extra holes or electrons are introduced and these can hop around without causing double occupancy: these holes/electrons can delocalize (figure 5.1c). This is actually a basic aspect of the physics of the high T_c superconductors. It was already announced in chapter III that band structure theory fails in describing a 'parent' material like La_2CuO_4. The reason is that the electrons in the CuO_2 layers are in a Mott-Hubbard insulating state. These parent insulators are doped (for instance, by substituting Sr^{2+} for La^{3+} in the inert layers), introducing holes in the CuO_2 planes. These holes can now hop around without causing double occupancy. This turns these insulators in metals which superconduct at 'high' ($\simeq$ 100K) temperatures. It is widely believed that the physics of the metallic and superconducting state lies outside the scope of the conventional paradigm which is the subject of these lectures - it represents the most urgent problem in contemporary quantum condensed matter physics.

Anoher way to fight the charge commensuration is by involving more bands. The tightly-bound d and f electrons typically satisfy the Mott-Hubbard criterium of large U's and small bandwidths, while the more extended s/p (nearly free) electrons are in the small U/W limit. Because the latter electrons have large bandwidths, it happens quite often that both the f/d and the s/p bands are partly filled,

This causes a non-integer occupancy of the d or f states. For instance, in figure 5.2 the density of states of a metal like Ni is indicated. The electronic configuration of a Ni atom is $3d)^9 4s)^1$. Because the s band crosses E_F in Ni metal, the local electron distribution becomes more like $3d)^{9.4} 4s)^{0.6}$. Accordingly, there are many free holes (fig. 5.1c). The d-electrons can therefore easily delocalize and one finds an itinerant ferromagnet instead of a Mott-Hubbard insulator. One can push this to extremes. In many rare-earth and actinide materials it appears possible to tune the f-occupancy very close to a charge commensuration point while there are still other

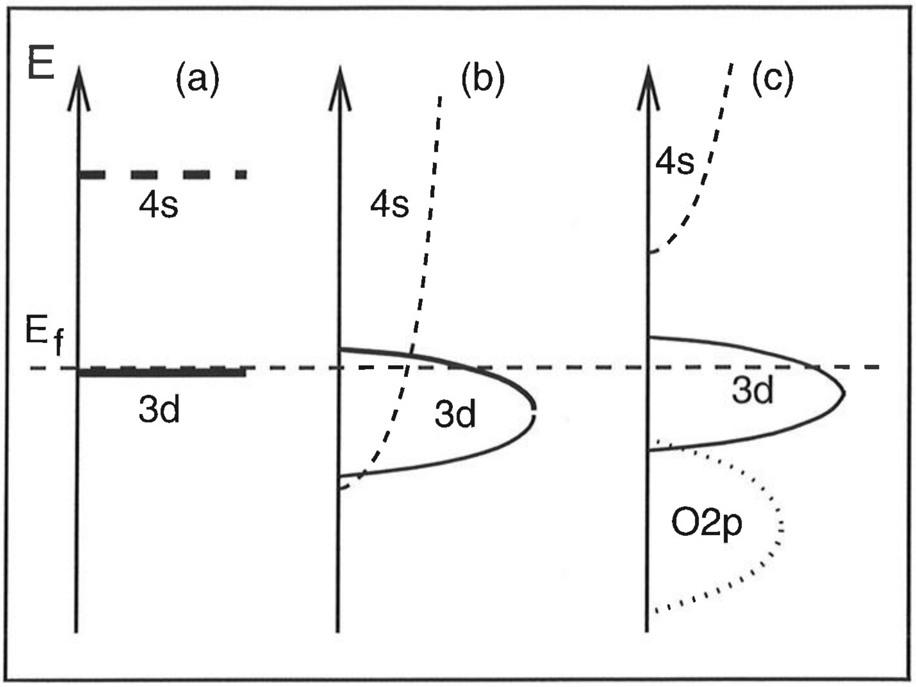

Figure 5.2: *Schematized band structure density of states of (a) an isolated Ni atom, (b) metallic Ni: both the 3d bands and the s/p nearly free electron band are partly filled, (c) the Mott-Hubbard insulator NiO; the 4s electrons are pushed away from the Fermi-energy by the presence of the electronegative counter-ion.*

bands at E_F. Under these conditions one finds the phenomenon of heavy fermions. At low temperatures, a Fermi-liquid state (chapter VII) is realized, characterized by quasiparticles with a mass exceeding 1000 electron masses!

The phenomena occurring in the 'strongly correlated metallic state', as I just summarized, are poorly understood and are still subject to a large scale research effort. There is only one subject which is very well understood: the Mott-Hubbard insulating state itself. Where are these insulators found in nature? One has to avoid the uncorrelated electrons of figure 5.2, so that only the correlated electrons are found near E_F. To get rid of these uncorrelated electrons one needs electronegative counter ions like O, F, Cl: Mott-Hubbard insulators are typically found in ionic substances like oxides, fluorides etcetera. For instance, consider the $3d$ oxides (CuO, NiO, Fe_2O_3 (rust), etcetera). Take ZnO as a reference : in this material the $3d$-band is just filled and this is a band insulator with a filled O $2p$ valence band (O^{2-}) and an empty Zn $4s$ conduction band, separated by a large band gap $\sim$ 10 eV. In Cu there is one more hole on the metal ion and this is accomodated in the $3d$ band, which becomes partly filled $(3d)^9$ (Figure 5.2c). There is precisely one $3d$ hole per Cu atom (charge commensuration) and because of the large effective interactions, these holes become localized[5]. Going further to the left in the 3d series, the d-band is gradually emptied

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[5] In La_2CuO_4, the orbital character of these localized holes is $x^2 - y^2$ - band structure theory predicted this aspect correctly (chapter III). It turns out that in cuprates the occupied $O2p$ states lie closer to E_F than the doubly occupied $3d$ states. Accordingly, the low lying valence band states

untill one arrives at CaO which is again a band insulator. All monoxides involving transition metal ions are Mott-Hubbard insulators.

5.2 Strong coupling: Mott-Hubbard insulators.

In the previous section I already hinted at a remarkable phenomenon occurring in the Mott-Hubbard insulators: starting out with strongly interacting electrons at high energies one ends up in a low energy universe where only the spin degrees of freedom of the electrons have survived. In this section I will present the rigorous way to transform electrons into spins by a 'projective renormalization'. The basic idea is, that we can use the presence of an energy scale (U) to renormalize away (or 'integrate out') the electrons in a controlled manner by perturbation theory. This 'canonical perturbation theory' is similar to the canonical transformation, introduced in the context of polaron physics (section 4.5).

With the principle of adiabatic continuity in mind, we should invent the simplest possible high energy model, fulfilling the basic requirements of symmetry and dimensionality of Hilbert space. For the Mott-Hubbard insulator these are: (i) fermions carrying spins, (ii) charge commensuration, (iii) strong local interactions. These requirements can be fulfilled by the so-called (single band) Hubbard model,

$$H = -t \sum_{\vec{i},\vec{\delta},\sigma} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} + U \sum_{\vec{i}} n_{\vec{i}\uparrow} n_{\vec{i}\downarrow}, \tag{5.2}$$

$c^{\dagger}_{\vec{i}\sigma}(c_{\vec{i}\sigma})$ creates (annihilates) an electron with spin $\sigma(=\{\uparrow,\downarrow\})$ on a lattice site $\vec{i}$, and $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. This is nothing else than the single band tight-binding model (3.39), augmented with an interaction term of the form discussed in the previous section: it costs an energy U to put two electrons on the same site. When $U = 0$ it is trivial to solve (5.2): according to the discussion in section 3.3, we solve the problem for one particle: $c^{\dagger}_{\vec{k}\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{i}} e^{i\vec{k}\cdot\vec{i}} c^{\dagger}_{\vec{i}\sigma}$ and the many electron states are of the form $|0\rangle = \Pi^{k_F}_{\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma} |vac.\rangle$. These are, however, not eigenstates of the interaction term and if $U \gtrsim W$, while the electron density is high, it is even not a good idea to use $|0\rangle$ as a zero-th order in a perturbation theory. Here we will consider the opposite limit: the interaction U is very large compared to the bandwidth W: 'strong coupling'. We do so because the problem is easier to understand in this limit. In section 5.4 it will be explained how the results derived here are continued into the more complex intermediate and weak coupling regimes. When the interactions dominate, the Hilbert space is organized in a different way than is the case in the non-interacting problem. U acts in real space, and it is instructive to choose a basis in terms of real space electron configurations ('configuration space'): all possible ways to distribute N_e electrons over N sites with the constraint that a single site is at most occupied by a pair of electrons with opposite spins. A basis is choosen such that every state

---

have a predominant O $2p$ character while the conduction band is $3d$ like. These insulators are called 'charge transfer insulators'.

in Hilbert space corresponds with one particular state in configuration space. For example, ($\uparrow\sim$ spin up, $\downarrow\sim$ spin down, $0\sim$ empty site, $\uparrow\downarrow\sim$ doubly occupied site),

$$\begin{aligned} |l\rangle &= |\ldots \uparrow_{i-1}\downarrow_i 0_{i+1}\ldots\rangle \\ &= \ldots c^\dagger_{i-1\uparrow}c^\dagger_{i\downarrow}\ldots|vac.\rangle \qquad (5.3)\\ |l'\rangle &= |\ldots \uparrow\downarrow_{i-1} 0_i 0_{i+1}\ldots\rangle \\ &= \ldots c^\dagger_{i-1\uparrow}c^\dagger_{i-1\downarrow}\ldots|vac.\rangle \qquad (5.4)\end{aligned}$$

⇒ Excercise 5.1

To get some feeling, let us consider the interacting version of the two level model for the hydrogen molecule of section 2.3. The two site version of the Hubbard model is actually quite a good model for real H_2,

$$H = -t\sum_\sigma (c^\dagger_{1\sigma}c_{2\sigma} + c^\dagger_{2\sigma}c_{1\sigma}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}) \qquad (5.5)$$

Let us first attempt to solve this in terms of the wavefunctions of the non interacting problem. The hopping term is diagonalized and bonding- ($b^\dagger_\sigma$, at -t) and antibonding states ($a^\dagger_\sigma$, at $+t$) are found,

$$\begin{aligned} b^\dagger_\sigma &= \frac{1}{\sqrt{2}}(c^\dagger_{1\sigma} + c^\dagger_{2\sigma}) \qquad (5.6)\\ a^\dagger_\sigma &= \frac{1}{\sqrt{2}}(c^\dagger_{1\sigma} - c^\dagger_{2\sigma}) \qquad (5.7)\end{aligned}$$

In the presence of one electron, the ground state is $|0; N=1\rangle = b^\dagger_\sigma|vac\rangle$. Consider now two electrons. We studied this already for $U=0$ (section 2.3),

$$\begin{aligned} |0; N=2\rangle &= b^\dagger_\uparrow b^\dagger_\downarrow|vac\rangle \qquad (5.8)\\ &= \frac{1}{2}(c^\dagger_{1\uparrow}c^\dagger_{1\downarrow} + c^\dagger_{2\uparrow}c^\dagger_{2\downarrow} + c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} + c^\dagger_{2\uparrow}c^\dagger_{1\downarrow})|vac\rangle \qquad (5.9)\end{aligned}$$

In the second line, the wave function is written explicitely in real space configurations. We find that the choice of single particle 'momentum' eigenstates (5.8) implies that the 'singly occupied' configurations $\sim c^\dagger_1 c^\dagger_2|vac\rangle$ carry exactly the same weight in the wave function as the 'doubly occupied' configurations $c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}|vac\rangle$ $(i=1,2)$. Obviously, if $U \neq 0$ the latter are energetically unfavourable and their relative weight in the ground state wave function has to decrease.

It is simple to solve the 'Hubbard hydrogen molecule' exactly.

⇒ Excercise 5.2

For large U/t the ground state is found to be,

$$|0; N=2\rangle = \frac{1}{\sqrt{2(1+4t^2/U^2)}}[(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} - c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}) + \frac{2t}{U}(c^\dagger_{1\uparrow}c^\dagger_{1\downarrow} + c^\dagger_{2\uparrow}c^\dagger_{2\downarrow})]|vac\rangle \quad (5.10)$$

In this limit, the singly occupied configurations are dominating in the ground state. The admixture of doubly occupied states becomes very small if $U >> t$. This means that electron 1 is always at site 1 while electron 2 is at site 2, while the remaining fluctuations are of the virtual kind: one of the electrons can make a detour to the other atom as long as it does not leave its 'home' atom for a time longer than $\sim 1/U$.

In the excercise (5.2) another low lying eigenstate is found

$$|T; N = 2\rangle = \frac{1}{\sqrt{2}}(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} + c^\dagger_{1\downarrow}c^\dagger_{2\uparrow})|vac\rangle \tag{5.11}$$

which costs only an excitation energy $\sim\ 2t^2/U$, while all other excitations cost an energy $\sim U$. (5.10) is clearly a spin-singlet state, while (5.11) is a triplet: the low energy solutions of the electronic problem (5.5) look like spin wavefunctions. This is no accident, as will soon be demonstrated.

$\Rightarrow$ Excercise 5.3

The size of the Hilbert space increases very rapidly if the number of sites increases. For instance, the largest Hubbard systems which can be exactly diagonalized with state of the art supercomputers have 20 sites and 20 electrons. It is nevertheless possible to use the largeness of U to simplify the problem considerably by integrating out doubly occupied configurations perturbatively. This results in the so-called $t-J$ model which is still unsolvable, except at the charge commensuration point $N_e = N$ where it reduces to a spin-only Heisenberg model.

(t/U) is the small parameter, and in the same spirit as in chapter 4 we first consider the (classical) limit where the interactions dominate: $U/t \longrightarrow \infty$. In this limit, the total Hilbert space is split up in sectors characterized by the total number of doubly occupied sites. These 'Hubbard' sectors are separated from each other by large gaps $\sim U$ (figure 5.3).

Let us specialize on the case that $N_e \leq N$. The sector with the lowest energy is the one containing configurations of only empty and singly occupied sites, and doubly occupied sites are *excluded.* The next sector (at energy U) contains all configurations with a single doubly occupied site somewhere in space. N_e is kept fixed and therefore an extra empty site is found somewhere else. In this way we continue, building up Hilbert space: at $2U$ there is a sector with two doubly occupied sites, at $3U$ a sector with three doubly occupied sites, and so on. The key observation is that the low lying sectors remain well separated from each other for finite t, as long as t/U is a small number. Quantum-mechanics does make a difference: for $t = 0$, the states within a Hubbard sector are degenerate. This classical degeneracy is lifted by quantum mechanics ($t \neq 0$). As long as the sectors do not overlap, this problem can be treated perturbatively (perturbation theory cannot change the dimension of Hilbert space !). Although the 'intra-Hubbard sector' problem found in this way is still quite untrivial, its Hilbert space is dramatically smaller than the Hilbert space of the full electronic problem. At least at half-filling, the problem will be simplified to such an extent that it becomes tractable again.

Let us now formulate the perturbation theory. The Hamiltonian is divided in a zero-th order part describing the physics *within* a Hubbard sector (H_0), and a perturbation

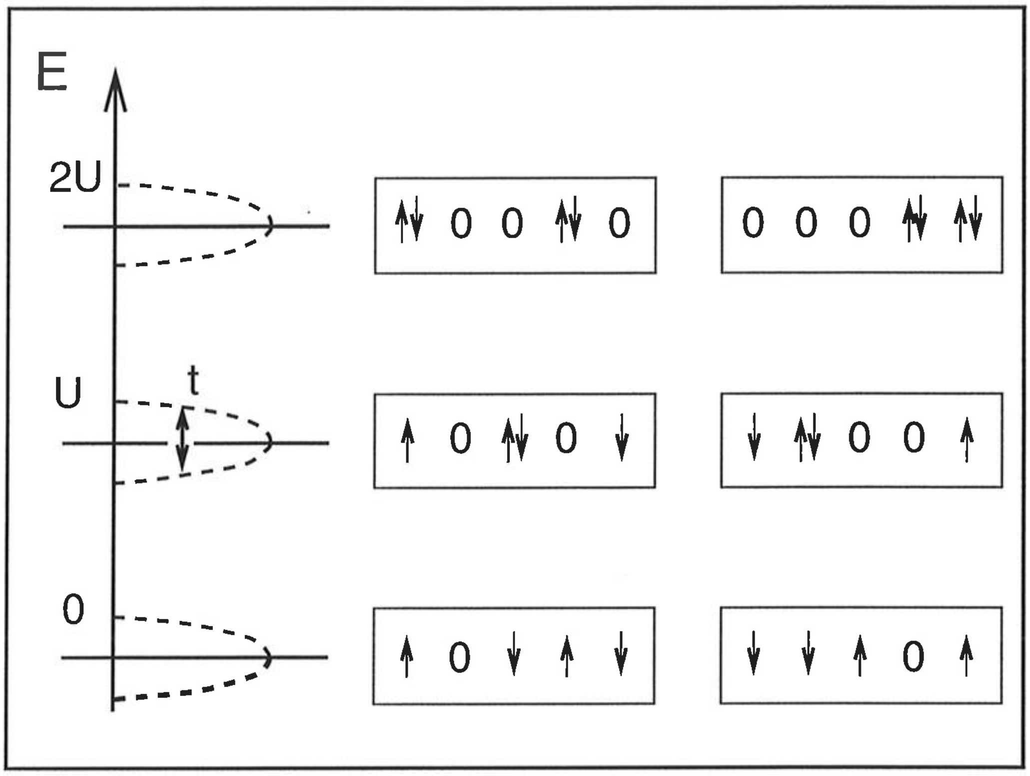

Figure 5.3: *When the atomic Coulomb interactions dominate, the Hilbert space splits in 'Hubbard sectors', characterized by an energy nU, where n is the number of doubly occupied sites. Some typical configurations are indicated in the figure as well.*

describing the fluctuations (H_1) *between* Hubbard sectors, (if $\sigma =\uparrow$, then $\bar{\sigma} =\downarrow$ and vice versa)

$$
\begin{aligned}
H &= H_0 + H_1 && (5.12)\\
H_0 &= V + T_0 \\
V &= U \sum_{\vec{i}} n_{\vec{i}\uparrow} n_{\vec{i}\downarrow} \\
T_0 &= -t \sum_{\vec{i},\vec{\delta},\sigma} \{(1 - n_{\vec{i}\bar{\sigma}}) c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} (1 - n_{\vec{i}+\vec{\delta}\bar{\sigma}}) + n_{\vec{i}\bar{\sigma}} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} n_{\vec{i}+\vec{\delta}\bar{\sigma}}\} && (5.13)
\end{aligned}
$$

and

$$
\begin{aligned}
H_1 &= T_+ + T_- && (5.14)\\
T_+ &= -t \sum_{\vec{i},\vec{\delta},\sigma} n_{\vec{i}\bar{\sigma}} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} (1 - n_{\vec{i}+\vec{\delta}\bar{\sigma}}) && (5.15)\\
T_- &= -t \sum_{\vec{i},\vec{\delta},\sigma} (1 - n_{\vec{i}\bar{\sigma}}) c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} n_{\vec{i}+\vec{\delta}\bar{\sigma}} && (5.16)
\end{aligned}
$$

⇒ Excercise 5.4

What do these expressions mean? The hopping term T_0, included in H_0, describes hopping processes within a Hubbard sector. For instance, $c_{\vec{i}+\vec{\delta}\sigma}(1 - n_{\vec{i}+\vec{\delta},\bar{\sigma}})$ means:

an electron with spin σ can only be annihilated at site $\vec{i}+\vec{\delta}$ if there is no electron with spin $\bar{\sigma}$ present on the same site. Otherwise, a doubly occupied state would be annihilated. In the same way, $(1-n_{\vec{i}\bar{\sigma}})\, c^{\dagger}_{\vec{i}\sigma}$ takes care that no doubly occupied state appears if the electron is created. The first term in T_0 describes therefore the exchange of an empty- and singly occupied site (figure 5.1c). The second term in T_0 describes the exchange of doubly- and singly occupied sites. All other hoppings change the number of doubly occupied sites, and these are collected in the perturbation H_1: T_+ adds a doubly occupied site and T_- removes a doubly occupied site.

⇒ Excercise 5.5

As in the case of the polaron (section 4.5), we again introduce a canonical transformation,

$$H_{\text{eff}} = e^S H e^{-S} \tag{5.17}$$

but now to construct a perturbation theory taking into account the effects of H_1. We assume that t/U is small, such that the corrections to H_0 are small. S has to be of order $0\left(\frac{t}{U}\right)$, and

$$e^S \simeq 1 + S + \frac{1}{2}\, S^2 + \dots \tag{5.18}$$

has to converge rapidly. Recall (4.89),

$$H_{\text{eff}} = H + [S,H] + \frac{1}{2}\, [S,[S,H]] + 0(S^3) \tag{5.19}$$

As in (4.91), the fermions transform 'with' the Hamiltonian

$$\tilde{c}^{\dagger}_{i\sigma} = e^S c^{\dagger}_{i\sigma} e^{-S} \tag{5.20}$$

acting on a transformed Fock space. For the case (5.12) - (5.16), H_{eff} is explicitely up to first order in t/U,

$$H^{(1)}_{\text{eff}} = H_0 + T_+ + T_- + [S^{(1)},H] + 0(S^2) \tag{5.21}$$

We demand that up to this order $H^{(1)}_{\text{eff}} = H_0$: with one hop (first order) we would leave the Hubbard sector under consideration. From this requirement the explicit form of S follows, up to first order,

$$T_+ + T_- = -[S^{(1)},H] \tag{5.22}$$

We assumed that S carries a small prefactor ($S^{(1)} \sim t/U$). Because $T_+ + T_-$ has a prefactor t, (5.22) has to be equal to

$$T_+ + T_- = -[S^{(1)},V] \tag{5.23}$$

This equation determines $S^{(1)}$, and all what remains is to 'pull' $S^{(1)}$ 'out of the commutator '. It follows,

$$S^{(1)} = \frac{1}{U}(T_+ - T_-) \tag{5.24}$$

⇒ Excercise 5.6

S is now determined up to first order in (t/U), but we still have to derive the transformed Hamiltonian. Because of (5.22) it is excluded that H_{eff} describes fluctuations between Hubbard sectors. Hence, the Hamiltonian has to be evaluated up to second order because one needs at least two hops, one to leave the Hubbard sector under consideration, and the other to return. For instance: $\uparrow_i \; \downarrow_{i+\delta} \xrightarrow{t} 0_i \; \uparrow\downarrow_{i+\delta} \xrightarrow{t} \uparrow_i \; \downarrow_{i+\delta}$. In analogy with Rayleigh-Schrödinger perturbation theory, one only needs S up to first order to obtain the Hamiltonian up to second order. Define

$$S^{(2)} = S^{(1)} + S' \tag{5.25}$$

with $S' \sim 0\left(\frac{t^2}{U^2}\right)$. (5.19) is expanded up to second order, using (5.25)

$$H^{(2)}_{\text{eff}} = H_0 + H'_{\text{eff}} + 0\left(\frac{t^3}{U^2}\right) \tag{5.26}$$

with the contributions $\sim t^2/U$ collected in,

$$H'_{\text{eff}} = [S^{(1)}, T^+ + T^-] + [S^{(1)}, T^0] + \frac{1}{2}[S^{(1)}, [S^{(1)}, V]] + [S', V] \tag{5.27}$$

using $[S', H] \to [S', V]$ such that $S' \sim (t/U)^2$ (compare (5.23))

This simplifies to

$$H'_{\text{eff}} = \frac{1}{U}[T^+, T^-] + [S^{(1)}, T^0] + [S', V] \tag{5.28}$$

⇒ Excercise 5.7

$H^{(2)}_{\text{eff}}$ should not contain terms describing fluctuations between Hubbard sector. The term $[T^+, T^-] = T^+T^- - T^-T^+$ is therefore allowed because these describe processes where the system always ends up in the same Hubbard sector where the fluctuation departed. On the other hand, $[S^{(1)}, T^0]$ causes transitions to the nearest-neighbour sectors which are not allowed in $H^{(2)}_{\text{eff}}$ and S' has to take care of this term. This implies that

$$[S^{(1)}, T^0] = -[S', V] \tag{5.29}$$

defining S' (compare (5.23)). We do not need S' explicitely to determine the Hamiltonian up to second order. Combining (5.26), (5.28) and (5.29) yields the result,

$$H^{(2)}_{\text{eff}} = T^0 + V + \frac{1}{U}[T^+, T^-] + O(\frac{t^3}{U^2}) \tag{5.30}$$

This expression describes the intra-Hubbard sector physics of all sectors. In first instance, we are interested in the lowest lying sector, containing the macroscopic, low energy properties of the system. T^+T^- drops out: T^- removes a doubly occupied state and in the '0' sector the number of doubly occupied sites is already as small as possible. Take $N_e \leq N$ ($N_e \geq N$ follows immediately from particle-hole conjugation), such that there are no doubly occupied sites present in '0'. (5.30) becomes for the lowest Hubbard sector in terms of the fermion operators,

$$\begin{aligned} H^{(2)}_{\text{eff}} &= -t \sum_{\vec{i},\vec{\delta},\sigma} (1 - n_{\vec{i}\bar{\sigma}}) c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} (1 - n_{\vec{i}+\vec{\delta}\bar{\sigma}}) \\ &\quad - \frac{J}{2} \sum_{\vec{i},\vec{\delta},\vec{\delta}',\sigma,\sigma'} (1 - n_{\vec{i}+\vec{\delta}'\bar{\sigma}'}) c^{\dagger}_{\vec{i}+\vec{\delta}'\sigma'} c_{\vec{i}\sigma'} n_{\vec{i}\bar{\sigma}'} n_{\vec{i}\bar{\sigma}} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} (1 - n_{\vec{i}+\vec{\delta}\bar{\sigma}}) \end{aligned} \tag{5.31}$$

$J = 2t^2/U$ is the energy scale associated with the virtual hopping fluctuations between Hubbard sectors and this quantity is called the 'superexchange interaction'. The problem (5.31) is known as the '(extended) $t - J$ model'.

⇒ Excercise 5.8

How to interpret (5.31)? Let us first consider the half-filled/charge commensurate point $N_e = N$: the lowest Hubbard sector corresponds with the configurations where every site is occupied by precisely one electron. The hopping term $\sim t$ in (5.31) vanishes: every single hop would cause a doubly occupied site (figure 5.1 b). For the same reason, one has to take $\vec{\delta} = \vec{\delta}'$ in the second term ($\sim J$), because the electron has to return on the site where it started to hop to avoid double occupancy. In the '0' sector the projections $\sim (1 - n_{i+\delta,\bar{\sigma}})$ are automatically satisfied and (5.1) simplifies at half-filling to,

$$H^{(2)}_{\text{eff}} = -\frac{J}{2} \sum_{\vec{i},\vec{\delta},\sigma,\sigma'} c^{\dagger}_{\vec{i}+\vec{\delta}\sigma'} c_{\vec{i}\sigma'} n_{\vec{i}\bar{\sigma}'} n_{\vec{i}\bar{\sigma}} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} \tag{5.32}$$

The creation and annihilation operators acting on the same site occur in this expression in pairs: *the electrons are localized and charge transport is not possible.* This is not surprising because we already observed that the electron had to return to the site where it started its hopping excursion, as a ramification of the Hilbert space projection. This is the mathematical version of the intuitive explanation of the Mott-Hubbard insulating state, as presented in the previous section. In addition, (5.32) describes a spin-only problem. Recall the definition of the $su(2)$ algebra for $S = 1/2$ in terms of fermion operators,

$$S^z_i = \frac{1}{2} \left(c^{\dagger}_{i\uparrow} c_{i\uparrow} - c^{\dagger}_{i\downarrow} c_{i\downarrow} \right) \tag{5.33}$$

$$S^+_i = c^{\dagger}_{i\uparrow} c_{i\downarrow} \tag{5.34}$$

$$S^-_i = c^{\dagger}_{i\downarrow} c_{i\uparrow} \tag{5.35}$$

We leave to the reader to show that (5.32) can be written as

$$H^{(2)}_{\text{eff}} = J \sum_{\vec{i},\vec{\delta}} \left(\vec{S}_{\vec{i}} \cdot \vec{S}_{\vec{i}+\vec{\delta}} - \frac{1}{4} \right) \tag{5.36}$$

$\Rightarrow$ Excercise 5.9

The above is a mathematically rigorous proof of the fact that at half-filling electrons (as objects carrying free spin *and* charge) no longer exist at energies $\ll U$. Instead, the system is described entirely in terms of the spins of the electrons. One should appreciate the radical changes which have occurred. For instance, the electrons at high energy are fermions while the low energy spins obey the $su(2)$ algebra, which describes neither fermions nor bosons. The statistics has changed! This finds its origin in the Hubbard projections which change completely the dimensionality of the Hilbert space associated with the low energy physics. At half-filling the Hilbert space of the non-interacting problem has a dimensionality $\sim (2N)!/(N!)^2$ (the number of ways to distribute N objects over 2N possibilities). After the Hubbard projection, the spin-degrees of freedom of the electrons are left and there are 'only' 2^N ways to distribute up- and down spins over N lattice sites.

According to (5.36), the virtual hopping fluctuations (the remainders of the kinetic energy) causes the spins to *interact*. These 'kinetic' spin-spin interactions are in fact easy to understand. Because we assumed U to be large, the hopping excursions have to be short ranged and we only have to consider nearest-neighbor sites. Let us consider two neighbouring sites occupied by electrons with anti-parallel spins. The hopping 'histories', bringing the system back to the '0' sector after two hops, are of the kind: $| \uparrow_i \downarrow_{i+\delta}\rangle \xrightarrow{t} |0_i \uparrow\downarrow_{i+\delta}\rangle \xrightarrow{t} | \downarrow_i \uparrow_{i+\delta}\rangle$. This yields a contribution $\sim (t^2/U)\ S_i^- S_{i+\delta}^+$ (compare with (5.34,5.35)). The *sign* of the spin-spin interaction can also be directly established. Because of the Pauli-principle, this second order fluctuation is *forbidden* if both spins are parallel ($| \uparrow_i \uparrow_{i+\delta}\rangle$) and the fluctuation leads of course to an energy gain. Therefore, the spin-spin interaction favours anti-parallel arrangements: an anti-ferromagnetic ($J > 0$) spin system is found. Notice that this kinetic exchange mechanism is quite different from the familiar Hund's rule exchange mechanism of atomic physics. The latter applies to strongly overlapping electrons: if the spins of the electrons are parallel, the Pauli principle causes them to stay further apart at average than would be the case for antiparallel spins (the exchange hole) which reduces the effective (repulsive) Coulomb interaction. This exchange mechanism tends to favour ferromagnetism. This is also relevant in condensed matter physics: in itinerant magnets the electrons are in extended, strongly overlapping states and nearly all metallic magnets are ferromagnets. In the magnetic insulators the electrons barely overlap and, with equally few exceptions, these are all antiferromagnets.

One reason to feel more comfortable with spin systems than with correlated electrons comes from the habit of spins to conform to the classical paradigm of section 1.2: spins freeze out in classical condensates with nearly the same ease as atoms. This tendency to form classical states should be understood to be a consequence of their relatively 'small' Hilbert space, which is rather sparsely connected: compared to a full electron problem there are far fewer states to go to, starting out with the wave function of the classical state. What happens if one dopes the Mott-Hubbard insulating state? This is described as well by the $t-J$ Hamiltonian (5.31) and we leave it to the reader to show that one finds hopping holes like the one in figure 5.1c, next to the interacting spins.

⇒ Excercise 5.10

When the density of free carriers increases, a dramatic increase of the quantum-fluctuations is found[6]. It is believed that any finite density of free carriers causes a melting of the classical spin state and what comes in its place is still a mystery[7].

⇒ Excercise 5.11

5.3 Classical spin condensation.

Compared to electrons, spins are relatively weakly fluctuating objects and they tend to form classical states: the ordered magnets. Despite their complicated algebra ($su(2)$), spin systems are much easier to understand theoretically than full electrons or full atoms. A first reason is that the simple Heisenberg Hamiltonian (5.36) is already quite realistic. Although it might be hard to calculate J numerically, symmetry demands that the operators are spin operators, while the largeness of the gap will take care of the local (nearest-neighbor) nature of the interaction. More importantly, spins are more easy to handle mathematically than fermions or bosons, because of the smallness of their Hilbert space. In this section we will force the spins in the paradigm of the classical state of section 1.2 and this will be a repetition of the first three sections of the previous chapter. Only at two instances magnets look different from crystals: (i) What to use for the $Y^\dagger$'s? (ii) How to discover harmonic oscillator bosons in a $su(2)$ algebra? These aspects will be heavily emphasized: everything else is just the same as in crystals, at least in antiferromagnets. Ferromagnets are special, as will be explained.

Generalized spin coherent states

In this section we will follow the pragmatic strategy which we learned to appreciate in the previous section: let us ask advice from mother nature regarding the answer, to work our way backwards by constructing the wave-function of the semi-classical state, subsequently studying the internal consistency of this state. The answer is well known from neutron scattering or magnetic force microscopy: condensates exists in spin systems, where every spin has turned into a magnetic dipole, indicated by an arrow pointing towards a particular direction in space, and these dipole moments

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[6] The case of a single free hole is quite well understood. Qualitatively, an analogue of the polaron of section 4.5 is formed, with the difference that the polarization cloud now corresponds with a *droplet of quantum spin liquid*, surrounding the hole. See E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).

[7] Already on the classical level, condensates are found which are far more complicated than antiferromagnets. It can be shown that in the classical spin limit, domain walls are spontaneously formed to which the carriers bind and these 'charged domain walls' form a regular pattern in space: the 'striped phase' (J. Zaanen and O. Gunnarsson, Phys. Rev. B **40**, 7391 (1989)). These striped phases have been observed recently in a variety of materials (e.g., J. M. Tranquada et al, Nature **375**, 561 (1995)) and current theoretical activity focusses on the hard task of developing the quantum theory of stripes.

form a pattern which is periodic in space and static in time. This has to be explained, starting from the quantum Hamiltonian (5.31),

$$\begin{aligned} H_{\text{spin}} &= J\sum_{\vec{i},\vec{\delta}} \vec{S}_{\vec{i}} \cdot \vec{S}_{\vec{i}+\vec{\delta}} \\ &= J\sum_{\vec{i},\vec{\delta}} \left(S^z_{\vec{i}} \cdot S^z_{\vec{i}+\vec{\delta}} + \frac{1}{2}(S^+_{\vec{i}} S^-_{\vec{i}+\vec{\delta}} + S^-_{\vec{i}} S^+_{\vec{i}+\vec{\delta}}) \right) \end{aligned} \tag{5.37}$$

where the S^α's obey a $su(2)$ Lie algebra,

$$\begin{aligned} \left[S^+_{\vec{i}},\, S^-_{\vec{j}}\right] &= 2S^z_{\vec{i}}\delta_{\vec{i},\vec{j}} \\ \left[S^z_{\vec{i}},\, S^+_{\vec{j}}\right] &= S^+_{\vec{i}}\delta_{\vec{i},\vec{j}} \\ \left[S^z_{\vec{i}},\, S^-_{\vec{j}}\right] &= -S^-_{\vec{i}}\delta_{\vec{i},\vec{j}} \end{aligned} \tag{5.38}$$

What is the connection between the classical arrows and this algebra? Clearly, this has to be related to a special kind of quantum-mechanical states of single spins which can take the role of the $Y^\dagger$'s in the construction of the classical state. Because of the complicated form of the algebra, these states are less simple than the Gaussian wave packets of the crystalline state. We need the 'spin-coherent states', which are defined for arbitrary total spin S (section 2.5) as[8]

$$|\hat{\Omega}\rangle = e^{-i\phi S^z} e^{i\theta S^y} |S, S\rangle \tag{5.39}$$

where $|S, S>$ is the maximum weight state, while $|\hat{\Omega}\rangle$ describes the coherent superposition of quantum mechanical spin states which is in fact the definition of the classical spin. The classical variables $\{\eta_i\}$ now describe an arrow pointing at a point on a sphere with diameter S, and

$$\hat{\Omega} = (sin\theta cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{5.40}$$

is the vector doing this, parametrized in terms of the two Euler angles θ and ϕ.

To see that the set of states (5.39) indeed relates to classical spins, let us consider the simple $S = 1/2$ case. As a first step, we express the eigenstates of S^y ($|\sigma\rangle_y$) in terms of the eigenstates of S_z,

$$\begin{aligned} |1/2, 1/2\rangle_y &= \frac{1}{\sqrt{2}}(|1/2, 1/2\rangle - i|1/2, -1/2\rangle) \\ |1/2, -1/2\rangle_y &= \frac{1}{\sqrt{2}}(|1/2, 1/2\rangle + i|1/2, -1/2\rangle) \end{aligned} \tag{5.41}$$

with $S^y|1/2, \pm 1/2\rangle_y = \pm 1/2|1/2, \pm 1/2\rangle_y$, and these are used to evaluate,

$$\begin{aligned} |\hat{\Omega}\rangle &= e^{-i\phi S^z} e^{i\theta S^y}|1/2, 1/2\rangle \\ &= e^{-i\phi S^z}\frac{1}{\sqrt{2}}\left(e^{\frac{i\theta}{2}}|1/2, 1/2\rangle_y + e^{\frac{-i\theta}{2}}|1/2, -1/2\rangle_y\right) \end{aligned}$$

---

[8] In the standard definition, an additional phase $e^{i\chi}$ is included, multiplying the state as a whole. This factor is inconsequential in the present context.

$$
\begin{aligned}
&= e^{-i\phi S^z}\left(\cos(\frac{\theta}{2})|1/2,1/2\rangle + \sin(\frac{\theta}{2})|1/2,-1/2\rangle\right) \\
&= e^{\frac{-i\phi}{2}}\cos(\frac{\theta}{2})|1/2,1/2\rangle + e^{\frac{i\phi}{2}}\sin(\frac{\theta}{2})|1/2,-1/2\rangle \qquad (5.42)
\end{aligned}
$$

The meaning of these spin coherent states becomes clear if one evaluates the expectation values of the spin operators, $\vec{S} = (S^x, S^y, S^z)$,

$$
\begin{aligned}
\langle\hat{\Omega}|\vec{S}|\hat{\Omega}\rangle &= \frac{1}{2}(\sin(\theta)\cos(\phi),\ \ \sin(\theta)\sin(\phi),\ \ \cos(\theta)) \\
&= \frac{1}{2}\hat{\Omega} \qquad (5.43)
\end{aligned}
$$

Hence, the spin coherent states translate the $su(2)$ algebra into the appropriate classical object. Keep in mind that these coherent states are quite unreasonable from the perspective of exact quantum mechanics - they are introduced only, because nature tells us that they might become reasonable in the thermodynamic limit, if a classical state is realized.

$\Longrightarrow$ Excercise 5.12

Having identified the $Y^\dagger$'s, it becomes straightforward to construct the wave function of the classical spin condensate. For $S = 1/2$ we might as well write the spin coherent state in terms of the fermion operators, describing the localized electrons,

$$
Y^\dagger_{\vec{i}}(\hat{\Omega}_{\vec{i}}) = e^{\frac{-i\phi_{\vec{i}}}{2}}\cos(\frac{\theta_{\vec{i}}}{2})c^\dagger_{\vec{i}\uparrow} + e^{\frac{i\phi_{\vec{i}}}{2}}\sin(\frac{\theta_{\vec{i}}}{2})c^\dagger_{\vec{i}\downarrow} \qquad (5.44)
$$

and the wave function of the classical spin system is (N is the number of lattice sites),

$$
|\Phi^0_{Cl}(\{\hat{\Omega}\})\rangle = \Pi^N_{\vec{i}} Y^\dagger_{\vec{i}}(\hat{\Omega}_{\vec{i}})|vac\rangle \qquad (5.45)
$$

It follows directly from (5.43) that the classical energy of the Heisenberg Hamiltonian (5.37) is given by (in fact, for arbitrary S)

$$
\begin{aligned}
H^{Cl}_{spin} &= \langle\Phi^0_{Cl}(\{\hat{\Omega}\})|H_{spin}|\Phi^0_{Cl}(\{\hat{\Omega}\})\rangle \\
&= JS^2\sum_{\vec{i},\vec{\delta}}\hat{\Omega}_{\vec{i}}\cdot\hat{\Omega}_{\vec{i}+\vec{\delta}} \\
&= JS^2\sum_{\vec{i},\vec{\delta}}\Big(\sin(\theta_{\vec{i}})\sin(\theta_{\vec{i}+\vec{\delta}})(\cos(\phi_{\vec{i}})\cos(\phi_{\vec{i}+\vec{\delta}}) + \sin(\phi_{\vec{i}})\sin(\phi_{\vec{i}+\vec{\delta}})) + \\
&\quad \cos(\theta_{\vec{i}})\cos(\theta_{\vec{i}+\vec{\delta}})\Big) \qquad (5.46)
\end{aligned}
$$

$\Longrightarrow$ Excercise 5.13

The classical ground state now depends on the lattice, the details of the couplings, etcetera. Considering cubic lattices and nearest-neighbour exchange couplings, there are only two possibilities:

(1) $J < 0$: the energy is minimized by the configuration of $\hat{\Omega}$'s where all arrows point in the same direction, with an energy $E_0 = -\frac{Nz}{2}|J|S^2$. This is the ferromagnetic state. Choosing the z-axis as preferred direction, the order parameter is simply

$$O_{FM} = \frac{1}{N}\langle\Phi^0|\sum_{\vec{i}} S^z_{\vec{i}}|\Phi^0\rangle \tag{5.47}$$

(ii) $J > 0$: the nearest-neighbour arrows align in an antiparallel fashion. A cubic lattice is bipartite: it can be divided in two sublattices ('A' and 'B'), where the sites on the A sublattice only have B sublattice neighbours, and vice versa. Hence, all magnetic bonds are satisfied if we take the spins to be parallel *on* the sublattices, while the spins on the A sublattice have the opposite orientation from the spins on the B sublattice. The classical ground state energy is the same as in the ferromagnetic state, and this state is called the antiferromagnetic of Néel state. The Néel (or 'staggered') order parameter is, again taking the z-axis as a reference,

$$O_{AFM} = \frac{1}{N}\langle\Phi^0|\sum_{\vec{i}\epsilon A} S^z_{\vec{i}} - \sum_{\vec{i}\epsilon B} S^z_{\vec{i}}|\Phi^0\rangle \tag{5.48}$$

On a square lattice these states look as follows,

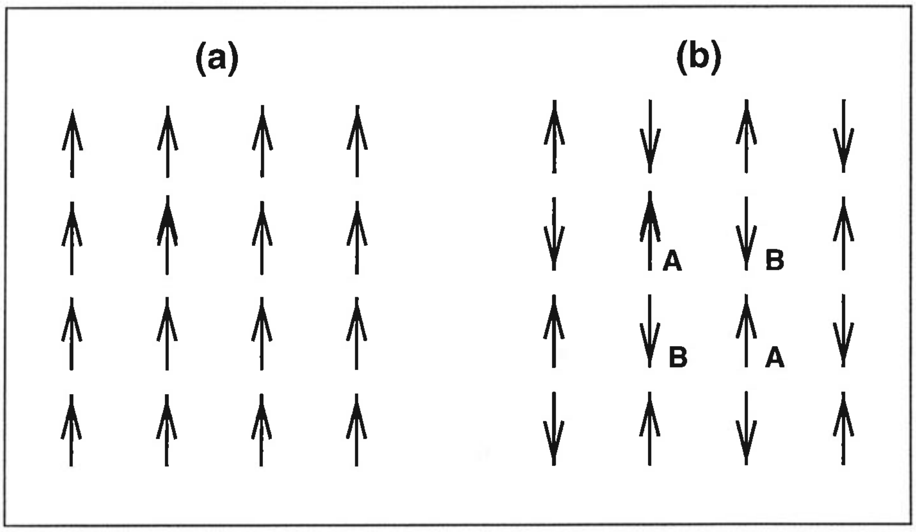

Figure 5.4: *Ferromagnetic- (a) and antiferromagnetic (b) condensates.*

As long as the exchange interactions have negative signs, the ferromagnetic state is always found, regardless the type of lattice. This is different for antiferromagnets. For positive J's one needs a bipartite lattice to stabilize the Néel state.

⟹ Excercise 5.14

The ferromagnet as an exact quantum state.

In the ferromagnet as well as in the antiferromagnet, spin-rotational symmetry is broken. Individual spins cannot rotate freely anymore, although the absolute orientation of the order parameter is still undetermined: we expect zero-modes, having a long wavelength limit where the spin system as a whole rotates freely. Despite this similarity, these states are completely different fundamentally. As will be proven in the next section, the Néel state is not an eigenstate of the Hamiltonian, in the same sense as that crystals or superconductors are not diagonalizing Hamiltonians, and it will become clear soon that the Néel state shares the universal properties of the classical state (like a linear mode spectrum, etcetera) with these other condensates. The ferromagnet is, however, very different and in fact exceptional: *the ferromagnetic state is an eigenstate of the Hamiltonian*! This is very easy to understand. We are free to choose the microscopic spin quantization axis in the same direction as the direction of the spontaneous magnetization. The z-component of the collective spin state becomes as large as possible: $\sum_{\vec{i}} S^z_{\vec{i}} |S_{tot} NS\rangle = NS|S_{tot} NS\rangle$ and this implies that this state is also an eigenstate of $S^2_{tot} = \sum_{\vec{i}} S^2_{\vec{i}}$, with $S^{tot} = NS$. In fact, the ferromagnet at zero-temperature is one of the very few exact macroscopic quantum states which exist (have been identified?) in nature. This exactness of the ground state leads to a number of consequences which makes the ferromagnet rather outstanding. First, it is not necessary to study quantum fluctuations because the ground state is an eigenstate and all off-diagonal matrix elements between the ground state and the remainder of the universe are zero. Secondly, the ferromagnet still carries collective excitations which look like collective modes ('spin waves') but are actually quite different. These 'modes', again corresponding with the lowest lying excitations of the system, are easy to calculate. We consider $S = 1/2$ and the vacuum is

$$|0\rangle = \Pi_{\vec{i}}^{N} c^{\dagger}_{\vec{i}\uparrow} |vac.\rangle = |S^{\text{tot}} = \frac{N}{2}\ ;\ M^{\text{tot}} = \frac{N}{2}\rangle \tag{5.49}$$

We now consider the set of N states, derived from the vacuum by flipping one spin somewhere on the lattice,

$$|\vec{i}\,\rangle = S^-_{\vec{i}} |0\rangle \tag{5.50}$$

These are states characterized by $S^{tot} = N/2$ and $M^{tot} = (N-2)/2$. The Hamiltonian acts as follows

$$H_{spin} |\vec{i}\,\rangle = (NE_0 + z|J|)|\vec{i}\,\rangle - \sum_{\vec{\delta}} \frac{|J|}{2} |\vec{i} + \vec{\delta}\,\rangle \tag{5.51}$$

This problem is easy to solve, because there are no matrix elements to states living outside the single spin-flip Hilbert subspace (5.50). Fourier transforming (5.51),

$$|\vec{q}\,\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{i}} e^{i\vec{q}\cdot\vec{i}} |\vec{i}\,\rangle \tag{5.52}$$

diagonalizes the Hamiltonian,

$$\begin{aligned} H_{\text{spin}} |\vec{q}\,\rangle &= (NE_0 + \hbar\omega_{\vec{q}})|\vec{q}\,\rangle \\ \hbar\omega_{\vec{q}} &= 2|J| \sum_{\alpha=1}^{d} \sin^2\left(\frac{1}{2} q_\alpha\right) \end{aligned} \tag{5.53}$$

$\Longrightarrow$ Excercise 5.15

For small $\vec{q}$ the dispersion becomes,

$$\hbar\omega_q = cq^2 \tag{5.54}$$

Instead of the linear mode dispersions of the genuine classical state, the 'magnons' of the ferromagnet show a 'particle'-like (q^2) behaviour! Notice that the theory of ferromagnetism is only simple if very few of these magnons are excited. If temperature is raised, these magnons occur at relatively high densities and they interact rather strongly with each other. It turns out that this is much harder to describe than the finite temperature quantum-antiferromagnet[9]. In the remainder of this chapter we further ignore ferromagnetism. Let us return to anti-ferromagnets.

Classical modes of the antiferromagnet

Since Néel condensates belong to the same general class as crystalline solids, we anticipate again the existence of modes. Different from the crystalline state, these modes are now a consequence of the breaking of *spin-rotational* symmetry. Physically, they represent precessional motion of the spins around the Néel ordered state. As in chapter IV, let us first study the linearized classical dynamics. Let us directly consider the quantum-mechanical equations of motions - as a general rule, one recovers the classical equations of motions if the operators are afterwards interpreted as the classical variables. Consider the time evolution of the flip operator S^+ on a particular site,

$$\begin{aligned} \dot{S}^+_{\vec{i}} &= \frac{1}{i}\,[S^+_{\vec{i}}, H_{\text{spin}}] && (5.55)\\ &= \frac{2J}{i}\,[-S^z_{\vec{i}+\vec{\delta}}\,S^+_{\vec{i}} + S^+_{\vec{i}+\vec{\delta}}\,S^z_{\vec{i}}] && (5.56) \end{aligned}$$

We assume the Néel order parameter (5.48) to be oriented along the z-axis, and in the classical limit all spins are pointing, say, upward on the A sublattice and downward on the B sublattice. In this limit we can therefore take $S^z \rightarrow +S$ on the A sublattice and $S^z \rightarrow -S$ on the B sublattice. This is substituted in (5.56) and we find the equations of motion for the spin flips on the two sublattices to be

$$\dot{S}^+_{\vec{i}\epsilon A} = \frac{JS}{i}\,[zS^+_{\vec{i}\epsilon A} + \sum_\delta S^+_{\vec{i}+\vec{\delta}\epsilon B}] \tag{5.57}$$

$$\dot{S}^+_{\vec{i}\epsilon B} = -\frac{JS}{i}[zS^+_{\vec{i}\epsilon B} + \sum_\delta S^+_{\vec{i}+\vec{\delta}\epsilon B}] \tag{5.58}$$

As in the case of the lattice vibrations, we write

$$S^+_{\vec{i}\epsilon A,B} = u_{A,B}\; e^{i(\vec{q}\cdot\vec{i}_{\epsilon A,B} - \omega_{\vec{q}}\,t)} \tag{5.59}$$

---

[9] For further reading, the book by D.C. Mattis, 'The Theory of Magnetism I' is recommended.

we find the dynamical matrix of this problem to be

$$\begin{pmatrix} zJS - \omega_{\vec{q}} & zJS\gamma_{\vec{q}} \\ -zJS\gamma_{\vec{q}} & -zJS - \omega_{\vec{q}} \end{pmatrix} \begin{pmatrix} u_A \\ u_B \end{pmatrix} = 0 \tag{5.60}$$

with

$$\gamma_{\vec{q}} = \frac{1}{z} \sum_{\vec{\delta}} e^{i\vec{q}\cdot\vec{\delta}} \tag{5.61}$$

Diagonalizing (5.61) yields the dispersion relation

$$\omega_{\vec{q}} = zJS\sqrt{1 - \gamma_{\vec{q}}^2} \tag{5.62}$$

⇒ Excercise 5.16

These are the spin-waves (or 'anti-ferromagnons') and it can be checked that they describe infinitisimal amplitude, precessional motions of the spins. Their general behaviour is very familiar: in the limit $q \rightarrow 0$ they correspond with the Goldstone-mode with $\omega = cq$ and a spin-wave velocity $c = zJS$. Although the language is different, this repeats precisely the story of the previous chapter.

Quantizing the spin-waves: Holstein-Primakoff.

As in the case of the crystals, there is no a-priori reason why the classical dynamics of the previous paragraph should make sense. This is actually a more interesting issue in the context of spin. Harmonic oscillators follow naturally in the case of crystals because of the Heisenberg algebra: momentum and position are the conjugate variables of the particles and one only needs to discover a harmonic potential in the collective problem. In the present context, spins do not know about $[p, x]$, and instead all one has is the $su(2)$ algebra. It is nevertheless possible to extract harmonic oscillators from spins, by a somewhat shaky procedure discovered by Holstein and Primakoff.

It starts out with the observation that harmonic oscillator bosons and spins have a ladder-like spectrum in common. The bosons have eigenstates $|n\rangle$ with n a non-negative integer ($n\epsilon\{0, 1, 2, \cdots, \infty\}$). For a given S, the spectrum of single spin states is characterized by $S^z|S, m_s\rangle = m_s|S, m_s\rangle$ with $m_s = S, S-1, \cdots, -S+1, -S$, in total $2S+1$ states. These two spectra have in common that the jumps involve integer numbers: Δm_s is also an integer. Starting with the maximum weight state, the action of S^- looks similar to the action of a boson creation operator,

$$\begin{aligned} S^-|S, m_s\rangle &\sim |S, m_s - 1\rangle \\ b^\dagger|n\rangle &\sim |n+1\rangle \end{aligned} \tag{5.63}$$

There is, however, a fundamental difference. The spectrum of harmonic oscillator states is unbounded from above, while the spin spectrum is *bounded* - it stops if S^- hits the minimum weight state: $S^-|S, -S\rangle = 0$. *The dimensionality of the Hilbert spaces of spin- and harmonic oscillator problems is completely different!* This should in principle give rise to fundamentally different physics: this is the problem. On a formal level, this problem can be circumvented by the introduction of a projection operator which removes all harmonic oscillator states with $n > 2S$ from the boson Hilbert space,

$$P = 1 - \sum_{n=2S+1}^{\infty} |n\rangle\langle n| \tag{5.64}$$

This is as dirty as it looks. Later on we will find good reasons to not worry about these projections. The manipulations which now follow are only valid in this projected space.

We take the maximum weight state as a reference to write,

$$S^z_{\vec{i}} = S - b^\dagger_{\vec{i}} b_{\vec{i}} \tag{5.65}$$

where the $b^\dagger$'s are associated with a boson: in the absence of a boson $S^z_{\vec{i}}|0\rangle = S|0\rangle$, one boson present $S^z_{\vec{i}}|1\rangle = (S-1)|1\rangle$, etcetera. We now need other operators, in terms of bosons, which form together with (5.65) a $su(2)$ algebra. The answer is [10]

$$S^+_{\vec{i}} = (2S)^{\frac{1}{2}} \sqrt{1 - \frac{b^\dagger_{\vec{i}} b_{\vec{i}}}{2S}}\, b_{\vec{i}} \tag{5.66}$$

$$S^-_{\vec{i}} = (2S)^{\frac{1}{2}} b^\dagger_{\vec{i}} \sqrt{1 - \frac{b^\dagger_{\vec{i}} b_{\vec{i}}}{2S}} \tag{5.67}$$

It is easily checked that the 'Holstein-Primakoff transformed bosons' (5.65-5.67) do form a $su(2)$ algebra in the projected boson Hilbert space.

Let us apply this transformation to the antiferromagnetic quantum Heisenberg problem (5.37). We anticipate on the existence of Néel order. On the A sublattice we can take the $|S,S\rangle$ states as the vacuum. However, on the B sublattice it has to be $\langle S^z \rangle = -S$, en here we cannot use (5.65) directly. This is simple to cure: rotate the quantization axis of the spins on the B sublattice by $\theta = 180^o$ with regard to he x-axis such that $M_s = -S \rightarrow S$

$$S^z_{\vec{i}\epsilon B} \rightarrow -S^z_{\vec{i}\epsilon B} \tag{5.68}$$

$$S^\pm_{\vec{i}\epsilon B} \rightarrow S^\mp_{\vec{i}\epsilon B} \tag{5.69}$$

and the Heisenberg Hamiltonian becomes,

$$H_{spin} = J \sum_{\vec{i},\vec{\delta}} \left[-S^z_{\vec{i}} S^z_{\vec{i}+\vec{\delta}} + \frac{1}{2}(S^+_{\vec{i}} S^+_{\vec{i}+\vec{\delta}} + S^-_{\vec{i}} S^-_{\vec{i}+\vec{\delta}}) \right] \tag{5.70}$$

This allows us to substitute (5.65-5.67). Next to terms bilinear in the bosons, one finds also terms of the form $b^\dagger b^\dagger b b$ (and higher order), describing boson-boson interactions.

---

[10] One needs the Schwinger boson formalism to derive this directly. See D. C. Mattis, 'The theory of Magnetism I'

These are the equivalents of the anharmonic terms in the phonon problem. Also in this case, they can be neglected if the interest is in the long wavelength properties.

⇒ Excercise 5.17

Neglecting the boson interactions, the substitution yields

$$\begin{aligned} H^{LSW}_{spin} &= J\sum_{\vec{i},\vec{\delta}}\left[-S^2 + S(b^\dagger_{\vec{i}}b_{\vec{i}} + b^\dagger_{\vec{i}+\vec{\delta}}b_{\vec{i}+\vec{\delta}} + b^\dagger_{\vec{i}}b^\dagger_{\vec{i}+\vec{\delta}} + b_{\vec{i}}b_{\vec{i}+\vec{\delta}})\right] && (5.71)\\ &= -\frac{z}{2}NJS^2 + SJ\sum_{\vec{i}\vec{\delta}}\left(b^\dagger_{\vec{i}}b_{\vec{i}} + b^\dagger_{\vec{i}+\vec{\delta}}b_{\vec{i}+\vec{\delta}} + b^\dagger_{\vec{i}}b^\dagger_{\vec{i}+\vec{\delta}} + b_{\vec{i}}b_{\vec{i}+\vec{\delta}}\right) && (5.72)\end{aligned}$$

LSW is an acronym for 'linear spin waves'. The classical energy is recovered, and in addition a fluctuation term is found, characterized by pairs of bosons. This term also contains combinations of two creation- and two annihilation operators, next to the usual bilinears. We need the Bogoliubov transformation of section 2.4!

The bosons are transformed to momentum space,

$$b^\dagger_{\vec{i}} = \frac{1}{\sqrt{N}}\sum_{\vec{i}} e^{i\vec{k}\cdot\vec{i}}b^\dagger_{\vec{k}} \tag{5.73}$$

and the Hamiltonian is in $\vec{k}$ space,

$$H^{LSW}_{spin} = -\frac{z}{2}NJS^2 + \frac{z}{2}SJ\sum_{\vec{k}>0}\left(b^\dagger_{\vec{k}}b_{\vec{k}} + b^\dagger_{-\vec{k}}b_{-\vec{k}} + \gamma_{\vec{k}}(b^\dagger_{\vec{k}}b^\dagger_{-\vec{k}} + b_{-\vec{k}}b_{\vec{k}})\right) \tag{5.74}$$

The second term is diagonalized by the boson version of the Bogoliubov transformation (2.108-2.110),

$$\begin{aligned} a_{\vec{k}} &= \cosh(u_{\vec{k}})b_{\vec{k}} + \sinh(u_{\vec{k}})b^\dagger_{-\vec{k}} && (5.75)\\ a^\dagger_{-\vec{k}} &= \sinh(u_{\vec{k}})b_{\vec{k}} + \cosh(u_{\vec{k}})b^\dagger_{-\vec{k}} && (5.76)\end{aligned}$$

and the inverse tranformation

$$\begin{aligned} b_{\vec{k}} &= \cosh(u_{\vec{k}})a_{\vec{k}} - \sinh(u_{\vec{k}})a^\dagger_{-\vec{k}} && (5.77)\\ b^\dagger_{-\vec{k}} &= -\sinh(u_{\vec{k}})a_{\vec{k}} + \cosh(u_{\vec{k}})a^\dagger_{-\vec{k}} && (5.78)\end{aligned}$$

In analogy with phonons $u_{\vec{k}} = u_{-\vec{k}}$. Substituting (5.77,5.78) into (5.74) and insisting that the transformed Hamiltonian takes a diagonal form yields a condition on the $u_{\vec{k}}$'s,

$$\tanh(2u_{\vec{k}}) = \gamma_{\vec{k}} \tag{5.79}$$

and the Hamiltonian becomes in diagonal form

$$H^{LSW}_{spin} = -\frac{z}{2}NJS(S+1) + \sum_{\vec{k}>0}\hbar\omega_{\vec{k}}\left(a^\dagger_{\vec{k}}a_{\vec{k}} + \frac{1}{2}\right) \tag{5.80}$$

with

$$\hbar\omega_{\vec{k}} = zJS\sqrt{1-\gamma^2_{\vec{k}}} \tag{5.81}$$

⇒ Excercise 5.18

Finally, let us calculate the Néel order parameter (5.48). We assumed that all sites on a particular sublattice are equivalent, and because of the rotation (5.70),

$$\begin{aligned} O_{AFM} &= \frac{1}{N}\langle\sum_{\vec{i}\epsilon A} S^z_{\vec{i}} + \sum_{\vec{i}\epsilon B} S^z_{\vec{i}}\rangle \\ &= \langle S^z_{\vec{i}}\rangle \\ &= S - \langle b^\dagger_{\vec{i}} b_{\vec{i}}\rangle \end{aligned} \tag{5.82}$$

where the last line follows from (5.65). When the local boson states would be unoccupied, we would recover the classical Néel state, with order parameter magnitude S! Notice that the existence of the order parameter is hard wired in the Holstein-Primakoff transformation itself. It is better to view this in the reverse order: if the order parameter exists, the transformation yields a well behaved theory, in the sense that no infinities show up in the perturbation expansion. In the absence of Néel order, the theory in terms of the bosons becomes highly singular and rather useless - I come back to this in a moment.

It is again expected that the Gaussian fluctuation is the most dangerous one. The order parameter fluctuation is nothing else than the local boson occupancy of (5.82) and on the Gaussian level at zero temperature,

$$\delta S = \frac{\langle b^\dagger_{\vec{i}} b_{\vec{i}}\rangle}{S} \tag{5.83}$$

$$= \frac{1}{NS}\sum_{\vec{k}}\langle b^\dagger_{\vec{k}} b_{\vec{k}}\rangle \tag{5.84}$$

$$= \frac{1}{NS}\sum_{\vec{k}}\sinh^2(u_{\vec{k}}) = \frac{1}{2NS}\sum_{\vec{k}}\left(\sqrt{\frac{1}{1-\gamma^2_{\vec{k}}}} - 1\right) \tag{5.85}$$

Making use of (5.78) and (5.79) to evaluate the expectation values of the bare boson occupancies.

Despite the different appearance of the formalism, we have obtained a physical picture which is in qualitative respects identical to what was found in the context of the crystalline state:

1. Although somewhat hidden in the formalism, the above manipulations are controlled by the finiteness of the Néel order parameter. In the context of crystals, we found that the classicalness of the state was at the end controlled by the largeness of the atomic mass. δS has the same status as the mean square fluctuation $\sqrt{\gamma}$, discussed in section 4.6, and we find that the prefactor (dimensionless coupling constant) is now $1/S$ (5.85): *the quantum fluctuation of the Néel state vanishes if the size of the spin becomes infinite* - S is much like a mass. It is easy to understand why the Néel state becomes more classical for larger spin.

We have first to identify a second way of approaching the classical limit. A subset of the classical states (5.39) is formed by the eigenstates of the total z-component of the spins: $S^z_{tot} = \sum_{\vec{i}} S^z_{\vec{i}}$. These states are also eigenstates of the Ising Hamiltonian which only contains the $S^z_{\vec{i}}$ operators: $H_{Ising} \sim \sum_{<ij>} S^z_{\vec{i}} S^z_{\vec{j}}$. and the *exact* ground state of the antiferromagnetic Ising model is the Néel state oriented along the z-axis. The spin-flip terms $\sim S^+_i S^-_j$ appearing in the Heisenberg model are therefore responsible for the quantum-spin fluctuations - see (5.65-5.72). What is the relationship between largeness of spin and the effects of spin-flips?

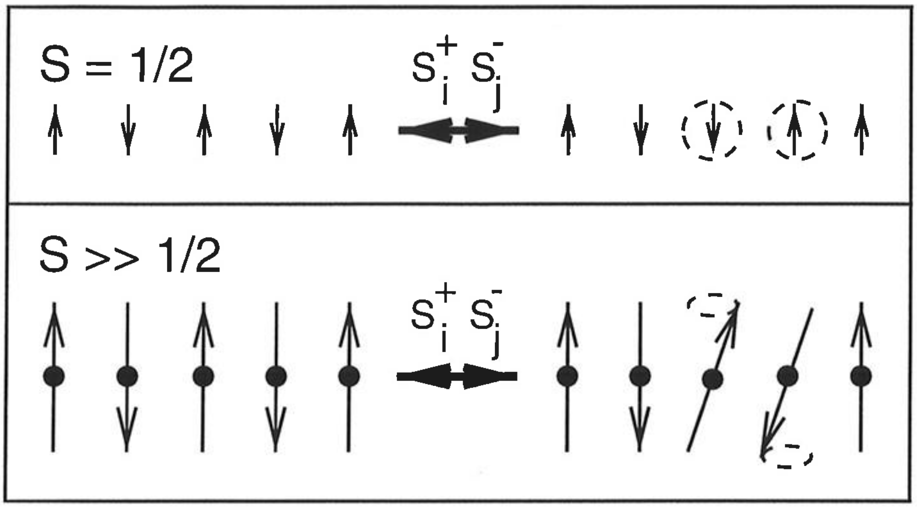

Figure 5.5: *In the case of $S = 1/2$, the fluctuation term in the Heisenberg Hamiltonian causes a complete reversal of two spins, while for large S it only gives rise to a small 'displacement'.*

Consider first $S = 1/2$. When $S^+_{i\epsilon B} S^-_{i+\delta\epsilon A}$ acts on the Néel state, it *reverses* the order parameter locally. On the other hand, for large spin the spin-flips only cause a small 'displacement' of the Néel order. $|\langle S^z \rangle|$ is reduced from $|S|$ tot $|S| - 1$, as illustrated in figure 5.5.

2. From (5.81) it is inferred that the dispersion relation of the antiferromagnons is identical to that of classical spin waves (5.62). Stronger, the large wavelength behaviour is identical to that of acoustical phonons: $\omega(k) = ck$. The deep reason is that antiferromagnets and crystals (as well as superconductors and Fermi-liquids) belong to the same class of classical condensates with long range order, and the zero-modes are a generic consequence of the nature of this vacuum. We save us here the effort to calculate the magnon-lifetime - we are sure that this will not pose a problem.

3. Let us now consider the order parameter fluctuation δS (5.83-5.85) in more detail. The integral in (5.85) is again dominated by the long wavelength modes

> because $\sqrt{1-\gamma_k^2} \sim k$ and the asymptotic behavior is governed by
>
> $$\delta S \sim \frac{1}{2S}\left[\int \frac{d^d\vec{k}}{k} - 1\right] \tag{5.86}$$
>
> As in crystals, δS is again divergent in $d = 1$ and Néel order cannot exist in one dimension. In larger dimensions the stability of the Néel state is again a matter of numbers.

Different from the crystalline case, the existence of Néel order can be proven in large regions of parameter space. Before we turn to this subject, let me comment on what happens if the Néel state does not survive. This is generically the case in one space dimension, as can already be inferred from the simple Gaussian argument (5.86). The investigation of one dimensional spin systems is one of the frontiers of physics: one finds 'quantum spin liquids' which can be quite a bit more interesting than the floating solids as explained in section 4.6. What was the crucial step in the 'derivation' of the Néel state? We assumed that the density of bosons (or spin flips) is low, which allowed us to make the step (5.70) to (5.71). We found this to be indeed the case for large S. For small S this is in principle no longer the case. In higher dimensions, the Néel state still wins. This is not as well understood as one would like and fortunately we can rely on some mathematical results which are summarized in the next section. In one dimension, the fluctuations get truely out of hand. The local displacements are no longer small and one has to worry about anharmonicities. Much worse, if the spin deviations become large it is no longer reasonable to close the eyes for the completely different dimensionality of the Hilbert spaces of bosons and spins. In terms of the bosons, the fluctuations would give rise to a massive invasion of the unphysical parts of the Hilbert space! This cannot be repaired with perturbation theory, because one needs infinitely large interactions between the bosons to get rid of these states: the problem becomes 'non-perturbative'. The spin wave bosons become irrelevant for the physics of these systems, and instead one finds a host of peculiar 'quantum-worlds'. A discussion of these phenomena would fill up most of the (non-existent) second volume of this lecture series[11].

5.4 The Néel state by theorem.

Next to causing conceptual difficulties, the smallness of the spin Hilbert space has a benefit: the powerfull machinery of mathematical physics has a chance to succeed. Accordingly, spin systems have been high on the agenda of this discipline for quite some time, with some remarkable outcomes. It has been *proven* that (a) the exact

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[11] I refer to the books by E. Fradkin: 'Field theories of condensed matter systems' (Addison-Wesley, Reading, 1991), and A. Auerbach 'Interacting electrons and quantum magnetism' (Springer, New York, 1994). A pedestrian introduction to the space-time condensation underlying the incompressible fluids can be found in: J. Zaanen, 'Quantum werelden, groot en klein' (jaarboek akademie-onderzoekers, Amsterdam, 1996: in press).

ground states of antiferromagnetic nearest-neighbour Heisenberg systems are non-degenerate spin-singlets for all values of S and in all dimensions[12] and (b) that Néel long range order exists in $d \geq 3$ for all values of S[13] and in $d = 2$ for $S \geq 3/2$[14].

⇒ Excercise 5.19

Giving it a minute of thought, this should sound like a paradox. *Néel states are never eigenstates of total spin:* $(\sum_{\vec{i}} S_{\vec{i}})^2$. This is simple to see. Take for instance the two-spin Heisenberg problem. We learned in section 2.5 that the *singlet* eigenstate $\sim (1/\sqrt{2})(\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2)$: this is a coherent superposition of the two Néel states constructed from two spins. The macroscopic singlets, as proven to be the exact ground states by Lieb and Mattis, are much more complicated than this simple example, but they share the property that they are linear superpositions of large numbers of Ising-like configurations. The Néel condensate violates total S, in the same sense as the crystalline state violates total momentum. How is it possible that one can proof at the same time that the Néel state nevertheless exists?

The aforementioned proofs are far too involved to be reproduced here. The essence of the physics can, however, be seen from a model which is mathematically far simpler than the Heisenberg model, the so-called Lieb-Mattis model (N is the number of lattice sites):

$$\begin{aligned} \vec{S}_A &= \sum_{\vec{i}\epsilon A} \vec{S}_{\vec{i}} \\ \vec{S}_B &= \sum_{\vec{i}\epsilon B} \vec{S}_{\vec{i}} \\ H_{LM} &= \frac{2J}{N} \vec{S}_A \cdot \vec{S}_B \end{aligned} \tag{5.87}$$

Every spin on the A sublattice interacts with the same strength with *all* spins on the B sublattice, and vice versa. Because every spin communicates with an infinity of other states, this really helps the collective (= classical) behaviour and this is the source of simplifications. Notice that the exchange coupling $\sim 1/N$ in order to keep the system extensive ($E_0 \sim N$). We introduce the total spin S,

$$\vec{S} = \vec{S}_A + \vec{S}_B \tag{5.88}$$

and it follows directly that

$$H_{LM} = \frac{J}{N} \left(\vec{S}^2 - \vec{S}_A^2 - \vec{S}_B^2 \right) \tag{5.89}$$

We now observe that $\vec{S}_A^2$, $\vec{S}_B^2$, $\vec{S}^2$ and S^z all commute with the Hamiltonian, and with (5.89) we have solved the problem! The eigenstates are completely specified by $|S_A, S_B, S, M_S\rangle$ (in an obvious notation) and the exact eigenvalues are

$$E(S_A, S_B, S) = \frac{J}{N} \left[S(S+1) - S_A(S_A+1) - S_B(S_B+1) \right] \tag{5.90}$$

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[12] E. H. Lieb and D. C. Mattis, J. Math. Phys. **3**, 749 (1962).

[13] F. J. Dyson, E. H. Lieb and B. Simon, J. Stat. Phys. **18**, 335 (1978).

[14] E. Neves and J. F. Perez, Phys. Lett. **114A**, 331 (1968).

Assuming spin 1 (it works for any spin) and a bipartite lattice, the ground state becomes the state with $S_A = S_B = N/2$ (maximum S on both sublattices) and total $S = 0$, a singlet state! The energy of this state is $E_0 = -J(N/2+1)$[15].

Hence, it is easy to proof that the ground state of the Lieb-Mattis model is a non-degenerate singlet. We also observe that the operator measuring the staggered magnetization,

$$\vec{M}_s = \vec{S}_A - \vec{S}_B \tag{5.91}$$

does *not* commute with the Hamiltonian. This is a fluctuating quantity and we are assured that the Néel order parameter, corresponding with the ground state expectation value of $\vec{M}_s$ (5.48) has to be zero. At the same time, the classical analysis (magnons around the Néel state) would actually indicate that the quantum fluctuations are harmless: (5.87) should be Néel ordered. Because of the long range interactions, the spectrum of spin waves becomes gapped, and even dispersionless and it is even so that the magnons do not mix into the pure Néel state ($O_{AFM} = 1$). At first sight, one would think that there has to be something really wrong with our understanding of the classical state!

⇒ Excercise 5.20

The confidence in the classical state can be restored, but this involves a very subtle argument. We start out with adding to the Hamiltonian a *symmetry breaking* term,

$$H \;=\; H_{LM} - B_s(S^z_A - S^z_B) \tag{5.92}$$

This extra term causes the Néel state, oriented along the z-axis, to be inequivalent from all other states. In the presence of the 'staggered' field (or 'order parameter field') B_s there is no longer a symmetry reason for the non-existence of the Néel order parameter: the Néel state is stabilized by hand. Fields like B_s (or equivalent fields like the 'crystalline' field forcing atoms to be on particular positions in space) do not exist in nature and (5.92) looks rather unphysical. The subtlety is, that the existence of the classical state depends *on the order in which one takes the thermodynamic limit $N \to \infty$ and the limit $B_s \to 0$*. More precisely,

$$\begin{aligned} \lim_{N\to\infty}\lim_{B_s\to 0}\langle\Phi_0|M^z_s|\Phi_0\rangle &= 0 \\ \lim_{B_s\to 0}\lim_{N\to\infty}\langle\Phi_0|M^z_s|\Phi_0\rangle &= 1 \end{aligned} \tag{5.93}$$

where $|\phi_0\rangle$ now corresponds with the exact quantum ground state. This is rather easy to proof for (5.92)[16]. We consider again $S = 1$ and it follows directly from (5.90) that in the absence of the staggered field: (i) it costs an energy of at least $O(J)$ to change the magnetization on one of the sublattices[17]. (ii) Initially, the states

---

[15] This turns out to be a crucial step in the original proof of Lieb and Mattis of the singlet nature of the ground state. The remainder of the proof, extending to whole classes of models, relates to the unique nodal (sign) structure of this kind of singlet wavefunction.

[16] This was discovered rather recently, see: C. Kaiser and I. Peschel, J. Phys. A **22**, 4257 (1989); T. A. Kaplan, W. von der Linden and P. Horsch, Phys. Rev. B42, 4663 (1990).

[17] This is actually the magnon 'mass' originating in the long range interactions, see excercise 5.20..

with S different from zero are separated by energies of order J/N. Since $E \sim S^2/N$, there is an infinity of states becoming degenerate with the singlet ground state if $N \rightarrow \infty$ and one needs $S \sim \sqrt{N}$ before these states become true excitations[18]. The essence of what follows is, that the Néel state can be reconstructed from the subset of eigenstates of the Hamiltonian in the absence of the staggered field, which become degenerate with the ground state singlet in the thermodynamic limit.

Only the set of eigenstates (5.90) has to be considered, characterized by maximum sublattice spin, $S_A = N/2, S_B = N/2$, and a total $M_S = 0$. This leaves only S as a variable quantum number, and we abbreviate $|S\rangle \equiv |S_A, S_B, S, M_S\rangle$. For a finite staggered field, these states are no longer eigenstates of (5.92). One has to determine the matrix elements of the Néel operator in the space of states $|S\rangle$. This involves a rather tedious excercise in vector addition, but the result is known. Only states where S differs by unity are coupled, by the matrix element,

$$\langle S|S_A^z - S_B^z|S-1\rangle = -S\sqrt{\frac{(N+1)^2 - S^2}{4S^2 - 1}} \tag{5.94}$$

As will become clear later, the important states are the ones with $1 << S << N$ (for N large), and (5.94) simplifies to $\langle S|M_s^z|S-1\rangle = -N/2$. In this space of low lying states, (5.92) becomes,

$$H = \sum_{S=0}^{N} \left[|S\rangle \frac{JS^2}{N} \langle S| - \frac{NB_s}{2} (|S\rangle\langle S+1| + h.c.) \right] \tag{5.95}$$

counting from the ground state energy in zero field E_0, and again assuming that the smallest S states are unimportant. (5.95) looks like a simple tight-binding problem, except that the diagonal energies increase quadratically with S: this is actually a discrete version of the harmonic oscillator. Because the splittings between the states become very small for large N we might as well take a continuum limit. The eigenstates in the presence of the field are written as $|\Psi\rangle = \sum_S \Phi(S)|S\rangle$ and the Schrödinger equation becomes,

$$-\frac{N}{2} B_s (\Phi(S-1) + \Phi(S+1)) + \frac{JS^2}{N}\Phi(S) = \varepsilon \Phi(S) \tag{5.96}$$

In the continuum limit,

$$\Phi(S+1) + \Phi(S-1) - 2\Phi(S) \rightarrow \frac{\delta^2 \Phi(S)}{\delta S^2} \tag{5.97}$$

and (5.96) can be written as

$$-\frac{1}{2}\frac{\delta^2\Phi(S)}{\delta S^2} + \frac{1}{2}\omega^2 S^2 \Phi(S) = \nu \Phi(S) \tag{5.98}$$

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[18] These states get lost in the standard classical analysis - they are believed to be present in real magnets, crystals, superconductors, etcetera. This is no problem, because they do not contribute in the thermodynamic limit. Their contribution to the partition function $Z_{thin} = \sum_{S=0}^{N}(2S+1)exp(-\beta E(S))$ and it is easy to show that $\beta F_{thin} = (1/N) ln Z_{thin} \rightarrow 0$ if $N \rightarrow \infty$. This is called a 'thin spectrum'.

with the parametrization,

$$\omega = \frac{1}{N\sqrt{B_s/J}} \tag{5.99}$$

$$\nu = \frac{(\varepsilon/J) + N(B_s/J)}{N(B_s/J)} \tag{5.100}$$

This is nothing else than Eq. (2.40) (with $m = \hbar = 1$) and we directly infer the spectrum of the states in the presence of the field: $\nu_n = (n + 1/2)\omega$. We have now to realize that S is positive definite, and only the harmonic oscillator wavefunctions with a node at the origin are admitted. The ground state is therefore the state with $n = 1$, corresponding with a wavepacket with width $\Delta S \sim N^{\frac{1}{2}}(B_s/J)^{\frac{1}{4}}$ and $\nu_0 = 3\omega/2$. The energy of the system is

$$E_0 + \varepsilon = E_0 - NB_s + \frac{3}{2}\sqrt{B_s J} \tag{5.101}$$

From this expression, the dependence on the order of taking the limits (5.93) becomes clear. The first limit is trivial: we of course recover that the ground state is a singlet by first taking $B_s \rightarrow 0$, before taking $N \rightarrow \infty$. The other limit is the interesting one: if one lets $N \rightarrow \infty$ in a finite field, the last term can be neglected and one finds that $\varepsilon = NB_s$: this is only possible if the Néel order is fully developed because this amount of energy can only be gained in a fully ordered Néel antiferromagnet.

⇒ Excercise 5.21

The above offers a rigorous way of understanding the phenomenon of rigidity. The argument is remarkable: in terms of the exact eigenstates, a classical system is characterized by a large number of excitations which become nearly degenerate with the exact ground state in the thermodynamic limit. Although these states are invisible in the thermodynamics, they allow for the existence of classical order because only a small (on the scale of N) subset of those is needed to reconstruct the symmetry broken state. In the present example, only the $\sim N^{\frac{1}{2}}(B_s/J)^{\frac{1}{4}}$ lowest states are needed, out of the total Hilbert space build from N $S = 1$ spins with dimension 3^N. The staggered field is of course unphysical and is only introduced as a mathematical device to demonstrate, via (5.93), that the ordered state becomes degenerate in the thermodynamic limit with the exact state satisfying the symmetry requirements. Nature might quite well be in the exact singlet state. The above demonstrates that the symmetry restoring fluctuations, making up the difference between the Néel state and the singlet, are of a highly collective kind. They correspond with a uniform precession of all the spin together and since the energy differences for finite N between the Néel- and the exact state are of order J/N, the collective precession frequency is very, very small. For instance $J \sim 10^{14}s^{-1}$ and $N \sim 10^{23}$ yields $1/\omega \sim 100$ years.

5.5 Weak coupling: condensation in momentum space.

Let us descend again to the level of the (semi) classical theory. Both in chapter IV and in this chapter, systems have been discussed where the *interaction energies* are much larger than the kinetic energies associated with the quantum-mechanical zero-point motions of the particles. For this reason, the latter could be taken into account perturbatively, giving rise to small corrections on the scale of the interaction energies. A major achievement has been the discovery that the classical paradigm of section 1.2 also applies to the opposite limit, where the quantum kinetic energies dominate over the interaction energies: the 'weak coupling limit'. The discovery of the microscopic theory of superconductivity by Bardeen, Cooper and Schrieffer (BCS) has played a key role in this development and in hinsight one could claim that they really deserved their Nobel price because they showed how to construct the classical state from the microscopic quantum soup.

The reason to introduce weak-coupling theory in the context of magnetism is that anti-ferromagnets both occur in their weak coupling ('spin density waves') and strong coupling versions in nature - crystals only occur in the strong coupling limit, and superconductors only in the weak coupling limit. Magnetism is the ideal playing ground to demonstrate the equivalence of the macroscopic physics in both limits: at long wavelengths and small energies it is all the same. The difference is that in weak coupling the classical features are first seen at a length scale (the 'coherence' length) and a time scale (the 'gap') much larger than the atomic scales. Up to these scales one has to take quantum-mechanics very seriously - beyond these scales it is (classical) business as usual. This complicates the formalism appreciably. In the general case, it is always worthwhile to first consider the strong coupling limit, to understand the general nature of the collective state, to continue the theory subsequently to weaker couplings. The benefits of this approach will become particularly obvious in the next chapter dealing with superconductivity.

Mean-field theory.

In the weak coupling limit, the kinetic energy dominates and the natural starting point is *single particle momentum space.* In forming the classical condensates, one needs now coherent superpositions of the single particle momentum states in order to construct the $Y^\dagger$ states needed for the condensate wave functions. Although the wave functions can be constructed, this is technically rather clumsey and a much more efficient approach exists: semi-classical mean-field theory, or 'Hartree-Fock'[19]. Let us illustrate this approach in the context of spin condensates. The starting point is again the Hubbard model,

$$H = t \sum_{\vec{i}\vec{\delta}\sigma} c^\dagger_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} + U \sum_{\vec{i}} n_{\vec{i}\uparrow} n_{\vec{i}\downarrow} \tag{5.102}$$

The central step in mean-field theory is straightforward. The existence of Néel order is anticipated. Orienting the staggered order parameter along the z-axis, its presence

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[19] The vocabulary is ambiguous: this amounts to the classical level of section 1.2 and one still has to calculate the fluctuations around these states, as we will be explained later. For this reason one would like to call this 'classical mean field theory', but this is usually associated with the mean-field theories in classical statistical mechanics. The best language is the field-theoretic one: 'integrating out the fermions around the classical saddlepoint of the Hubbard-Stratanovich auxiliary fields'. See Fradkin's 'Field theories of condensed matter systems'.

implies that the operator $S^z_{\vec{i}}$ acquires a finite expectation value ('vacuum amplitude') on every site. In terms of the fermion operators (recall (2.142)), this means

$$\langle S^z_{\vec{i}} \rangle = \frac{1}{2}\left(\langle n_{\vec{i}\uparrow} \rangle - \langle n_{\vec{i}\downarrow} \rangle \right) \neq 0 \tag{5.103}$$

One anticipates that on the the A sublattice $\langle n_{\vec{i}\uparrow} \rangle > \langle n_{\vec{i}\downarrow} \rangle$ and on the B sublattice $\langle n_{\vec{i}\uparrow} \rangle < \langle n_{\vec{i}\downarrow} \rangle$, or vice versa. The crucial step in mean-field theory is to use the finiteness of the vacuum amplitudes to derive a new, effective Hamiltonian where the important effects of the interactions are 'eaten by the order parameter'. We define

$$n_{\vec{i}\sigma} \equiv O_{\vec{i}\sigma} + \delta \hat{O}_{\vec{i}\sigma} \tag{5.104}$$

$O_{\vec{i}\sigma}$ is the scalar vacuum amplitude,

$$O_{\vec{i}\sigma} = \langle n_{\vec{i}\sigma} \rangle \tag{5.105}$$

and $\delta \hat{O}_{\vec{i}\sigma}$ is the operator describing the quantum fluctuation of $O_{\vec{i}\sigma}$. These play the same role as the spin- or lattice displacements as we discussed in the strong coupling cases. Explicitely,

$$\delta \hat{O}_{\vec{i}\sigma} = n_{\vec{i}\sigma} - \langle n_{\vec{i}\sigma} \rangle \tag{5.106}$$

Using (5.104,5.106), the Hamitonian can be rewritten as,

$$H = t \sum_{\vec{i}\vec{\delta}\sigma} c^\dagger_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} + U \sum_{\vec{i}} \left(O_{\vec{i}\uparrow} n_{\vec{i}\downarrow} + O_{\vec{i}\downarrow} n_{\vec{i}\uparrow} - O_{\vec{i}\uparrow} O_{\vec{i}\downarrow} + \delta \hat{O}_{\vec{i}\uparrow} \delta \hat{O}_{\vec{i}\downarrow} \right) \tag{5.107}$$

As long as the order parameter exists, it should be possible to treat the effects of the fluctuations perturbatively - as in strong coupling this has to be checked afterwards and this will be discussed in the next section. The classical limit is reached if the fluctuation term $\delta \hat{O}_{\vec{i}\uparrow} \delta \hat{O}_{\vec{i}\downarrow}$ is neglected. This defines the 'mean-field Hamiltonian'

$$H^{MF} = t \sum_{\vec{i}\vec{\delta}\sigma} c^\dagger_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} + U \sum_{\vec{i}} \left(O_{\vec{i}\uparrow} n_{\vec{i}\downarrow} + O_{\vec{i}\downarrow} n_{\vec{i}\uparrow} - O_{\vec{i}\uparrow} O_{\vec{i}\downarrow} \right) \tag{5.108}$$

With these simple manipulations we obtain a remarkable physical insight. We learned to respect the difficulties coming from the combination of the interaction term $\sim U$ and the kinetic term $\sim t$ in section 5.2. As long as the order parameter is finite, (5.107) is far simpler. The difficulties associated with the electron correlations, in so far they are not 'eaten by the order parameter', are absorbed in the term fluctuating the order parameter and we learned how to handle those. What remains is (5.108): the effects of the electron-electron interactions have been absorbed in simple single electron potential scattering terms, representing the scattering of the electrons against the order parameter. (5.108) is an independent electron ('band structure') problem which can be solved in principle. The mean-field structure of the Hamiltonian is equivalent to the statement that the classical state corresponds with single determinant wave functions (Eq. 1.3, section 1.2). The beauty is, that much of the work of sections (5.2) and (5.3) is now done in one simple, algebraic manipulation.

(5.108) can be written in a more transparent form by introducing scalars which refer directly to the local z-axis spin- ($\Omega^z_{\vec{i}}$) and charge ($2\bar{n}_{\vec{i}}$) density

$$\begin{aligned} \Omega^z_{\vec{i}} &= \frac{1}{2}\left(O_{\vec{i}\uparrow} - O_{\vec{i}\downarrow}\right) \qquad (5.109) \\ \bar{n}_{\vec{i}} &= \frac{1}{2}\left(O_{\vec{i}\uparrow} + O_{\vec{i}\downarrow}\right) \qquad (5.110) \end{aligned}$$

because

$$\begin{aligned} O_{\vec{i}\uparrow} &= \bar{n}_{\vec{i}} + \Omega^z_{\vec{i}} \\ O_{\vec{i}\downarrow} &= \bar{n}_{\vec{i}} - \Omega^z_{\vec{i}} \qquad (5.111) \end{aligned}$$

the mean-field Hamiltonian becomes

$$H^{MF} = t\sum_{\vec{i}\vec{\delta}\sigma} c^\dagger_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} + U\sum_{\vec{i}} \Big(\bar{n}_{\vec{i}}(n_{\vec{i}\uparrow} + n_{\vec{i}\downarrow}) - \Omega^z_{\vec{i}}(n_{\vec{i}\uparrow} - n_{\vec{i}\downarrow}) - \bar{n}^2_{\vec{i}} + (\Omega^z_{\vec{i}})^2\Big) \qquad (5.112)$$

This should somehow relate to the classical spin Hamiltonian (5.46) and at first sight it seems that the spin-rotational invariance got lost. In the above 'decoupling' one has to take care that one respects the symmetries of the original Hamiltonian. In the present case, this means that one should also consider the ordering of the interaction term $\sim -U\sum_{\vec{i}} c^\dagger_{\vec{i}\uparrow} c_{\vec{i}\downarrow} c^\dagger_{\vec{i}\downarrow} c^\dagger_{\vec{i}\uparrow}$. Such a term is decoupled by $c^\dagger_{\vec{i}\uparrow} c_{\vec{i}\downarrow} (\equiv S^+_{\vec{i}}) \equiv \Omega^+_{\vec{i}} + \delta\Omega^+_{\vec{i}}$ and $c^\dagger_{\vec{i}\downarrow} c_{\vec{i}\uparrow} (\equiv S^-_{\vec{i}}) \equiv \Omega^-_{\vec{i}} + \delta\Omega^-_{\vec{i}}$. The interaction term becomes in this spin-rotational invariant decoupling,

$$\begin{aligned} U\sum_{\vec{i}} n_{\vec{i}\uparrow} n_{\vec{i}\downarrow} &= U\sum_{\vec{i}} \Big(\bar{n}_{\vec{i}}(n_{\vec{i}\uparrow} + n_{\vec{i}\downarrow}) - \Omega^z_{\vec{i}}(n_{\vec{i}\uparrow} - n_{\vec{i}\downarrow}) - \Omega^+_{\vec{i}} c^\dagger_{\vec{i}\downarrow} c_{\vec{i}\uparrow} - \Omega^-_{\vec{i}} c^\dagger_{\vec{i}\uparrow} c_{\vec{i}\downarrow} \\ &\quad -\bar{n}^2_{\vec{i}} + (\Omega^z_{\vec{i}})^2 + \Omega^+_{\vec{i}}\Omega^-_{\vec{i}} + fluctuations\Big) \qquad (5.113) \end{aligned}$$

It is easily checked that this decoupling obeys spin rotational invariance.

⟶ Excercise 5.22

Notice also the presence of an average charge density ($\bar{n}_{\vec{i}}$). Except for some exceptional cases, this average always exists. The reason is an underlying discrete symmetry in the charge sector, as will be further explained in the next chapter.

Given (5.112) or (5.113), how to proceed? In fact, this is nothing else than a convenient reformulation of the general procedure of section 1.2:

(i) Choose a set of classical variables $\bar{n}_{\vec{i}}$ and $\hat{\Omega}_{\vec{i}}$ which can in principle be different on every lattice site with the only restriction that $\bar{n}$, $|\hat{\Omega}| \leq 1/2$: this is the classical field configuration.

(ii) Every choice of classical variables, (5.112,5.113) defines an independent electron problem. The eigenstates of this problem are therefore single-determinant states - the ground state for every choice of classical field variables is nothing else than $|\Phi^0_{Cl}(\{\bar{n}, \hat{\Omega}\})\rangle$ (eq. 1.8, section 1.2). Diagonalizing the effective independent particle problem is called 'integrating out the fermions'.

(iii) Find the minimum of the classical energy $E_{Cl}(\{\bar{n}, \hat{\Omega}\})$ in classical field configuration space. In terms of the eigenstates of the independent particle problem, the classical energy is simply the sum over the N_e lowest lying single particle energies ('band energy'), plus the contribution of the 'potential energy' $\sim U(-\bar{n}^2_{\vec{i}} + \hat{\Omega}^2_{\vec{i}})$. In this minimization step one obtains implicit equations for the classical variables which can be solved by iteration (compare with the discussion in section 4.1).

This procedure can be illustrated in the now familiar context of the half-filled Hubbard model on a (hyper)cubic lattice. In principle one should allow for every possible field-configuration. However, for an arbitrary configuration the single particle problem becomes very complicated and this can be only handled numerically. In fact, the half-filled case has been thoroughly investigated and it turns out that the ground state indeed corresponds with the Néel state, with an uniform charge density. Hence, we limit ourselves to the part of configuration space with $\bar{n}_{\vec{i}} = \bar{n}$, $\forall \vec{i}$, $\hat{\Omega}_{\vec{i}} = (0, 0, +\Omega)$, $\vec{i} \epsilon A$ and $\hat{\Omega}_{\vec{i}} = (0, 0, -\Omega)$, $\vec{i} \epsilon B$ (staggered orderparameter in the z direction). $\bar{n}$ and Ω still remain to be determined. From (5.112) it follows immediately that the up-electron sees a potential $\sim U(\bar{n} - \Omega)$ on the A sublattice and $\sim U(\bar{n} + \Omega)$ on the B sublattice. The down electron sees the same potential, except that the A and B sublatices have been exchanged. The following *band structure* problem has to be solved,

$$H^{MF}_{Neel} = t \sum_{\vec{i}\vec{\delta}\sigma} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} + U \sum_{\vec{i}\epsilon A,B} \left(\bar{n}(n_{\vec{i}\uparrow} + n_{\vec{i}\downarrow}) \mp \Omega(n_{\vec{i}\uparrow} - n_{\vec{i}\downarrow}) - \bar{n}^2 + \Omega^2 \right) \quad (5.114)$$

This is very similar to the two-band models which were discussed in chapter III: it is just a tight-binding model on a cubic lattice with a unit cell containing two sites.

Let us first consider the simple one dimensional case - one should not take this too litteral, because this is precisely the case where the classical theory is bound to fail because of the order parameter fluctuation. The up- and down electrons see the following potential,

We learned how to obtain the bandstructure for a tight-binding problem of this kind (Eq.'s (3.44)-(3.47)) and we find in k-space

$$\begin{aligned} H^{MF} \;=\; & \sum_k \left[2t \cos(\frac{k}{2}) \sum_{\sigma} (c^{\dagger}_{Ak\sigma} c_{Bk\sigma} + h.c.) \right] \\ & + U(\bar{n} - \Omega)(c^{\dagger}_{kA\uparrow} c_{kA\uparrow} + c^{\dagger}_{kB\downarrow} c_{kB\downarrow}) + U(\bar{n} + \Omega)(c^{\dagger}_{kA\downarrow} c_{kA\downarrow} + c^{\dagger}_{kB\uparrow} c_{kB\uparrow}) \\ & + U(\Omega^2 - \bar{n}^2) \qquad (5.115) \end{aligned}$$

introducing A and B fermions living on the A and B sublattices. $k \epsilon \{-\pi, \pi\}$ is defined in the new Brillouin zone with absolute dimensions $\{-\frac{\pi}{2a}, \frac{\pi}{2a}\}$ (a is the lattice constant).

(5.115) is diagonalized by,

$$\gamma^{\dagger}_{k\uparrow} \;=\; \cos\phi_k c^{\dagger}_{kA\uparrow} + \sin\phi_k c^{\dagger}_{kB\uparrow} \qquad (5.116)$$

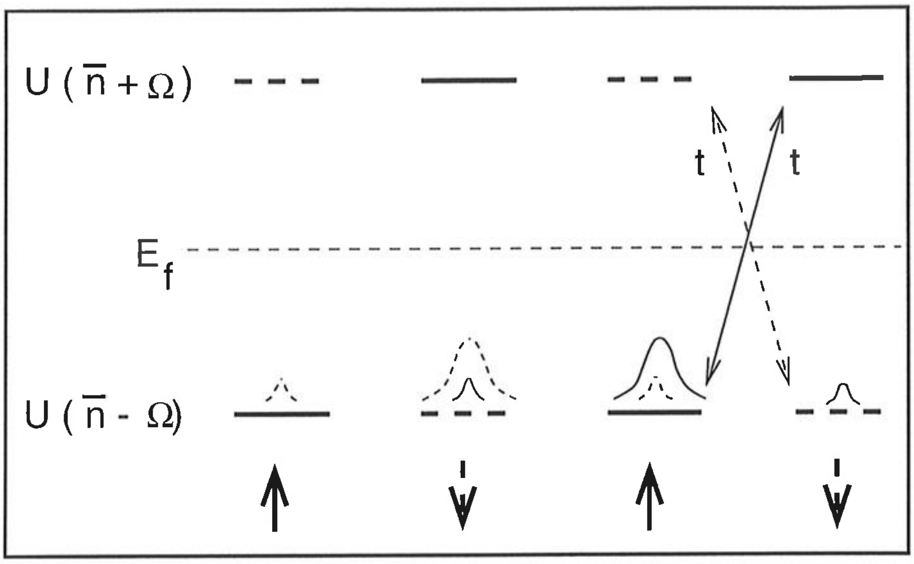

Figure 5.6: *Potentials as seen by the up- (full lines) and down (dashed line) electrons, caused by the presence of the Néel order parameter in the one dimensional chain problem. Also the charge density of two tightly localized 'spin-quasiparticles' is indicated, as they appear in the strong coupling limit ($U >> t$).*

$$\bar{\gamma}^\dagger_{k\uparrow} = \sin\phi_k c^\dagger_{kA\uparrow} - \cos\phi_k c^\dagger_{kB\uparrow} \tag{5.117}$$
$$\gamma^\dagger_{k\downarrow} = \cos\phi_k c^\dagger_{kB\downarrow} + \sin\phi_k c^\dagger_{kA\downarrow} \tag{5.118}$$
$$\bar{\gamma}^\dagger_{k\downarrow} = \sin\phi_k c^\dagger_{kB\downarrow} - \cos\phi_k c^\dagger_{kA\downarrow} \tag{5.119}$$

associating $\gamma^\dagger_{k\sigma}$ with the low lying ('bonding') occupied states, and $\bar{\gamma}^\dagger_{k\sigma}$ with the high lying unoccupied states. The Hamiltonian becomes in diagonal form,

$$H^{MF} = \sum_{k\sigma}\left[\omega^-_k(\bar{n},\Omega)\gamma^\dagger_{k\sigma}\gamma_{k\sigma} + \omega^+_k(\bar{n},\Omega)\bar{\gamma}^\dagger_{k\sigma}\bar{\gamma}_{k\sigma}\right] + NU(\Omega^2 - \bar{n}^2) \tag{5.120}$$

with (compare eq. (3.47))

$$\omega^\pm_k(\bar{n},\Omega) = U\bar{n} \pm \sqrt{U^2\Omega^2 + 4t^2\cos^2\frac{k}{2}} \tag{5.121}$$

This represents the same band structure as the one shown in Figure 3.8b, where the gap is now of order $U\Omega$, instead of $|\varepsilon_p - \varepsilon_d|$. Both bands are spin degenerate; a difference with the discussion in chapter 3 is that the potential is now spin dependent. For large $U\Omega/t$, the lower band now corresponds with the up- and down electrons being mainly on the A- and the B sublattice, respectively (see also Fig. 5.6). At half-filling, there is one up- and one down electron per (two site) unit cell, and the lower lying band is therefore exactly filled.

We still have to determine $\bar{n}$ and Ω. The lowest lying band of eigenstates is precisely filled up and the classical energy is,

$$E(\bar{n},\Omega) = \frac{\langle H^{MF}\rangle}{N} = \frac{1}{N}\sum_{k=-\pi}^{\pi}\omega^-_k(\bar{n},\Omega) + U(\Omega^2 - \bar{n}^2) \tag{5.122}$$

Making use of the fact that the problem is identical for spin up on the A sublattice and spin down on the B sublattice to write the energy per lattice site. From this expression we can already infer the energy balance. Due to the presence of the antiferromagnetism, the occupied states are pushed downwards. This energy gain is balanced by the potential energy term $\sim U\Omega^2$. Minimizing (5.122) to Ω and $\bar{n}$ yields the 'saddle-point equations',

$$\frac{\delta E(\bar{n},\Omega)}{\delta \bar{n}} = -2\bar{n}U + \frac{1}{N}\sum_k \frac{\delta}{\delta \bar{n}}\omega_k^-(\bar{n},\Omega) = 0 \tag{5.123}$$

$$\frac{\delta E(\bar{n},\Omega)}{\delta \Omega} = 2\Omega U + \frac{1}{N}\sum_k \frac{\delta}{\delta \Omega}\omega_k^-(\bar{n},\Omega) = 0 \tag{5.124}$$

One sees that these amount to implicit equations: Ω and $\bar{n}$ are given in terms of functions of Ω and $\bar{n}$. Let us first consider (5.123). Because of (5.110), we can deduce the answer without doing any calculation. We have assumed that the charge-density $2\bar{n}$ is the same on every site. At half filling, we therefore should find $2\bar{n} = 1$ (one electron per site). From (5.123) together with (5.121) it follows directly that,

$$2\bar{n} = \frac{1}{N}\sum_k 1 = 1\ ! \tag{5.125}$$

The Néel order parameter is less trivial. (5.124) together with (5.121) yields the implicit expression for the order parameter amplitude Ω,

$$\frac{1}{2N}\sum_k \frac{1}{\sqrt{U^2\Omega^2 + 4t^2\cos^2\frac{k}{2}}} = \frac{1}{U} \tag{5.126}$$

or

$$\frac{1}{2\pi}\int_0^\pi \frac{dk}{\sqrt{1 + (\frac{2t}{U\Omega})^2\cos^2\frac{k}{2}}} = \Omega \tag{5.127}$$

This equation can be solved by iteration - start with some value for Ω on the left hand side of this equation to calculate the right hand side, and use this new value again on the left hand side, etcetera, untill Ω no longer changes: (5.127) is an explicit way of looking at the self-consistency requirement which was already discussed in section 4.1. The physical picture is actually quite similar.

⇒ Excercise 5.23

Let us first consider *strong coupling*: $U >> t$. This is very important: there is no instance in the derivation leading to (5.127) that we demanded anything from U/t. All we needed was the existence of the Néel state, and this is controlled by $1/S$ and the dimensionality. It is quite often claimed that the above mean-field theory is only correct for small U/t (weak coupling) and this is a gross misunderstanding. It is controlled by classicalness. I will now demonstrate that mean-field theory precisely reproduces the result of the exact strong coupling expansion of section 5.2, given that the spins in the result (5.36) are taken to be classical.

(5.127) can be expanded for small t/U as

$$\begin{aligned} \Omega &\simeq \frac{1}{2\pi}\int_0^\pi dk \left[1 - 2(\frac{t}{U\Omega})^2 \cos^2\frac{k}{2}\right] \\ &= \frac{1}{2}\left(1 - (\frac{t}{U\Omega})^2\right) \qquad (5.128) \end{aligned}$$

In the limit $t/U \to 0$, $\Omega \to 1/2$, its maximum value, as one would expect. Let us expand the classical energy (5.122) to the same order, making use of (5.125),

$$\begin{aligned} E(\frac{1}{2},\Omega) &\simeq \frac{1}{\pi}\int_0^\pi dk \left[\frac{U}{2} - U\Omega(1 + 2(\frac{t}{U\Omega})^2 \cos^2\frac{k}{2})\right] + U\left(\Omega^2 - \frac{1}{4}\right) \\ &= \frac{U}{2} - U\Omega - \frac{t^2}{U\Omega} + U\left(\Omega^2 - \frac{1}{4}\right) \qquad (5.129) \end{aligned}$$

To lowest order in t/U we should take $\Omega = 1/2$ (see (5.128)), and it follows that $E = -t^2/U$ per site. This is identical to what we find from the exact expression (5.36) for classical spins ($\vec{S}_i \to \Omega^z = 1/2$): $J\sum_{i\delta}(\vec{S}_i\cdot\vec{S}_{i+\delta} - 1/4) \to -JN/2 = -Nt^2/U$! This is no accident; for every possible configuration of classical spins $\{\hat{\Omega}\}$, one will find a one-to-one correspondence with the energies calculated form the exact expression (5.36) and the mean-field energies.

⇒ Excercise 5.24

Although in technical regards more awkward, one might as well look at mean-field theory from the wavefunction perspective of section 1.2. Occupying the N lowest lying states of the mean-field Hamiltonian amounts to writing the ground state wavefunction of the condensate as

$$|\Phi^0_{Cl}(\vec{n},\Omega)\rangle = \Pi_k \gamma^\dagger_{k\uparrow}\gamma^\dagger_{k\downarrow}|vac.\rangle \qquad (5.130)$$

Different from the real space single particle operators of the localized magnets or crystals, the condensate is constructed from *momentum space* single particle states! This is the generalization needed to understand superconductors and Fermi-liquids, as well as the spin density waves which will be explained in a moment. For large U/t, however, this reduces again to a real space affair. All the states in (5.130) are separated from the other states by a gap which is much larger than the width of the occupied band (fig. 3.8). Under these conditions, we can transform the set of occupied states to obtain *localized* wave packets: Wannier wave functions. Consider first $U/t \to \infty$: the low lying spin-up and spin-down states on the A and B sublattices, respectively, are isolated from the rest of the universe by infinite potential barriers (fig. 5.6). For large, but finite U/t, these localized states will start to leak out to the high energy states on the neighbouring sites on the 'wrong' sublattice (see figure 5.6). These states can be written as,

$$\gamma^\dagger_{\vec{i}\epsilon A\uparrow} = c^\dagger_{\vec{i}\epsilon A\uparrow} - \frac{t}{U}\sum_{\vec{\delta}} c^\dagger_{\vec{i}+\vec{\delta}\epsilon B\uparrow}$$

$$\gamma^{\dagger}_{\vec{i}\epsilon B\downarrow} = c^{\dagger}_{\vec{i}\epsilon B\downarrow} - \frac{t}{U}\sum_{\vec{\delta}} c^{\dagger}_{\vec{i}+\vec{\delta}\epsilon A\downarrow} \tag{5.131}$$

and the wave function of the Néel condensate becomes in this limit,

$$|\Phi^{0}_{Cl}(\bar{n},\Omega)\rangle = \Pi_{\vec{i}\epsilon A}\gamma^{\dagger}_{\vec{i}\uparrow}\Pi_{\vec{i}\epsilon B}\gamma^{\dagger}_{\vec{i}\downarrow}|vac\rangle \tag{5.132}$$

Because a density of $\sim (t/U)^2$ of down-spin electron leaks out on the up-sublattice and the same amount of up-spin electron on the down spin lattice, the order parameter gets reduced: $\Omega \rightarrow 1/2(1-(t/U)^2)$, compare (5.128). I leave it to the reader to show that (5.132), together with the recipy of section 1.2, is precisely equivalent to the mean-field approach.

⇒ Excercise 5.25

What happens if the coupling is further reduced? We could in principle improve (5.131) by spreading out the localized wave functions further and further: as long as the gap is present it is always possible to construct Wannier states. This is, however, quite clumsy and it is much more convenient to work in momentum space. We have in fact already done all the hard work for the one dimensonal case and all what remains is to solve (5.127). Imagine that we want to solve this equation by iteration for a moderate or even small value of U/t. Let us start with the fully saturated (strong coupling) value $\Omega = 1/2$ on the left hand side. This would yield an Ω on the right hand side which is smaller (e.g., (5.127)). We understand now why: the wave-functions start to leak out to the wrong sublattices, thereby decreasing the sublattice magnetization. This in turn makes the gap ($\sim U\Omega$) smaller and in the next iteration round the electrons spread out even further, further diminishing the order parameter, etcetera - the similarity with the discussion in section 4.1 should be clear. In essence, it involves a trade off between kinetic energy gain (the spreading of the wavefunction), at the expense of an increased amount of double occupancy: if the order parameter is large there is only one electron per site, and no double occupancy. The question arises: if U/t is further and further decreased, is there a point where Ω vanishes? In the general case there is such a critical U/t where the Néel condensate vanishes. The one dimensional case is, however, special: neglecting the collective quantum fluctuations, Ω is finite for any finite U!

Let us consider the limit $U/t \rightarrow 0$ in one dimension. It is expected that only the states very close to E_F are affected, and in analogy with the Debye model for phonons, the details of the electron states at high energies can be neglected. The states close to E_F can be *linearized.* Consider the bands in the folded zone at $U = 0$ and count momentum from $k_F = \pi$ (in units of $2a$): $k' = k - k_F$. The dispersion $\omega_k = 2|t\cos(k/2)|$ can now be written as $\omega_k = v_F k'$ for the occupied- and $-v_F k'$ for the unoccupied band (see Figure 5.7), with $v_F = |t|$ (or $2a|t|$ in absolute units). A high energy cut-off momentum k'_0 is choosen which reproduces the bandwidth: $v_F k'_0 = 2t$.

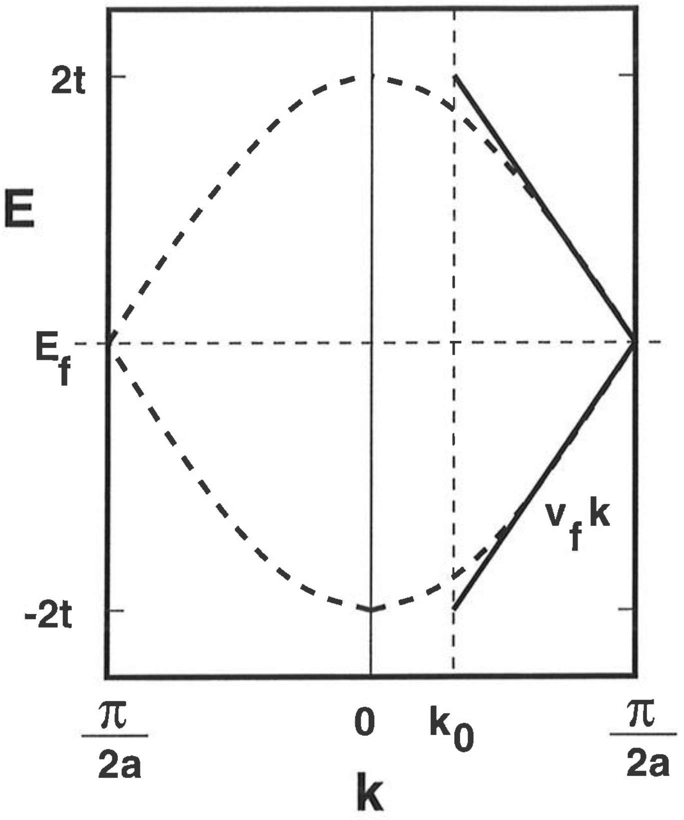

Figure 5.7: *linearizing the one dimensional tight binding bands (compare with figure 3.8).*

With these assumptions, (5.126) simplifies to,

$$\begin{aligned}\frac{1}{U} &= \frac{1}{2\pi|v_F|}\int_0^{k_0'} \frac{dk'}{\sqrt{\frac{U^2\Omega^2}{v_F^2}+(k')^2}} \\ &= \frac{1}{2\pi|v_F|} arcsinh(\frac{|v_F k_0'|}{U\Omega}) \qquad (5.133)\end{aligned}$$

such that

$$U\Omega = \Delta = \frac{|v_F k_0'|}{\sinh(\frac{2\pi|v_F|}{U})} \simeq 4|t|e^{-\frac{2\pi|t|}{U}} \qquad (5.134)$$

We have now to recall the discussion in section (3.2): we found there that at the Brilloun zone boundary always a gap appears regardless the strength of the periodic potential. In this case the potential is coming from the Néel orderparameter $U_K \sim U\Omega$ and the gap is twice this number. According to (5.134) this gap is finite for all $U > 0$! At the same time, the orderparameter Ω is finite, although it becomes very, very small for small U.

The form of the expression for the gap and the order parameter (5.134) is quite general - we will see it back, for instance, in the form of the famous BCS-gap equation for superconductivity. It is crucial for the existence of the weak coupling instability that the system is characterized by nesting: the gap opens everywhere at the Fermi-surface, because the Fermi-surface lies exactly at the new zone boundary, associated with the symmetry breaking. Under this condition, the band energy decreases initially linearly in Ω: all the occupied states closest to the Fermi-surface move downward with $U\Omega$ and this always outnumbers the potential term, which is quadratic in Ω, for small enough Ω. The novelty is that the linear 'driving force' is multiplied by a very small number $\sim \exp(-W/U)$ (W is bandwidth) - this is a consequence of the Pauli principle, which has forced the electrons in large kinetic energy states, which are hard to localize.

Despite its smallness, the gap is still there in the weak coupling limit, and as long as the gap spans the Fermi surface (as it does in $d = 1$) it is possible to construct Wannier states of localized spins. The difference with the localized spin wave packets in strong coupling (5.131) is their much larger spatial extent. Their linear dimension, the 'coherence length' ξ, is estimated by,

$$\frac{\xi}{a} \sim \frac{W}{2U\Omega} \tag{5.135}$$

Because the gap $2U\Omega$ is a very small fraction of the bandwidth W, the coherence length is quite large, typically like $1000a \sim 10^2$ nm. The orderparameter corresponds therefore with a superposition of $O(10^3)$ overlapping single particle spin states! This weak coupling antiferromagnet is called a 'spin density wave' (SDW): it is basically a Fermi-fluid (metal) with a tiny wave of spin density superimposed on it. Notice that these spin density waves also occur in one dimension at filling fractions, different from half filling. The difference is that the nesting occurs now at different wave numbers than $\pi/2a$ and instead of a simple doubling of the unit cell, a spin density wave is found with a wavelength $1/2k_F$, which is not necessarily an integer multiple of the lattice period ('incommensurate density waves'). Next to these spin density waves, one finds also charge density waves in one dimensional systems, which can be driven by electron-phonon interactions, and/or *attractive* electron-electron interactions.

⇒ Excercise 5.26

⇒ Excercise 5.27

Despite the strongly delocalized character of the electrons, the collective state falls still in the same class as the localized magnets at macroscopic scales. At energies less than the gap or length scales larger than the coherence length, the electrons 'disappear' (because of the gap) and all what remains are the collective spin degrees of freedom (magnons). The order parameter fluctuations behave qualitatively in the same manner as in strong coupling. In fact, the fluctuations are strongly reduced in weak coupling as will be further discussed in the next section.

The statements in the last paragraph are all true at zero temperature. At finite temperatures, there are important differences in the macroscopic properties of the strong coupling and weak coupling condensates. We learned in section 5.2 that at energies less than U only spins exists if U is large. It is possible to find a phase transition from the Néel state to the disordered spin state as function of temperature. Above this transition, occurring at the Néel temperature $T_N \sim J$, there are still spins and the difference is that their orientation is randomized. This is different in weak coupling. The gap is now very small, (5.134), and if temperature becomes of order $U\Omega$, the spins themselves have to disappear. In addition, if the spins disappear, the gap has to disappear as well! It turns out that this 'gap disappearance' transition occurs at a lower temperature than the spin-orientation transition: the spins have disappeared before they could loose their orientational order. This will be further discussed in the context of superconductivity, where it is of particular empirical relevance.

I already stressed that nesting is a necessary requirement to find condensation in the weak coupling limit. Nesting is special to one dimensional physics while it was already explained in section 3.2 to be exceptional in higher dimensions. With the exceptions of Fermi-liquids, superconductors, and bose superfluids, it is never possible to find a 'true' weak coupling condensate in higher dimensions, and one has always to exceed a critical coupling strength. This can be illustrated in the context of the Hubbard model on a square ($d = 2$) lattice - recall that the model with nearest neighbour hoppings showed an accidental nesting property (excercise 3.19). A and B sublattices are implied and the mean-field Hamiltonian for the two dimensional problem becomes,

$$
\begin{aligned}
H &= \sum_{\vec{k}} [2t\tilde{\gamma}_{\vec{k}} \sum_{\sigma} (c^{\dagger}_{\vec{k}A\sigma} c_{\vec{k}B\sigma} + h.c.) \\
&\quad + U(\bar{n} - \Omega)(c^{\dagger}_{\vec{k}A\uparrow} c_{\vec{k}A\uparrow} + c^{\dagger}_{\vec{k}B\downarrow} c_{\vec{k}B\downarrow}) + U(\bar{n} + \Omega)(c^{\dagger}_{\vec{k}A\downarrow} c_{\vec{k}A\downarrow} + c^{\dagger}_{\vec{k}B\uparrow} c_{\vec{k}B\uparrow})] \\
&\quad + NU(\Omega^2 - \bar{n}^2)
\end{aligned}
\qquad (5.136)
$$

with the dispersion relation,

$$
\omega^{\pm}_{\vec{k}}(\bar{n}, \Omega) = U\bar{n} \pm \sqrt{U^2\Omega^2 + 4t^2\tilde{\gamma}^2_{\vec{k}}} \qquad (5.137)
$$

and the saddle-point equation for Ω is,

$$
\frac{1}{2N} \sum_{\vec{k}} \frac{1}{\sqrt{U^2\Omega^2 + 4t^2\tilde{\gamma}^2_{\vec{k}}}} = \frac{1}{U} \qquad (5.138)
$$

while $2\bar{n} = 1$. The only difference with the one dimensional problem are the two dimensional integrals and a different dispersion relation,

$$
\tilde{\gamma}_{\vec{k}} = \cos(\frac{k_x + k_y}{2}) + \cos(\frac{k_x - k_y}{2}) \qquad (5.139)
$$

with $k_x, k_y \epsilon \{-\pi, \pi\}$ in the folded Brillioun zone The $U = 0$ bandstructure is indicated in figure 5.8 with the dashed lines (recall excercise 3.19),

For finite $U\Omega$, a gap appears along the boundary of the new Brillioun zone, as indicated with the dashed line in the figure. It is directly clear that the gap opens up everywhere at the Fermi-surface at the moment $U\Omega$ becomes finite. This Hubbard model is nested in two dimensions, at half filling! It is straightforward to show that

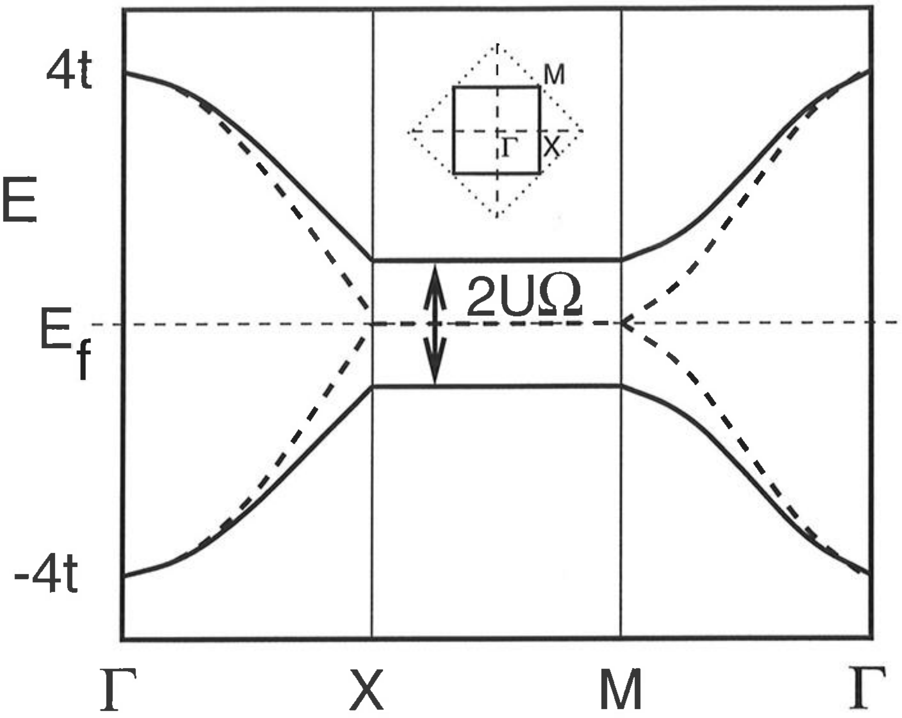

Figure 5.8: *Band structure of the mean-field Hubbard model on a square lattice, in the absence- (dashed lines) and presence (full lines) of the staggered order parameter. Notice that everywhere at the Fermi surface (X − M, etcetera) a gap opens up for a finite UΩ, because the fermi-surface coincidizes with the new Brillioun zone boundary (see also inset). This is a pathology of this model.*

this causes the same singularity as was found in $d = 1$[20]. We again focus on the states close to E_F, observing that the band at E_F is flat in the direction parallel to the Fermi-surface. Consider the side of the Fermi surface between $(\pi, -\pi)$ and (π, π) - the other pieces of the Fermi-surface are equivalent. The Fermi-velocity is finite in the perpendicular direction, and we linearize this problem in the same way as we did in the $d = 1$ example. Take an arbitrary $k_y \epsilon \{-\pi, \pi\}$, and define $k_x = \pi + k'_x$. For $U = 0$ and small k'_x,

$$\begin{aligned} \omega^-_{\vec{k}} &= -4|t| \cos\frac{k_x}{2} \cos\frac{k_y}{2} && (5.140) \\ &\simeq v_F(k_y) k'_x && (5.141) \end{aligned}$$

with

$$v_F(k_y) = -4|t| \cos\frac{k_y}{2} \qquad (5.142)$$

---

[20] This singularity is the infinity produced by integrals like (refco124) or (5.138) if $\Omega = 0$. This infinity implies a finite Ω for every finite U. This singularity shows up as well in the perturbation theory around the Fermi-liquid state - another example of perturbation theory revealing flaws in the vacuum state. An example is the Cooper instability which played an important role in the discovery of the BCS theory.

The k_y dependence of v_F is in first instance unimportant, and we can average the Fermi velocity along the k_y direction: $v_F(k_y) \rightarrow \bar{v}_F$ (similar as to the average sound velocity in the Debye model). This works the same for the other three sides of the Fermi-surface, and we find ($N = N_x N_y$),

$$\begin{aligned} \frac{1}{U} &= \frac{1}{2N_x N_y} \sum_{\vec{k}} \frac{1}{\sqrt{U^2\Omega^2 + 4t^2\tilde{\gamma}_{\vec{k}}^2}} \\ &\simeq \frac{1}{2N_x N_y} \sum_{k'_x, k_y} \frac{1}{\sqrt{U^2\Omega^2 + \bar{v}_F^2 (k'_x)^2}} \\ &= \frac{1}{2N_x} \sum_{k'_x} \frac{1}{\sqrt{U^2\Omega^2 + \bar{v}_F^2 (k'_x)^2}} \end{aligned} \qquad (5.143)$$

Precisely the same equation is obtained as in one dimension, except for unimportant corrections related to the averaging of the Fermi velocity.

The square Fermi-surface of the single band, nearest-neighbour hopping model is an artefact. At the moment one adds *anything* else (like a next-nearest-neighbour hopping) the Fermi surface will start to look more spherical. In these more realistic cases, the Fermi surface will only coincidize with *points* on the Brillouin zone boundary. Since we only found a logarithmic singularity in the nested case, the integrals will be *finite* for $\Omega = 0$ and the condensation will not occur for sufficiently small U. One needs a finite value of U to find spin-ordering. For instance, a finite t' in the present example (excercise 3.16) will cause a 'warp' in the band along the Brillioun zone boundary ($X - M$ direction) and U has to exceed this warp in order for the SDW instability to occur.

The central message is that weak-coupling antiferromagnets (or charge density waves) are special to the one dimensional world. This is a strong theoretical prediction which is confirmed by a large body of experimental evidence. One dimensional physics is littered with these collective density waves. Because of the arguments of section 4.6 and 5.3, the long wavelength quantum fluctuations will eventually destroy the classical order in one dimension. This is also what happens, but the resulting quantum fluids are best understood as floating solids (section 4.6) build from these density wave states. In the higher dimensional world, weak-coupling magnets nearly never occur: the only known examples are the so-called Bechgaard salts. Although these are nominally two dimensional, they are very anisotropic and not far from the one dimensional limit[21].

5.6 Fluctuations in weak coupling.

In the previous section, it was demonstrated that the Néel condensate could be studied with remarkable ease, by starting directly with the electronic Hamiltonian, combining

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[21] One encounters in these systems the so-called field induced spin density waves. Magnetic fields increase the anisotropy further and it turns out that spin density waves appear in these Bechgaard salts in external magnetic fields of some Teslas.

the projective renormalization and the construction of the condensate in one step. The crucial operation was the neglect of the fluctuation terms $\sim \delta\hat{\Omega}\delta\hat{\Omega}$, and I *stated* that these relate to harmless order parameter fluctuations (magnons). One would like to see this explicitely. Electrons are far more complicated than spins and the luck on the mean-field level ends at the moment one tries to calculate the fluctuations. Although the principles are straightforward, the calculation of the fluctuations around the electronic mean-field state is a tedious affair. One really profits from the efficient organization of perturbation theory in the field-theoretic formalism (diagrams) and in chapter VII I will present an example of a full calculation of this sort. To give some confidence already at this point, I will present in this section a rather special case where one can get at the answer, in finite time, without invoking the Green's functions: the spin waves around the electronic mean-field state in strong coupling. What follows is an example of a so-called 'Random Phase Approximation' (RPA) calculation.

The principle is straightforward: do a calculation of the type (5.55-5.62), now using the electronic vacuum amplitudes $\bar{n}, \Omega$ and the electronic fluctuations $\sim \delta\hat{\Omega}_\sigma$. This becomes relatively simple in strong coupling: as I discussed, it is possible to build up the Néel state in terms of real space wavepackets. Since the spin fluctuations involve small energies, also the fluctuation theory can be constructed in real space. Since these wave packets are tightly localized, we have only to consider two neighbouring sites (A, B). Next to the occupied wavefunctions (5.131), we now also need the unoccupied high energy states,

$$\begin{aligned}
\gamma^\dagger_{A\uparrow} &= C(c^\dagger_{A\uparrow} - \frac{t}{U} c^\dagger_{B\uparrow}) && (5.144)\\
\gamma^\dagger_{A\downarrow} &= C(c^\dagger_{A\downarrow} + \frac{t}{U} c^\dagger_{B\downarrow}) && (5.145)\\
\gamma^\dagger_{B\uparrow} &= C(c^\dagger_{B\uparrow} + \frac{t}{U} c^\dagger_{A\uparrow}) && (5.146)\\
\gamma^\dagger_{B\downarrow} &= C(c^\dagger_{B\downarrow} - \frac{t}{U} c^\dagger_{A\downarrow}) && (5.147)
\end{aligned}$$

with the normalisation factor $C = (1 + (t/U)^2)^{1/2}$.

We want to rediscover the magnons in the full electronic problem. The obvious idea would be to investigate the equations of motion of the spin-flip operator S^+. We might as well consider the non-local spin-flip, $c^\dagger_{\vec{i}\uparrow} c_{\vec{i}+\vec{\delta}\downarrow}$, and for the Hubbard Hamiltonian (5.2),

$$[c^\dagger_{\vec{i}\uparrow} c_{\vec{j}\downarrow}, H] = t \sum_{\vec{\delta}} (c^\dagger_{\vec{i}\uparrow} c_{\vec{j}+\vec{\delta}\downarrow} - c^\dagger_{\vec{i}+\vec{\delta}\uparrow} c_{\vec{j}\downarrow}) + U(-n_{\vec{i}\downarrow} c^\dagger_{\vec{i}\uparrow} c_{\vec{j}\downarrow} + c^\dagger_{\vec{i}\uparrow} c_{\vec{j}\downarrow} n_{\vec{j}\uparrow}) \qquad (5.148)$$

⇒ Excercise 5.28

It is not at all obvious what this expression has to do with the spin-only result (5.56). This actually makes sense - the bare electrons $\sim c^\dagger$ no longer exist at low energies in the insulator, and we ae looking at the wrong objects. Instead, we should focus on the localized electron states (5.144-5.147) and we should investigate the spin-flip operators which can be constructed from the states $\gamma^\dagger$

$$\begin{aligned} \hat{S}_A^+ &= \gamma_{A\uparrow}^\dagger \gamma_{A\downarrow} && (5.149) \\ \hat{S}_B^+ &= \gamma_{B\uparrow}^\dagger \gamma_{B\downarrow} && (5.150) \end{aligned}$$

and these will turn out to be equivalent to the localized electron spin-flips of section 5.3. One should first calculate the equation of motion (compare 5.55),

$$\dot{\hat{S}}_{A,B}^+ = \frac{1}{i}[\hat{S}_{A,B}^+, H] \qquad (5.151)$$

with the electronic Hamiltonian, and subsequently we should replace the operators by their vacuum amplitudes, to obtain the classical modes. Although the principle is straightforward, the calculation is already becoming tedious. It is convenient to first transform the Hamiltonian by the inverse of (5.144-5.147),

$$\begin{aligned} c_{A\uparrow}^\dagger &= C(\gamma_{A\uparrow}^\dagger + \frac{t}{U}\gamma_{B\uparrow}^\dagger) \\ c_{B\uparrow}^\dagger &= C(\gamma_{B\uparrow}^\dagger - \frac{t}{U}\gamma_{A\uparrow}^\dagger) \\ c_{A\downarrow}^\dagger &= C(\gamma_{A\downarrow}^\dagger - \frac{t}{U}\gamma_{B\downarrow}^\dagger) \\ c_{B\downarrow}^\dagger &= C(\gamma_{B\downarrow}^\dagger + \frac{t}{U}\gamma_{A\downarrow}^\dagger) && (5.152) \end{aligned}$$

The normalization factor $C^2 = 1$ up to order t/U and the Hamiltonian looks as follows up to second order ($J = 2t^2/U$),

$$H = U\hat{O}_U + t\hat{O}_t + J\hat{O}_J + O(\frac{t^3}{U^2}) \qquad (5.153)$$

with

$$\begin{aligned} \hat{O}_U &= \gamma_{A\uparrow}^\dagger\gamma_{A\uparrow}\gamma_{A\downarrow}^\dagger\gamma_{A\downarrow} + \gamma_{B\uparrow}^\dagger\gamma_{B\uparrow}\gamma_{B\downarrow}^\dagger\gamma_{B\downarrow} && (5.154) \\ \hat{O}_t &= (\gamma_{A\uparrow}^\dagger\gamma_{B\uparrow} + \gamma_{B\uparrow}^\dagger\gamma_{A\uparrow})(1 + \gamma_{A\downarrow}^\dagger\gamma_{A\downarrow} - \gamma_{B\downarrow}^\dagger\gamma_{B\downarrow}) \\ &\quad + (\gamma_{A\downarrow}^\dagger\gamma_{B\downarrow} + \gamma_{B\downarrow}^\dagger\gamma_{A\downarrow})(1 - \gamma_{A\uparrow}^\dagger\gamma_{A\uparrow} + \gamma_{B\uparrow}^\dagger\gamma_{B\uparrow}) && (5.155) \\ \hat{O}_J &= -\gamma_{A\uparrow}^\dagger\gamma_{A\uparrow} - \gamma_{B\downarrow}^\dagger\gamma_{B\downarrow} + \gamma_{A\uparrow}^\dagger\gamma_{A\uparrow}\gamma_{B\downarrow}^\dagger\gamma_{B\downarrow} + \\ &\quad \gamma_{A\downarrow}^\dagger\gamma_{A\downarrow} + \gamma_{B\uparrow}^\dagger\gamma_{B\uparrow} + \gamma_{B\uparrow}^\dagger\gamma_{B\uparrow}\gamma_{A\downarrow}^\dagger\gamma_{A\downarrow} + \\ &\quad \gamma_{A\uparrow}^\dagger\gamma_{A\downarrow}\gamma_{B\downarrow}^\dagger\gamma_{B\uparrow} + \gamma_{B\uparrow}^\dagger\gamma_{B\downarrow}\gamma_{A\downarrow}^\dagger\gamma_{A\uparrow} + \\ &\quad \gamma_{A\uparrow}^\dagger\gamma_{B\downarrow}\gamma_{A\downarrow}^\dagger\gamma_{B\uparrow} + \gamma_{B\uparrow}^\dagger\gamma_{A\downarrow}\gamma_{B\downarrow}^\dagger\gamma_{A\uparrow} && (5.156) \end{aligned}$$

At first sight, this does not look at all like a Heisenberg Hamiltonian. One should realize, however, that the transformation only makes sense in the presence of the vacuum amplitudes: $\gamma_{A\uparrow}^\dagger\gamma_{A\uparrow} \rightarrow \langle\gamma_{A\uparrow}^\dagger\gamma_{A\uparrow}\rangle = 1$ and $\gamma_{B\downarrow}^\dagger\gamma_{B\downarrow} \rightarrow \langle\gamma_{B\downarrow}^\dagger\gamma_{B\downarrow}\rangle = 1$, while $\gamma_{A\downarrow}^\dagger\gamma_{A\downarrow} \rightarrow 0, \gamma_{B\uparrow}^\dagger\gamma_{B\uparrow} \rightarrow 0$. Substituting these averages in (5.154) and (5.155), the terms $\hat{O}_U$ and $\hat{O}_t$ vanish - they are 'eaten' by the classical ground state. Only the last two lines of (5.156) survive, and these represent spin-flip terms ~ $S_A^+ S_B^-$: this demonstrates that the fluctuation terms $\delta\hat{\Omega}_A \delta\hat{\Omega}_B$, neglected on the mean-field level, do correspond with the operators describing the kinetic energy of the spins.

Using the representation (5.153) of the Hamiltonian to calculate the equation of motion (5.151) for the spin flips,

$$\begin{aligned} i\dot{\hat{S}}_A^+ &= [\hat{S}_A^+, H] \\ &= t(\gamma^\dagger_{A\uparrow}\gamma_{B\downarrow}(1 - \hat{n}_A + \frac{\hat{n}_B}{2} + \hat{S}^z_B) - \gamma^\dagger_{B\uparrow}\gamma_{A\downarrow}(\hat{n}_A - \frac{\hat{n}_B}{2} + \hat{S}^z_B) + \\ &\quad 2J((1 + \hat{S}^z_B)\hat{S}^+_A + \hat{S}^+_B \hat{S}^z_A) + O(\frac{t^3}{U^2}) \end{aligned} \tag{5.157}$$

using

$$\hat{n}_{A,B} = \gamma^\dagger_{A,B\uparrow}\gamma_{A,B\uparrow} + \gamma^\dagger_{A,B\downarrow}\gamma_{A,B\downarrow} \tag{5.158}$$

$$\hat{S}^z_{A,B} = \frac{1}{2}(\gamma^\dagger_{A,B\uparrow}\gamma_{A,B\uparrow} - \gamma^\dagger_{A,B\downarrow}\gamma_{A,B\downarrow}) \tag{5.159}$$

⇒ Excercise 5.29

This result is still exact for large U/t. In order to find the classical order parameter fluctuation, we have to insert the vacuum amplitudes $\hat{n}_A = \langle \hat{n}_A \rangle = 1$, $\hat{n}_B = \langle \hat{n}_B \rangle = 1$, $\hat{S}^z_A = \langle \hat{S}^z_A \rangle = 1/2$ and $\hat{S}^z_B = \langle \hat{S}^z_B \rangle = -1/2$. We obtain the classical equation of motion,

$$i\dot{\hat{S}}_A^+ = J(\hat{S}^+_A + \hat{S}^+_B) \tag{5.160}$$

This has to be repeated for every pair of neighbouring spins, and the complete classical equation of motion is,

$$i\dot{\hat{S}}^+_{\vec{i}\epsilon A} = J\sum_{\vec{\delta}}(\hat{S}^+_{\vec{i}\epsilon A} + \hat{S}^+_{\vec{i}+\vec{\delta}\epsilon B}) \tag{5.161}$$

identical with the result following from the Heisenberg model, (5.57)!

The above derivation has been taylored to deal with the low lying spin excitations. Much more can be done with RPA. For instance, one can also calculate the longitudinal spin fluctuation (fluctuation of the local moment $\hat{S}^z_{\vec{i}}$) or the charge fluctuation (fluctuation of $\hat{n}_{\vec{i}}$). These modes live at large energies ~ U and it is no longer possible to use a real space basis. At these energies, the electrons become delocalized and one has to pursue the calculations in momentum space, and it is much harder to calculate in k space (see chapter VII). The same problem is encountered even for the Goldstone modes in the weak coupling limit. However, as long as the gap is present, one recovers the same spin waves, etcetera, as in strong coupling at length scales larger than the coherence length, and energies smaller than the gap. These modes are quantized as usual, and the fluctuation behavior does not change qualitatively in going from strong- to weak coupling. There is, however, a quantitative difference: the order parameter fluctuations grow weaker for decreasing coupling! This might sound counterintuitive: the electrons themselves are more strongly delocalized and one might have anticipated more orderparameter kinetic energy as well. However, we saw in the previous section that the order parameter is composed of large numbers of overlapping electrons at scales less than the coherence length, and this acts in a similar way as long range interactions. Recall the Lieb-Mattis model of section 5.3, where we found that spatial non-locality surpresses fluctuations. The bottomline is that one should start to integrate at the ultraviolet momentum cut-off π/ξ, instead of π/a in fluctuation integrals like (5.85), which leads to a large reduction of the magnitude of the order parameter fluctuation.

5.7 Excercises

5.1 Assume that in (5.3) and (5.4) all sites, except the sites $i-1, i$ and $i+1$, are occupied in the same way. Using the fermion operators, show that $\langle l|H|l'\rangle = -t$ and $\langle l'|H|l'\rangle - \langle l|H|l\rangle = U$, where H is the Hubbard Hamiltonian (5.2).

5.2 a. Diagonalize the Hubbard hydrogen molecule (5.5) for two electrons.

  (i) Write the Hamiltonian in the configuration space basis: $|\uparrow\downarrow_1\ 0_2\rangle, |0_1\ \uparrow\downarrow_2\rangle, |\uparrow_1\ \downarrow_2\rangle$ and $|\uparrow_2\ \downarrow_1\rangle$.

  (ii) Show that $|T; N=2\rangle = (1/\sqrt{2})(|\uparrow_1\ \downarrow_2\rangle - |\uparrow_2\downarrow_1\rangle)$ and $|U; N=2\rangle = (1/\sqrt{2})(|\uparrow\downarrow_1\ 0_2\rangle - |0_1\ \uparrow\downarrow_2\rangle)$ are eigenstates of H.

  (iii) Because of (ii), only two states are left. Diagonalize this problem, to derive the ground state energy and wavefunction in the large U limit, up to order t/U (compare: (5.10)).

5.3 As was discussed in section 5.1, one finds quite often coexisting strongly-interacting and weakly interacting electrons. The toy model

$$H = \sum_\sigma [\varepsilon_s s^\dagger_\sigma s_\sigma + \varepsilon_f f^\dagger_\sigma f_\sigma + V(f^\dagger_\sigma s_\sigma + h.c.)] + U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow \qquad (5.162)$$

gives some insights about the factors influencing the correlation effects. It describes a f-like state (large U) and a s-like state which are hybridized. Solve this problem for two electrons, in the limits $U << t$ and $U >> t$. Discuss the strength of the electron-electron correlations using as criteria the surpression of double occupancy and the spin-like character of the low lying states, as function of $(\varepsilon_f - \varepsilon_s)/t$.

5.4 Verify that (5.12-5.16) is a precise decomposition of the Hubbard model (5.2).

5.5 Consider 2 electrons on a Hubbard triangle of three sites. Group the states in Hubbard sectors and use in addition the conservation of the z-component of the total spin. Solve the (intra-sector) problem for $U/t \to \infty$. How many states are found in total for 10 electrons on 20 sites? What would be the dimensionality of the lowest Hubbard sector in this case?

5.6 Show that (5.23) is solved by (5.24).

a. By substituting (5.24) in (5.23).

b. Systematically: (i) write $S^{(1)} = \sum_m S_m$, S_m being the operator creating or annihilating m doubly occupied sites for $m > 0$ or $m < 0$, respectively. Show that $[S_m, V] = -mUS_m$. (ii) It follows that $\sum_m mUS_m = T^+ + T^-$: argue that this implies (5.24).

5.7 Show that (5.27) reduces to (5.28): Prove that $\frac{1}{2}[S^{(1)}, [S^{(1)}, V]] = \frac{-1}{2U}[T^+ - T^-, T^+ - T^-]$, and (5.28) follows.

5.8 Derive (5.31) from (5.30).

5.9 Show that (5.32) reduces to (5.36). Why is $n_{\vec{i}\uparrow} + n_{\vec{i}\downarrow} = \hat{1}$?

5.10 Consider half-filling and create one additional hole ($N_e = N - 1$). Show that next to the T_0 term, an additional term appears $O(J)$, describing the delocalization of the hole. Notice that in the standard $t - J$ model this term is neglected, for no good reason.

5.11 The following extension of the simple model of excercise 3.1,

$$H = \sum_\sigma \left[\sum_{\vec{k}} \varepsilon(\vec{k}) c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \varepsilon_f f^\dagger_\sigma f_\sigma + \sum_{\vec{k}} V(f^\dagger_\sigma c_{\vec{k}\sigma} + h.c.) \right] + U f^\dagger_\uparrow f_\uparrow f^\dagger_\downarrow f_\downarrow \tag{5.163}$$

describes a single strongly interacting state, hybridizing (V) with a bath of conduction electrons with dispersion $\varepsilon(\vec{k})$. This is the 'Anderson impurity model' which is very important in the context of heavy fermion physics (Anderson's Nobel price work is actually based on this model). Assume large U, and in addition that ε_f and E_F are choosen such that $< n_f >= 1$. Use the results of section (5.2) to show that the effective low energy Hamiltonian becomes,

$$H \sim \sum_\sigma \sum_{\vec{k}} \varepsilon(\vec{k}) c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \frac{2V^2}{U} \sum_{\vec{k}\vec{k}'} \vec{S}_f \cdot \vec{s}_{\vec{k}\vec{k}'} \tag{5.164}$$

where $s^+_{\vec{k}\vec{k}'} = c^\dagger_{\vec{k}\uparrow} c_{\vec{k}'\downarrow}$, etcetera. This latter model is the equally famous Kondo model, describing a single impurity spin interacting with a Fermi-liquid.

5.12 Derive the following properties of the $S = 1/2$ spin-coherent states (5.42):

a. They are not orthogonal. Show that

$$\langle \hat{\Omega} | \hat{\Omega}' \rangle = \left(\frac{1 + \hat{\Omega} \cdot \hat{\Omega}'}{2} \right)^{1/2} e^{-i\psi} \tag{5.165}$$

where

$$\psi = arctan \left[tan(\frac{\phi - \phi'}{2}) \frac{cos[\frac{1}{2}(\theta + \theta')]}{cos[\frac{1}{2}(\theta - \theta')]} \right] \tag{5.166}$$

b. Show that the identity operator

$$\hat{1} = \frac{1}{2\pi} \int d\theta sin\theta d\phi |\hat{\Omega}\rangle\langle\hat{\Omega}| \tag{5.167}$$

c. Show that the spin operators are given by

$$\vec{S} = \frac{3}{4\pi}\int d\theta sin\theta d\phi \hat{\Omega}|\hat{\Omega}\rangle\langle\hat{\Omega}| \tag{5.168}$$

5.13 Repeat (5.41-5.46) for $S = 1$, using the results of excercise 2.35.

5.14 Consider a Heisenberg system with nearest-neighbour antiferromagnetic couplings on a *triangular* lattice (excercise 3.17). Consider only Ising configurations (spins oriented along the z-axis), and derive the classical ground state.

5.15 Verify (5.50-5.53).

5.16 Verify (5.55-5.62). Repeat this calculation for the ferromagnet.

5.17 The Holstein-Primakoff transformation. The unusual aspect of this transformation is the occurrence of the square roots in (5.66,5.67). These can only be defined in the projected Hilbert space. We use ($\hat{n}$ is the occupation number operator, f an arbitrary function),

$$f(\hat{n})|n\rangle = f(n)|n\rangle \tag{5.169}$$

a. What would happen in the *unprojected* Hilbert space?

b. The square root can be expanded as

$$\sqrt{1 - b^\dagger_{\vec{i}}b_{\vec{i}}/(2S)} = \alpha_0 + \alpha_1 b^\dagger_{\vec{i}}b_{\vec{i}} + \alpha_2(b^\dagger_{\vec{i}}b_{\vec{i}})^2 + \cdots \tag{5.170}$$

Determine the coefficients in this expansion for $S = 1/2$ en $S = 1$. What happens in the (classical) limit $S \to \infty$?

c. Show that (5.65-5.67) form a $su(2)$ algebra for all S.

d. Express the Heisenberg Hamiltonian in terms of the Holstein-Primakoff bosons for $S = 1/2$, including the boson interaction terms.

5.18 The Bogoliubov transformation for bosons.

a. Why are the hyperbolic functions used in (5.75-5.76), instead of the usual $\cos u_k/sinu_k$?

b. Verify (5.79-5.81).

5.19 In these mathematical proofs, inequalities play an important role. A simple example is the inequality due to Anderson for the ground state energy (E_0) of the antiferromagnetic Heisenberg model in d dimensions on a hypercubic lattice:

$$-NdS^2(1 + \frac{1}{2dS}) < \frac{E_0}{J} < -NdS^2 \tag{5.171}$$

This is proven as follows:

a. Show that the upper bound corresponds with the energy of the classical Néel state. Why is this energy an upper bound?

b. The lower bound is obtained as follows. The Heisenberg Hamiltonian can be written as $H = (1/2)\sum_{\vec{i}} H_{\vec{i}}$ where $H_{\vec{i}}$ describes a cluster of spins, consisting of the spin at $\vec{i}$, coupled to its $2d$ neighbours: $H_{\vec{i}} =$

$J\vec{S}_{\vec{i}} \cdot (\sum_{\vec{\delta}} \vec{S}_{\vec{i}+\vec{\delta}})$. Show that the ground state energy of $H_{\vec{i}}$ is $E_0^i = -JS(2dS+1)$. If $E_0 > (N/2)E_0^i$ the lower bound follows. Give the reason why this is the case.

Notice that it follows directly from this inequality that the Néel state becomes exact, both in the limits $S \to \infty$ *and* $d \to \infty$.

5.20 The classical limit of the Lieb-Mattis model. Interpret the spins in (5.87) as classical spins with magnitude $S = 1$.

a. Calculate the classical ground state energy. One already anticipates that the classical Néel state should be a good bet!

b. Calculate the classical modes, using (5.55-5.62).

5.21 Verify (5.95-5.101).

5.22 Use (5.45) to show that (5.113) describes a system of N_e free classical spins in the case that $t = 0$.

5.23 There is another (equivalent) way to derive the saddle point equations, which is used in cases where the classical energy is not available in closed form (e.g., numerical computations).

a. Show that according to (5.105,5.109,5.110) and (5.115)

$$\begin{aligned}\Omega &= \frac{1}{2}\sum_k \Big(\langle c^\dagger_{kA\uparrow} c_{kA\uparrow} \rangle - \langle c^\dagger_{kA\downarrow} c_{kA\downarrow} \rangle \Big) \\ \bar{n} &= \frac{1}{2}\sum_k \Big(\langle c^\dagger_{kA\uparrow} c_{kA\uparrow} \rangle + \langle c^\dagger_{kA\downarrow} c_{kA\downarrow} \rangle \Big)\end{aligned}$$

b. Use the inverse of (5.116-5.119) to express Ω, $\bar{n}$ in terms of ϕ_k.

c. ϕ_k is itself a function of Ω, $\bar{n}$. Derive this function and show that this yields, together with (a.), the saddle point equations (5.125) and (5.127).

5.24 Consider the ferromagnet in mean field theory (Ω the same everywhere). Derive the saddle point equations and show that one recovers in the large U limit the energy of the ferromagnet state as calculated from (5.36).

5.25 The classical ground state for large U.

a. Use (5.132) to calculate (5.129), following the prescription of section 1.2.

b. Determine the ground state wave function of the ferromagnet for large U/t, and calculate its energy, again using section 1.2.

5.26 The mean-field procedure is not restricted to electronic problems. It works equally well in the context of electron-phonon problems, where it even becomes more straightforward to interpret. Consider the SSH model (excercise 4.17). We consider a $d = 1$ chain, and neglect the kinetic energy of the ions,

$$H = \sum_{i\delta\sigma} t(1 + \alpha u_{i\delta}) c^\dagger_{i\sigma} c_{i+\delta\sigma} + \frac{K}{2}\sum_i u^2_{i\delta} \tag{5.172}$$

Use the fact that $u_{i\delta}$ is a classical quantity to show that for any α the chain will dimerize: the bond-lengths stagger, in chemist' notation $\cdots - . = . - . = \cdots$. This is the so-called 'Peierls instability'. Hint: calculate the energy of the dimerized state and minimize to the dimerization amplitude. Linearize, to find an expression similar to (5.134).

5.27 In principle, it is also possible to find *charge density waves* in electronic systems. This is associated with *attractive* interactions. Consider the *negative* U problem,

$$H = t \sum_{\vec{i}\vec{\delta}\sigma} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} - |U| \sum_{\vec{i}} n_{\vec{i}\uparrow} n_{\vec{i}\downarrow} \tag{5.173}$$

a. Consider half-filling and $t = 0$. Demonstrate that the lowest Hubbard sector consists entirely of configurations build from empty- and doubly occupied sites.

b. Consider strong coupling ($|t/U| << 1$). Give the qualitative reason why, on a bipartite lattice, the charge density tends to stagger: doubly occupied sites on the A sublattice and empty sites on the B sublattice.

c. Mean-field: consider a $d = 1$ chain.

   i. Show that $U n_{\vec{i}\uparrow} n_{\vec{i}\downarrow} \equiv (U/2)(n_{\vec{i}} n_{\vec{i}} - n_{\vec{i}})$, with $n_{\vec{i}} = n_{\vec{i}\uparrow} + n_{\vec{i}\downarrow}$.

   ii. Write $n_{\vec{i}} = O_{\vec{i}} + \delta O_{\vec{i}}$, with $O_{\vec{i}}$ a scalar, and show that

$$H = t \sum_{\vec{i}\vec{\delta}\sigma} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} - |U| \sum_{\vec{i}} \Big((O_{\vec{i}} - \frac{1}{2}) n_{\vec{i}} - \frac{1}{2} O^2_{\vec{i}} + \frac{1}{2} \delta O_{\vec{i}} \delta O_{\vec{i}} \Big) \tag{5.174}$$

   iii. Neglect the fluctuations and impose a two sublattice structure $O_{\vec{i}\epsilon A} > O_{\vec{i}\epsilon B}$. Solve the mean-field problem and derive analytical expressions for the charge order parameter $O_{CDW} = O_A - O_B$ and the energy, both in the weak- and the strong coupling limits.

Notice that this variety of density wave is probably not realized in nature: either the electron-phonon coupling interferes (excercise 5.26), or superconductivity takes over (next chapter).

5.28 Verify (5.148)

5.29 Verify (5.153-5.156). Repeat (5.157-5.160), but now for S^+_B - watch your personal minus sign problem!

6 Superconductivity: condensing the gauge.

Superconductivity and superfluidity (two manifestations of the same fundamental phenomenon) play a special role in the sociology of physics. When superconductivity is discovered in one or the other subfield, a flurry of activity follows instanteneously, and in no time this subfield has acquired the status of frontier of science[1]. I find this attention not quite justifyable.

I do not want to deny that superconductivity is a beautiful phenomenon, neither that its explanation is a triumph of physics. Above all, the phenomenon escapes from our daily intuition, build on the human senses. On the most superficial level, the mystique is helped by the fact that superconductivity only occurs at inhumanly low temperatures. Although large numbers of magnets and crystals persist at a comfortable temperature of 300 K, the room temperature superconductor is still a wishfull dream. Hence, we can only see the phenomenon through the window of a cryostat or in the mid of an interesting mist caused by liquid nitrogen (familiar from discotheques). This is the first reason to percieve superconductors as special - nanokelvin intellects would percieve persistent currents and the Meissner effect as unremarkable facts of life.

The next (more serious) confusion is found on the level of theoretical physics. For a long time it was believed that superconductivity is really very different from magnets or crystals. The latter would be 'just' classical physics, while superconductors are about wavefunctions, representing a singular opportunity to study quantum-mechanics on the macroscopic level. This is nonsense. Superconductivity is as classical as tables and chairs, and it fits precisely in the recipy of section 1.2.

The true beauty of superconductivity lies in its use as *demonstration* material: the power of abstraction, coming with the paradigm of section 1.2, becomes fully visible dealing with a subject as weird as superconductivity. The mathematical theory of superconductivity is actually quite close to that of magnetism. The difference is that one now deals with electrons which *attract* each other. Again a projective renormalization occurs, leading into a low energy Hilbert space which is now build from objects different from spin: 'Cooper pairs'. Interestingly, this Hilbert space has precisely the same dimension as the Hilbert space of spins, and these Cooper pairs are also subject to a $su(2)$ algebra, which is explicitely broken to $U(1)$ (on the classical level: $O(2)$, point on a circle) if the system is not electron-hole symmetric: attractive fermion systems are like XY spin systems. The real novelty is that these XY spins turn out to communicate with the vector potential of the electromagnetic field, and the local gauge symmetry of the field is broken in the classical condensate. This aspect is the key to the unusual physics of the superconducting state.

Having the lesson in mind of the previous chapter, we will first focus on the strong

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[1] An embarrassing example is the early history of high T_c superconductivity. The mere discovery of a relatively high transition temperature (35 K, instead of the previous record of 28 K) caused a mass movement which is unparallelled in the history of physics.

coupling limit (section 6.1). The theory becomes quite easy in this limit and a clear view will be obtained on the qualitative nature of superconductivity. This strong coupling limit is never approached in nature. Electrons repell each other in the physical vacuum, and to find attractions one needs at least virtual phonon exchange, as will be explained in section 6.2. Section 6.3 deals with the weak coupling limit, as described by the famous Bardeen-Cooper-Schrieffer (BCS) theory. Nature is quite often in this limit and, for reasons which will be explained, this theory gives a highly accurate, quantitative description of a large variety of measurable quantities.

6.1 The Zen of superconductivity.

In the previous chapter we learned that it is much easier to understand condensates in the strong coupling limit, than in intermediate or weak coupling. We will follow in this chapter the same strategy: first *understand* the phenomena in strong coupling to subsequently continue the theory to weak coupling. In the context of superconductivity this is particularly helpfull. The problem is with the electro-magnetic 'sector' of the theory which is about gauge invariance. I will show that it is rather easy to formulate a manifestly gauge invariant theory in strong coupling. To keep the theory tractable in weak coupling, one is forced into gauge fixing, and this makes the theory manifestly less beautiful, and somewhat unclear. Since strong coupling superconductivity is never realized in nature, we do not attempt to get any number right, and the analysis which follows is as qualitative as possible, on purpose!

Superconductivity is caused by *attractive* fermion-fermion intractions. We again start with a minimal model: the 'negative U Hubbard model',

$$H = \frac{1}{2} \sum_{\vec{i}\vec{\delta}\sigma} (t_i^\delta c^\dagger_{\vec{i}+\vec{\delta}\sigma} c_{\vec{i}\sigma} + (t_i^\delta)^* c^\dagger_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma}) - |U| \sum_{\vec{i}} n_{\vec{i}\uparrow} n_{\vec{i}\downarrow} \tag{6.1}$$

This model is identical to the standard Hubbard model, except that the sign of U is reversed. Notice also that we now insist on *complex* hopping parameters. This small fact will turn out to be of enormous importance later on. What happens when $|U|$ becomes large? We should again think in terms of the Hilbert space being split in Hubbard sectors. There is one big difference with section 5.2: because the interactions are attractive, *the lowest lying Hubbard sector is now the one containing the maximum possible number of doubly occupied sites.* With the thermodynamic potential we can force an average number of electrons per site $0 \leq n_e \leq 2$ and these electrons have to be distributed between empty and doubly occupied sites (figure 6.1).

There is in addition a 'first excited' Hubbard sector at $|U|$, containing two *singly* occupied sites, a sector at $2|U|$ containing 4 singly occupied sites, etcetera: it is the top-down version of the Hilbert space of the repulsive problem (fig. 5.3).

At half filling, there are precisely as many doubly occupied- as empty sides and the dimension of the ground state sector is 2^N: the Hilbert space has the same dimension as the Hilbert space of a $S = 1/2$ problem! This hints at a spin-like character of the physics at low energy. The crucial observation is, that the dynamics at energies

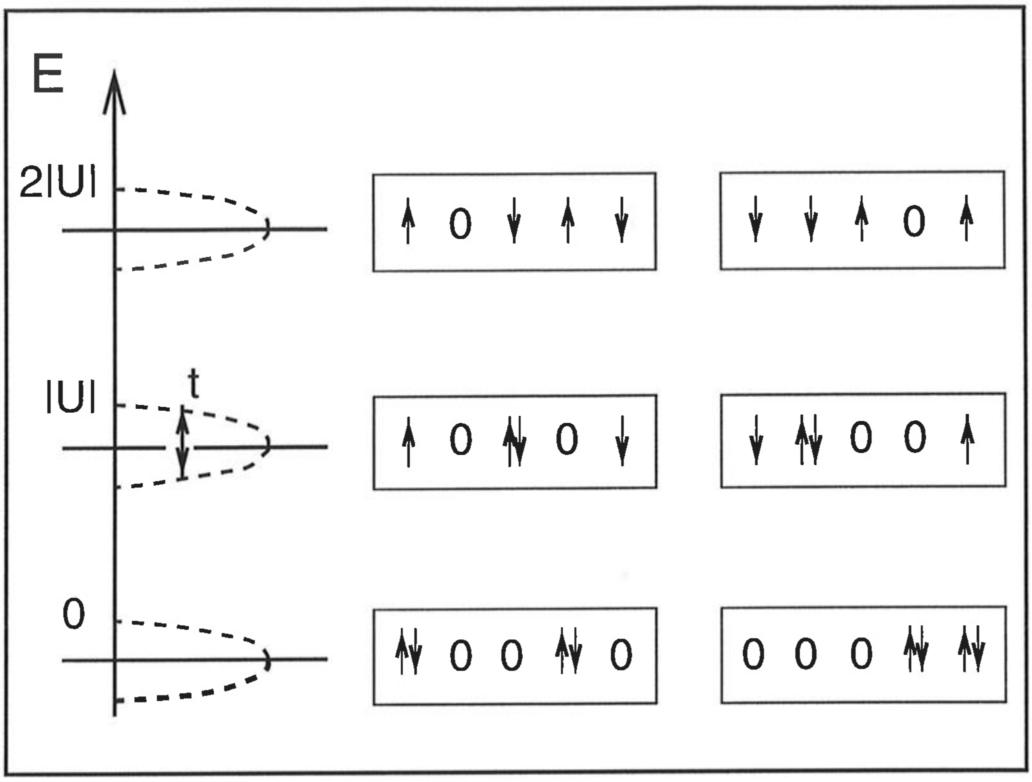

Figure 6.1: *Organization of Hilbert space for the negative U model. This is the 'bottom up' version of the Hilbert space of the repulsive problem (figure 5.3).*

$<< |U|$ can be complete described in a set of operators, obeying a $su(2)$ algebra. It is easy to deduce this algebra. In the projected Hilbert space it is only allowed to create a doubly occupied site from an empty site, or to annihilate the doubly occupied site to end up with an empty site. Let us try the operators,

$$T_{\vec{i}}^{+} = c^{\dagger}_{\vec{i}\uparrow} c^{\dagger}_{\vec{i}\downarrow} \tag{6.2}$$

$$T_{\vec{i}}^{-} = c_{\vec{i}\downarrow} c_{\vec{i}\uparrow} \tag{6.3}$$

Commuting (6.2-6.3) yields,

$$[T_{\vec{i}}^{+}, T_{\vec{i}}^{-}] = 2T_{\vec{i}}^{z} \tag{6.4}$$

$$T_{\vec{i}}^{z} = \frac{1}{2}(n_{\vec{i}\uparrow} + n_{\vec{i}\downarrow} - 1) \tag{6.5}$$

It is a mathematical fact that (6.2,6.3) and (6.5) form a $su(2)$ algebra. Let me call this the Cooper algebra, honoring the inventor of the two-fermion bound state.

$\Longrightarrow$ Excercise 6.1

To derive the strong coupling Hamiltonian, we have again to apply the canonical perturbation theory of section 5.2. Let me explain the principle, leaving the detailed calculation as an excercise for the reader. We observe that virtual hoppings can only occur between nearest-neighbour sites, if one of the sites is empty and the other

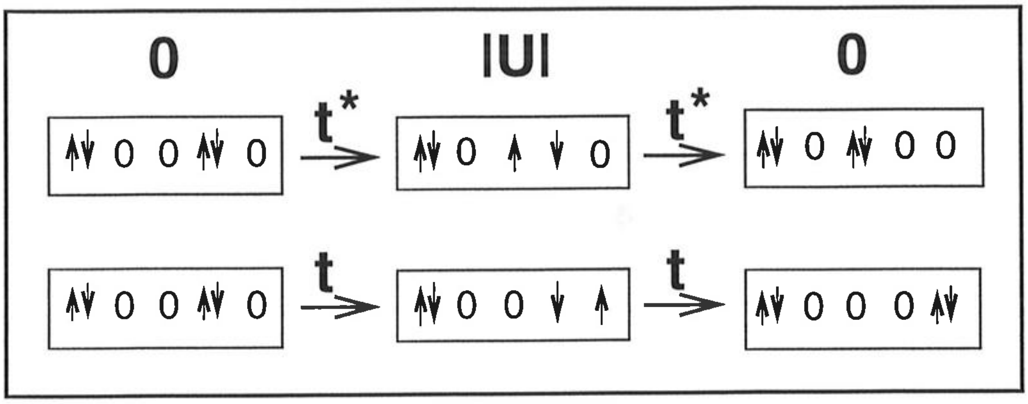

Figure 6.2:*Exchange of doubly occupied- and empty sites, giving rise to the spin-flip like terms in the Hamiltonian. Notice that the tunneling rate of the 'right moving' pair is the complex conjugate of that of the 'left moving' pair.*

doubly occupied (figure 6.1). The first possibility is to empty the doubly occupied site and to doubly occupy the empty site (figure 6.2).

Recalling the discussion in section 5.2, we directly recognize that these processes add terms to the effective Hamiltonian $\sim T^-_{\vec{i}} T^+_{\vec{i}+\vec{\delta}}$ with a prefactor $\sim t^2/|U|$. Compared to superexchange, there is a subtle but very important difference. In the superexchange process the electron jumped forth and back, ending up at the site where it started: using complex hoppings $J \sim tt^*/U = |t|^2/U$ and J is always a real quantity. In the attractive case, both electrons move in the same direction and the J is therefore a complex quantity if the t's are complex - this small fact will turn out to be responsible for the peculiarities of the superconducting state. Summarizing, the virtual hoppings of figure 6.2 contribute to the effective Hamiltonian the term,

$$H^{(2b)}_{eff} = \sum_{\vec{i}\vec{\delta}} \left(\frac{(t^{\delta}_{\vec{i}})^2}{|U|} T^+_{\vec{i}} T^-_{\vec{i}+\vec{\delta}} + \frac{((t^{\delta}_{\vec{i}})^2)^*}{|U|} T^-_{\vec{i}} T^+_{\vec{i}+\vec{\delta}} \right) \tag{6.6}$$

It is also possible for the electron to hop back to the lattice site where it started (figure 6.3). These 'stay at home' processes are equivalent to the non-spin reversing processes in the repulsive model, and they turn out to give rise to the same contribution as in the spin case (compare 5.36), but now in terms of the Cooper z-axis operators (6.5),

$$H^{(2a)}_{eff} = 2 \sum_{\vec{i}\vec{\delta}} \frac{|t^{\delta}_{\vec{i}}|^2}{|U|} \left(T^z_{\vec{i}} T^z_{\vec{i}+\vec{\delta}} - \frac{1}{4} \right) \tag{6.7}$$

Together with (6.6), this implies that at half-filling the attractive fermion system is precisely described in terms of a Heisenberg Hamiltonian, with the only difference that the physical meaning of the $su(2)$ algebra is now different.

A crucial difference with the repulsive problem is that the spin-like nature of the low energy sector is *not* restricted to the special, charge commensurate electron density. Regardless the filling, the low energy sector will always contain only doubly occupied- and empty sites and the 'fermionic' singly occupied sites are always projected out.

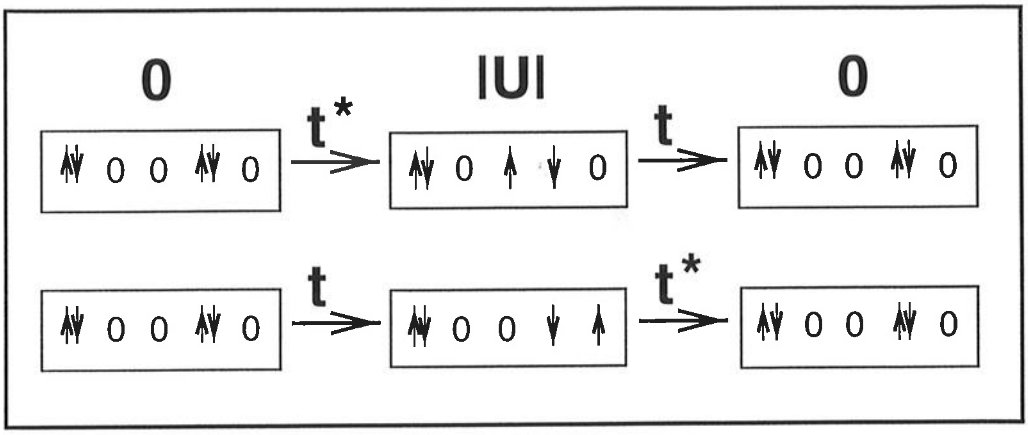

Figure 6.3: *Virtual fluctuations where the pair returns to the site where it started. These processes give rise to the Ising terms in the effective spin Hamiltonian.*

Hence, the system is completely described in terms of the $su(2)$ algebra at all fillings. In section 6.3 we will find that this is also true in the weak coupling limit: the attractive problem turns out to be automatically nested, and superconductivity occurs for every finite attractive interaction. The filling of the system has nevertheless a fundamental influence. Away from half-filling one looses the $su(2)$ global symmetry which characterizes the Hamiltonian (6.6-6.7): the 'spin' z-axis becomes inequivalent from the xy plane. This can be seen directly. The T^z operator (6.5) measures the electron density: the $m_s = -1/2$ state corresponds with an empty site and the $m_s = 1/2$ state with a doubly occupied state. When the average electron density $n_e \neq 1$ there are either more empty- ($n_e < 1$) or more doubly occupied sites ($n_e > 1$). Accordingly, there is always a net 'magnetization' due to the external influence of the thermodynamic potential. Using the definition of T^z, it is immediately seen that the Hamiltonian also contains the term,

$$H^0 = -(|U| + 2\mu) \sum_{\vec{i}} \left(T^z_{\vec{i}} + \frac{1}{2} \right) \tag{6.8}$$

The energy of an empty site ($m_s = -1/2$) is zero, while a doubly occupied site costs $-|U| - 2\mu$. The thermodynamic potential (μ) acts as an effective external magnetic field pointing along the z-axis, which only vanishes when $\mu = -|U|/2$, corresponding with half-filling! This expresses the simple fact that away from half-filling there is no electron-hole symmetry. What remains is the XY symmetry ($U(1)$) of (6.6) and this symmetry is spontaneously broken in the superconducting state[2].

$\Longrightarrow$ Excercise 6.2

Let us now turn to the classical sector of the problem (6.6-6.8). We have learned how to construct the classical limit of spin-problems in section 5.3. We again use the $S = 1/2$ spin coherent state (5.42) and the wave function of the classical state now becomes in terms of the fermion operators,

$$|\Phi^0_{Cl}(\{\hat{\Omega}\})\rangle = \Pi_{\vec{i}} \left(e^{-i\phi_{\vec{i}}/2} \sin(\theta_{\vec{i}}/2) + e^{i\phi_{\vec{i}}/2} \cos(\theta_{\vec{i}}/2) c^\dagger_{\vec{i}\uparrow} c^\dagger_{\vec{i}\downarrow} \right) |vac\rangle \tag{6.9}$$

The empty- and doubly occupied sites take the role of the up- and down fermions of the real spin problem. The hopping is parametrized in terms of an absolute value t which is uniform on the lattice and a phase $\psi^{\vec{\delta}}_{\vec{i}}$ which depends on the bond under consideration,

$$t^{\delta}_{\vec{i}} = t e^{i\psi^{\vec{\delta}}_{\vec{i}}} \tag{6.10}$$

and the classical energy becomes, using (5.43) ($J = 2t^2/|U|$),

$$\begin{aligned} H^{Cl}_{SC} &= \langle \Phi^0_{Cl}(\{\hat{\Omega}\}) | H^0 + H^{2a}_{eff} + H^{2b}_{eff} | \Phi^0_{Cl}(\{\hat{\Omega}\}) \rangle \\ &= -(|U| + 2\mu) \sum_{\vec{i}} \left(\frac{1}{2} (\cos(\theta_{\vec{i}}) + 1) \right) + \frac{J}{4} \sum_{\vec{i}\vec{\delta}} \Big(\cos(\theta_{\vec{i}}) \cos(\theta_{\vec{i}+\vec{\delta}}) \\ &\quad + \sin(\theta_{\vec{i}}) \sin(\theta_{\vec{i}+\vec{\delta}}) \cos(2\psi^{\delta}_{\vec{i}} - \phi_{\vec{i}+\delta} + \phi_{\vec{i}}) \Big) \end{aligned} \tag{6.11}$$

$\Longrightarrow$ Excercise 6.3

How to interpret this expression? When the system is half-filled ($\mu = -|U|/2$) the external field vanishes and we could choose the spins to lie along the z-axis. Because the interaction is 'anti-ferromagnetic' this would give rise to a staggering of the T^z component. According to (6.5), this state corresponds with a charge density wave: doubly occupied sites on the A sublattice and empty sites on the B sublattice. Going away from half-filling ($\mu \neq |U|/2$) the spins 'flop' to the xy-plane and the effective magnetic field cants the spins uniformly in the (positive or negative) z-direction, just as would be the case for a Heisenberg antiferromagnetic in a real magnetic field (figure 6.4). Although the z-component is fixed by the external field, it is still possible to rotate the spins in the xy-plane: the $O(3)$ symmetry is explicitely broken to $O(2)$ (point on a circle), corresponding with the free rotations in the xy-plane, parametrized by the phase angle $\phi_{\vec{i}}$. This $O(2)$ symmetry gets spontaneously broken. At energies or temperatures much smaller than $||U| + 2\mu|$, the 'diagonal' charge density $\langle T^z \rangle$

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[2] It is straightforward to show that non-local Coulomb interactions give rise to extra Ising-like contributions to the Hamiltonian. The fundamental symmetry in the charge sector is therefore not $SU(2)$, but instead $U(1)$. Notice that for this reason it is always possible to find a non-zero average charge-density: the symmetry is explicitely broken in the density channel T^z because there are more particles than holes in the universe. (6.1) at half-filling is exceptional: for instance, at half-filling the charge density would become a purely fluctuating quantity! Notice that in the presence of longer range interactions it is possible to stabilize either superconducting- or charge density wave order at half-filling: see R. Micnas, J. Ranninger and S. Robaszkiewicz, Rev. Mod. Phys. 62, 113 (1990).

does not fluctuate and $\theta_{\vec{i}}$ takes some uniform value. We find therefore the following effective problem at low energies,

$$H^{Cl}_{eff}(\{\phi_{\vec{i}}\}) = J\rho(t,U,\mu)\sum_{\vec{i}\vec{\delta}}\cos\left(2\psi^{\vec{\delta}}_{\vec{i}} - \phi_{\vec{i}+\vec{\delta}} + \phi_{\vec{i}}\right) \tag{6.12}$$

where the effects of the uninteresting z-axis interactions are stored in the density ρ - we only need that this quantity is finite. It is directly seen that the classical energy is minimized, taking

$$2\psi^{\vec{\delta}}_{\vec{i}} - (\phi_{\vec{i}+\vec{\delta}} - \phi_{\vec{i}}) = \pi\ ,\ \forall\vec{i},\vec{\delta} \tag{6.13}$$

the symmetry in the phase channel is spontaneously broken and (6.13) is the definition of the *superconducting order parameter.* To visualize this order, it is convenient to assume that $\psi^{\vec{\delta}}_{\vec{i}} = 0$ everywhere, and in this case the spin order is as indicated in figure 6.4.

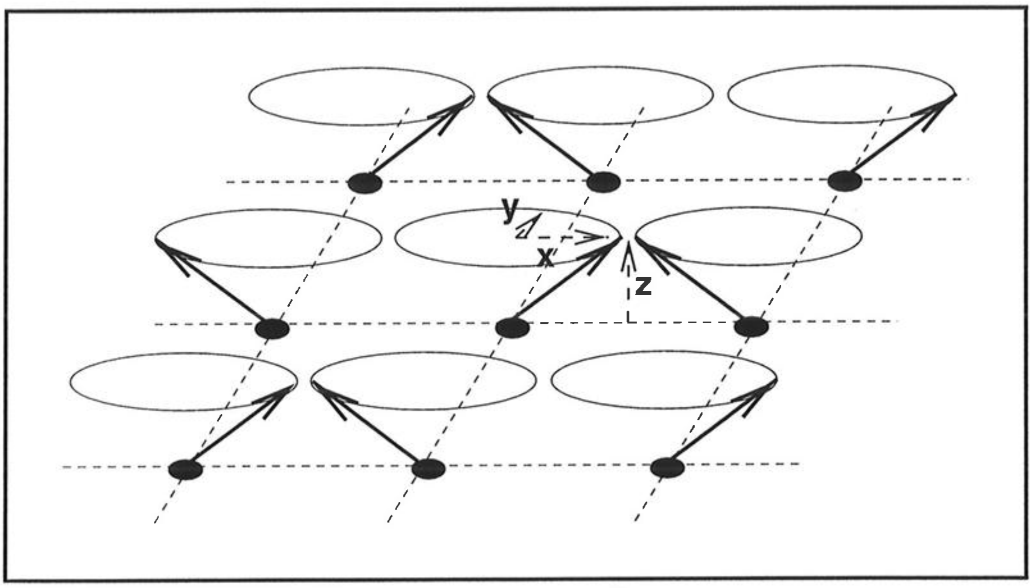

Figure 6.4: *The superconducting order parameter on a square lattice in terms of the 'Cooper' spins for a gauge* $\psi = 0$. *The spins are uniformly canted out of the* XY *plane and the z-component of the spin is a measure of the charge density, while the ordering in the* XY *direction causes the superconductivity. Notice that the orientation of the spin z axis with regard to the square lattice is arbitrary.*

Up to this point, the discussion of superconductivity appeared as a marginal extension of the spin-ordering as discussed extensively in the previous chapter. Nevertheless, the physical nature of the order (6.13) is completely different from magnetism. It is seen that (6.13) also amounts to a condition on the *phase of the hopping*: $2\psi^{\vec{\delta}}_{\vec{i}}$ has to be compensated by the difference of the intrinsic phases $\phi_{\vec{i}+\vec{\delta}} - \phi_{\vec{i}}$. Now it comes: *the phase of the hopping* $2\psi^{\delta}_{\vec{i}}$ *is directly proportional to the vector potential of* *the electromagnetic field.* The vector potential is usually gauge invariant, but (6.13) breaks this gauge invariance!

Electromagnetism, as all fundamental bosonic fields, is characterized by a local symmetry: gauge invariance. In case of the electromagnetic field, this means that that at every point in space a gradient of a function can be added to the vector potential, leaving the physics the same,

$$\vec{A}(\vec{r}) \rightarrow \vec{A}(\vec{r}) + \vec{\nabla} f(\vec{r}) \tag{6.14}$$

With the advent of quantum-mechanics, the meaning of this symmetry became clear. The interaction between charged matter and the electromagnetic field is expressed in the minimal coupling form,

$$\left[\frac{\hbar^2}{2m} (\vec{\nabla} + i\frac{e}{\hbar c}\vec{A}(\vec{r}))^2 + H_{pot} \right] \Psi = E\Psi \tag{6.15}$$

It is easy to check that the transformation (6.14) can be precisely cancelled by adjusting the sign of the wave function,

$$\begin{aligned} H(\vec{A}) &\rightarrow H(\vec{A} + \vec{\nabla} f) \\ \Psi &\rightarrow \Psi e^{-i\phi(\vec{r})} && (6.16) \\ \phi(\vec{r}) &= \frac{e}{\hbar c} f(\vec{r}) && (6.17) \end{aligned}$$

so that before and after the transformation $H\Psi = E\Psi$.

$\Longrightarrow$ Excercise 6.4

The gauge invariance of the field reflects the fact that it is not possible to determine the absolute phase of the wavefunction, because only the probability amplitude $|\Psi|^2$ relates to measurable quantities. This is true for all exact quantum-mechanical states, including the exact eigenstates of (6.5-6.7). We learned in the previous chapters that nevertheless non-exact 'classical' states are realized in the thermodynamic limit, which violate quantum-mechanical symmetry requirements. The specialty of the superconducting condensate (6.13) is that *it breaks the fundamental gauge symmetry (6.14,6.16,6.17)*!

To see how this works in the present strong coupling limit, we have first to find out how the vector potential appears in the Hubbard model. The vector potential influences the kinetic term in the Schrödiner equation (6.15), and we expect therefore that it enters in the hopping term. A minimal form for the interaction between the lattice fermions and the electromagnetic field is derived as follows (the 'Peierls construction'): we assume that we are dealing with well-localized tight-binding orbitals. In addition, we assume that the orbitals do not change their shape ('polarize') in the presence of the field. The shape of the electronic orbitals can only change by admixing other orbitals and because these are at high energy, the polarization due to the (small) field will be quite insignificant[3]. We choose the components A^δ of the vector potential $\vec{A}(\vec{r})$

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[3] Notice that these polarizations are responsible for the dielectric response of insulators.

along the bond axis and because the electronic wave functions on the sites can only acquire an overall phase, the hopping term transforms as

$$c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} \rightarrow e^{i\frac{e}{\hbar c}(f(\vec{R}_{\vec{i}}+a\vec{\delta})-f(\vec{R}_{\vec{i}}))} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} \tag{6.18}$$

under the gauge transformation (6.16-6.17). At the same time, because of (6.14),

$$\int_{\vec{R}_{\vec{i}}}^{\vec{R}_{\vec{i}}+a\vec{\delta}} dt A^{\delta}(t) \rightarrow \int_{\vec{R}_{\vec{i}}}^{\vec{R}_{\vec{i}}+a\vec{\delta}} dt A^{\delta}(t) + f(\vec{R}_{\vec{i}}+a\vec{\delta}) - f(\vec{R}_{\vec{i}}) \tag{6.19}$$

(6.18) and (6.19) imply that the hopping part of the Hamiltonian in the presence of a vector potential becomes,

$$H_{kin} = \sum_{\vec{i}\vec{\delta}\sigma} \left[e^{-i\frac{e}{\hbar c}\int_{\vec{R}_{\vec{i}}}^{\vec{R}_{\vec{i}}+a\vec{\delta}} dt A^{\delta}(t)} c^{\dagger}_{\vec{i}\sigma} c_{\vec{i}+\vec{\delta}\sigma} + h.c. \right] \tag{6.20}$$

This is the simplest gauge invariant lattice kinetic energy which can be imagined. We now understand the meaning of the phase of the complex hopping (6.10),

$$\psi^{\delta}_{\vec{i}} = \frac{e}{\hbar c} \int_{\vec{R}_{\vec{i}}}^{\vec{R}_{\vec{i}}+a\vec{\delta}} dt A^{\delta}(t) = \frac{e}{\hbar c} a \bar{A}^{\delta}_{\vec{i}} \tag{6.21}$$

$\psi^{\delta}_{\vec{i}}$ is proportional to the average of the vector potential $\bar{A}$ on the bond $\vec{i}, \vec{\delta}$!

The implication of the orderparameter (6.13) becomes now clear,

$$\bar{A}^{\delta}_{\vec{i}} = -\frac{\hbar c}{2e} \frac{\phi_{\vec{i}+\vec{\delta}} - \phi_{\vec{i}} - \pi}{a} \tag{6.22}$$

Considering length scales much larger than the lattice constant a, (6.22) can be written as (the factor π can be gauged away),

$$\vec{A}(\vec{r}) = -\frac{\hbar c}{2e} \vec{\nabla} \phi(\vec{r}) \tag{6.23}$$

The condensate *forces* the vectorpotential to take the form of the gradient of a function, while the function itself is still arbitrary! The magnetic field corresponds with the *rotation* of $\vec{A}$ and the gradient of a function is rotation free,

$$\vec{B} = \vec{\nabla} \times \vec{A} \sim \vec{\nabla} \times \vec{\nabla} \phi = 0 \tag{6.24}$$

A magnetic field cannot exist in the superconducting condensate ! This is the Meissner effect. The magnetic field expulsion is a manifestation of the classical *rigidity* of the superconducting state.

From its name it is already clear that a superconductor carries electric current. Usually, we associate conducting behaviour with fluids. In a deep sense, the superconductor is *not* a fluid. It is a special solid. The specialty of the (super)current in a superconductor is that it persists: it never stops flowing after it is set into motion. This is another manifestation of the *rigidity* of the superconducting state. The

Goldstone mode of the superconducting state carries current, and because Goldstone modes do not decay in a finite time (section 4.4), the supercurrent flows forever!

The current operator is the time derivative of the total polarization. The polarization operator ($\vec{P}_{tot}$) can be written as the sum of the products of the position vectors and the local charge densities. In the projected Hilbert space, the local charge densities can be expressed in terms of the operators measuring double occupancy,

$$\vec{P}_{tot} = \sum_{\vec{i}} \vec{R}_{\vec{i}}\, 2(T^z_{\vec{i}} + \frac{1}{2}) \tag{6.25}$$

and the current operator is given by,

$$\vec{J}_{tot} = -\frac{ie}{\hbar}\left[H, \vec{P}_{tot}\right] \tag{6.26}$$

$\vec{P}_{tot}$ commutes with (6.7) and (6.8), and

$$\begin{aligned}
\vec{J}_{tot} &= -\frac{ie}{\hbar}\left[H^{2b}_{eff}, \vec{P}_{tot}\right] && (6.27)\\
&= -\frac{2ie}{\hbar} J \sum_{\vec{i}\vec{\delta}} (\vec{R}_{\vec{i}+\vec{\delta}} - \vec{R}_{\vec{i}})(e^{2i\psi^{\delta}_{\vec{i}}} T^+_{\vec{i}} T^-_{\vec{i}+\vec{\delta}} - e^{-2i\psi^{\delta}_{\vec{i}}} T^-_{\vec{i}} T^+_{\vec{i}+\vec{\delta}}) && (6.28)
\end{aligned}$$

The total current is a macroscopic quantity and it therefore make sense to define the *classical* current as the expectation value of the current operator in the classical state (6.9) (fixing θ),

$$\begin{aligned}
\vec{J}^{Cl}_{tot} &= \langle \{\theta, \phi_{\vec{i}}\} | \vec{J}_{tot} | \{\theta, \phi_{\vec{i}}\} \rangle && (6.29)\\
&= \frac{4e}{\hbar} J\rho \sum_{\vec{i}} (\vec{R}_{\vec{i}+\vec{\delta}} - \vec{R}_{\vec{i}}) \sin\left(\frac{2ea}{\hbar c} \bar{A}^{\delta}_{\vec{i}} - (\phi_{\vec{i}+\vec{\delta}} - \phi_{\vec{i}})\right) && (6.30)
\end{aligned}$$

$\Longrightarrow$ Excercise 6.5

(6.30) is quite interesting. It states that the current is proportional to the sinus of the quantity

$$\chi^{\delta}_{\vec{i}} = \frac{2ea}{\hbar c} \bar{A}^{\delta}_{\vec{i}} - (\phi_{\vec{i}+\vec{\delta}} - \phi_{\vec{i}}) \tag{6.31}$$

summed over all bonds. On the other hand, the energy goes like the cosine of χ and we found $\chi^{\delta}_{\vec{i}} = \pi$, $\forall \vec{i}, \vec{\delta}$ (6.13) in the ground state. Hence, there is no current flowing in the ground state of the superconductor. Recall that in the superconducting condensate a continuous symmetry ($O(2)$) is broken. Because this is a non-exact symmetry breaking, there has to be a Goldstone mode present with a dispersion relation $\omega_q = cq$ and a diminishing decay rate in the long wavelength limit. Let us imagine that in some past time, Goldstone modes would have been excited at $\vec{q}$ and $-\vec{q}$ such that a standing Goldstone mode is frozen in in the superconductor. This standing wave corresponds with a slow, spatial precession of the XY arrows on the $O(2)$ circles. To visualize this, fix the gauge by $\bar{A} = \pi\hbar c/(2ea)$ and a standing

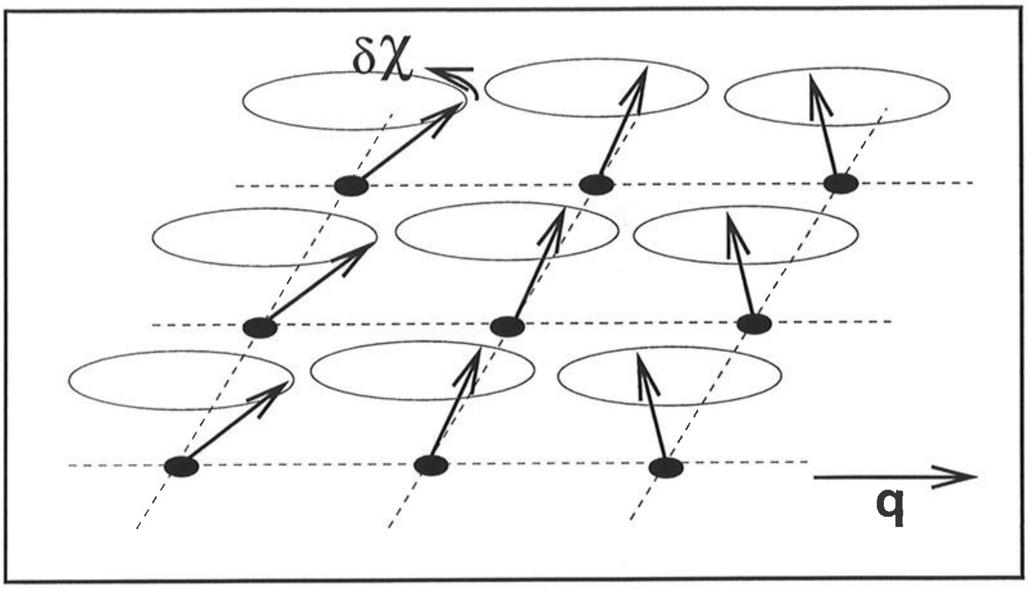

Figure 6.5: *The 'spin configuration' corresponding with a supercurrent flowing in the* q *direction, fixing the gauge at* $\bar{A} = \pi\hbar c/(2ea)$ *(exaggurated).*

Goldstone mode in the x direction in the lattice would appear as indicated in figure 6.5.

We observe that the differences between the relative orientations of spins on neighbouring sites is constant in space, and this is also true if we 'free' the gauge,

$$\begin{aligned} \chi^{\delta}_{\vec{i}} &= \pi + (\delta\chi^{\vec{\delta}}_{\vec{i}}) \\ &\rightarrow \pi + (\delta\chi^{\vec{\delta}}_{GM}) \end{aligned} \tag{6.32}$$

For large wavelength, $\delta\chi_{GM}$ becomes small and we can expand (6.12) and (6.30) as,

$$E^{Cl} \rightarrow E^{Cl}_0 + J\rho\sum_{\vec{\delta}}(\delta\chi^{\vec{\delta}}_{GM})^2 \tag{6.33}$$

$$J^{Cl}_{\vec{\delta}} \rightarrow -\frac{4Nea}{\hbar}J\rho(\delta\chi^{\vec{\delta}}_{GM}) \tag{6.34}$$

the potential energy increases quadratically with the displacement $\delta\chi$ and this implies that $\omega_q = cq$. The surprise is in (6.34): in the presence of the Goldstone mode, a current flows which increases when the wavelength of the Goldstone mode decreases!

Finally, how to put the supercurrent into motion? We already found that the magnetic field communicates with the rigidity of the superconducting state: it is the equivalent of a hammer exciting phonons in a crystal! We saw that in the bulk of the superconductor the vector field $\vec{A}$ should be rotation free. What happens near the surface of a superconductor? According to the Maxwell equations, it is not possible for the magnetic field to vanish suddenly. On the other hand, one needs electric currents to screen the magnetic field and in the superconductor this is the supercurrent. For a time independent field,

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c}\vec{J}^{Cl} \tag{6.35}$$

In general,

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{B}) = -\nabla^2 \vec{B} \tag{6.36}$$

On the left hand side of (6.36) we find the rotation of the supercurrent. The supercurrent on its turn is proportional to $(\delta \vec{\chi})$ which contains the variation of the gradient of the intrinsic phase $\vec{\nabla}\phi$ and the variation of $\vec{A}$ itself. Because the rotation of the gradient of ϕ vanishes, the rotation of the superconductor has to be caused by the rotation of the vector potential itself,

$$\vec{\nabla} \times \vec{J}^{Cl} \sim \vec{\nabla} \times (\delta \vec{A} - \delta \vec{\nabla} \phi) = \vec{\nabla} \times (\delta \vec{A}) = \vec{B} \tag{6.37}$$

Combining (6.36) and (6.37),

$$\nabla^2 \vec{B} = \frac{1}{\lambda_L^2} \vec{B} \tag{6.38}$$

This implies that the magnetic field decays exponentially in the superconductor as $B = B_0 e^{-x/\lambda_L}$, with a characteristic length scale λ_L (in this case, $\lambda_L = \hbar^2 c^2 / (32 \pi e^2 a^2 J \rho)$ in Gaussian units) which is called the "London penetration depth".

The above is all what can be said about the fundamental nature of the superconducting state. In fact, the above description is far superior to the standard treatment one finds in older books. The reason is that superconductivity is, for good reasons, realized in nature near to its *weak coupling* limit. We learned already in the previous chapter that the technical complications one faces in this limit tend to obscure a clear view on the physics. This is especially true in the case of superconductivity. The reason is that the vector potential is an *integral part* of the order parameter (6.13). Also in the condensate there is still a remnant of the gauge freedom, and this is visible in the above ('manifest gauge invariant') treatment. The meaning of gauge invariance is that $\vec{A}$ at some particular position in space can be changed from a small number to a large number at will, without changing the physics. This is still true in the superconducting state: $\vec{A}$ can be still changed from very small to very large, but in the condensate this transformation is constrained by the requirement that this change has to correspond with the gradient of the phase field ϕ. Recall the ambiguity in drawing the arrows in figures 6.4 and 6.6: for an arbitrary allowed gauge, these arrows would have pointed in many different directions and in order to draw a picture we had to fix the gauge $\vec{A} = 0$ or $\pi \hbar c / (2ea)$.

The problem in weak coupling is that it is very hard to formulate the theory in a gauge invariant way. Regauging the vector-potential appears in weak coupling as if one switches on very strong interactions. For instance, starting with $\vec{A} = 0$ on a particular bond, a genuine gauge transformation might change the phase of the hopping into π, thereby changing the sign of the hopping on this bond. At the end of the calculation this will not make a difference, but halfway the calculation one has to keep track of these phases and this is not easy. Instead, one chooses some particular gauge at the beginning of the calculation (gauge fixing). For instance, in the standard weak coupling theory (section 6.3) one picks $\vec{A} = \vec{\phi} = 0$, and in the linear response theory for measurable quantities one considers the vector potential as a small perturbation. This obscures the physics, and one is much better off in strong coupling: at large length scales, physics is invariant under coupling strength.

6.2 Attractive electron-electron interactions.

At the moment that attractive interactions are present in a fermion system, superconductivity becomes a nearly unavoidable fate. The undistinguishable fermions, relevant to condensed matter physics, have here a problem: they are subject to the electromagnetic interactions and these fermions repell each other because they carry equal charges. This is different in nuclear matter. The strong force is attractive and on short length scales it dominates over electromagnetic forces. As a consequence, superconducting correlations are common in nuclear matter. The most spectacular examples are neutron stars: they are believed to be balls of superfluid of truely cosmic dimension.

At low energies, the only fermions which are not locked in a crystalline state are the electron and ^3He, both characterized by repulsive bare interactions. The effective attractive interactions, giving rise to superconductivity/superfluidity in electron systems and ^3He, have to be therefore of a collective, 'emergent' nature, involving many particle physics. It follows immediately that the characteristic energy scales of these interactions have to be rather small. This is the reason that the phenomenon of superconductivity is only found at rather low temperatures[4].

The vast majority of superconductors are of the 'conventional' kind, where convential means (as usual) 'well understood'. The source of the attraction in these superconductors is the *virtual exchange of phonons between the electrons.* In chapter IV, we already found that the non-adiabatic corrections in the electron-lattice problem gave rise to the electron-phonon interaction, which looked quite similar to the minimal coupling between photons and charged particles underlying the electromagnetic interactions. As will be shown in detail in this section, there is an important difference between electromagnetism and the electron-phonon problem: the virtual exchange of phonons between low energy electrons gives rise to *attractive* interactions between the electrons. Next to this 'phonon-mediated' superconductivity, there is a class of superconductors/superfluids which is called unconventional. These include ^3He, heavy-fermion-, and organic superconductors and, last but not least, the oxide high T_c superconductors. All they have in common is that the mechanism leading to superconductivity is not quite understood. It is believed that in ^3He- and the heavy fermion systems, spin excitations play the role of the phonons of the conventional superconductors. The problem here is mainly of a technical nature: the theory of

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[4] In addition, superfluidity also occurs in the boson system ^4He. This is on the fundamental level the same as the fermionic superfluidity discussed up to now: the Cooper pair is like one boson with a hard-core interaction. Unfortunately, due to the persistent misunderstanding that Boson-superfluidity has something to do with Bose-Einstein condensation (which is not the case), the standard microscopic theory of ^4He is severely flawed. At present, this theory is under reconstruction by the author.

spin-fluctuation mediated superconductivity/superfluidity is much harder to control than the phonon version. In the organics and especially the high T_c superconductors the situation is much worse. The metallic reference state found at temperatures above the superconducting transition temperature seems unrelated to the Fermi-liquid state. In chapter VII it will be explained that the existence of a Fermi-liquid 'condensate' is a necessary requirement for the existence of fermionic (electron-like) low energy excitations. In the metallic state of the high T_c superconductors and the organics there are apparently no electrons! It is not at all clear what exists instead, let alone that one can address the superconducting instability of this mysterious state.

Let us turn to the conventional superconductors. The theory of those is one of the triumphs of conventional quantum condensed matter physics. The understanding of the full ('Eliashberg-Migdal-Gorkov') theory requires the diagrams and Green's functions as introduced in chapter VII. However, the qualitative features of this theory can be seen using less sophisticated means, as will be demonstrated in the remainder of this section, and in the next section. This form of superconductivity occurs as an instability of the Fermi-liquid state. This highly non-trivial state will be discussed in more detail in the next chapter, and in the present context you only need to know the rough features of this state:

1. Next to bosonic Goldstone modes (zero-sound, plasmons), the Fermi-liquid condensate also carries fermionic 'modes': the quasiparticles. In many regards, these look like band structure electrons. They have a dispersion, while they are counted as fermions, and they define a Fermi-energy and a Fermi-surface.

2. In contrast to the band-electrons, these quasiparticles are only well defined in the low energy limit - in this respect, they are like Goldstone modes. In the approach to the $\omega \to 0$ limit, their mutual interactions become weaker and weaker, to vanish when $\omega = 0$. Their energy is counted from the Fermi-energy: $\omega = E_F - \varepsilon_{\vec{k}}$ or $\omega = -E_F + \varepsilon_{\vec{k}}$ for quasiparticles or quasiholes, respectively.

3. In contrast to the quasiparticle-quasiparticle interactions, the electron-phonon interaction is unrenormalized on the scale of the Einstein frequency. At energies $\omega \sim \omega_E (<< E_F)$ the electron-phonon is of the same order as for real electrons. Going to lower energies, also the effective quasiparticle-phonon interactions become weaker and weaker, and the lowest energy quasiparticles are decoupled from the long-wavelength acoustic phonons.

The last statement applies to *real* phonons; it is still possible for the low energy quasiparticle to interact with *virtual* phonons at $\omega \sim \omega_E$, and this interaction is of the order of the bare interaction. The following model describes the essence of the problem,

$$
\begin{aligned}
H_{eff} &= H_0 + H_1 && (6.39)\\
H_0 &= \sum_{\vec{k}\sigma} (\varepsilon_{\vec{k}} - \mu) c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma} + \omega_E \sum_{\vec{q}} b^{\dagger}_{\vec{q}} b_{\vec{q}} \quad , && (6.40)\\
H_1 &= \mathcal{M} \sum_{\vec{k}\vec{q}\sigma} c^{\dagger}_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} \left(b_{\vec{q}} + b^{\dagger}_{-\vec{q}} \right) \quad , && (6.41)
\end{aligned}
$$

where $c^\dagger$ now creates a quasiparticle at energy $\varepsilon_{\vec{k}} - \mu$ (μ is the thermodynamic potential, $\mu = E_F$ at $T = 0$), while $b^\dagger_{\vec{k}}$ creates a localized 'Einstein' phonon. This model is quite similar to the Holstein model (4.83). Because the interest is in the phonons at the Einstein frequency, their dispersion might as well be neglected. For the same reason, the quasiparticle-phonon interaction H_1 can be taken to be local in space, compare with Eq. (4.79).

We now focus on the lowest lying quasiparticle excitations with energy $|\varepsilon_k - \mu| << \omega_E$. In direct analogy with the discussion in sections 5.2 and 6.1, we find that the Hilbert space of the problem splits up in sectors, which are now labelled by the number of excited phonons, instead of the number of doubly occupied sites. We span up the Hilbert space with the direct product of the quasiparticle- and phonon Fock spaces, to find a ground state sector characterized by zero-occupancy of the phonon state, and any configuration in quasiparticle Fock space, as long as its excitation energy is small compared to ω_E (figure 6.6). The first excited sector is characterized by one excited phonon, and any allowed quasiparticle configuration, etcetera.

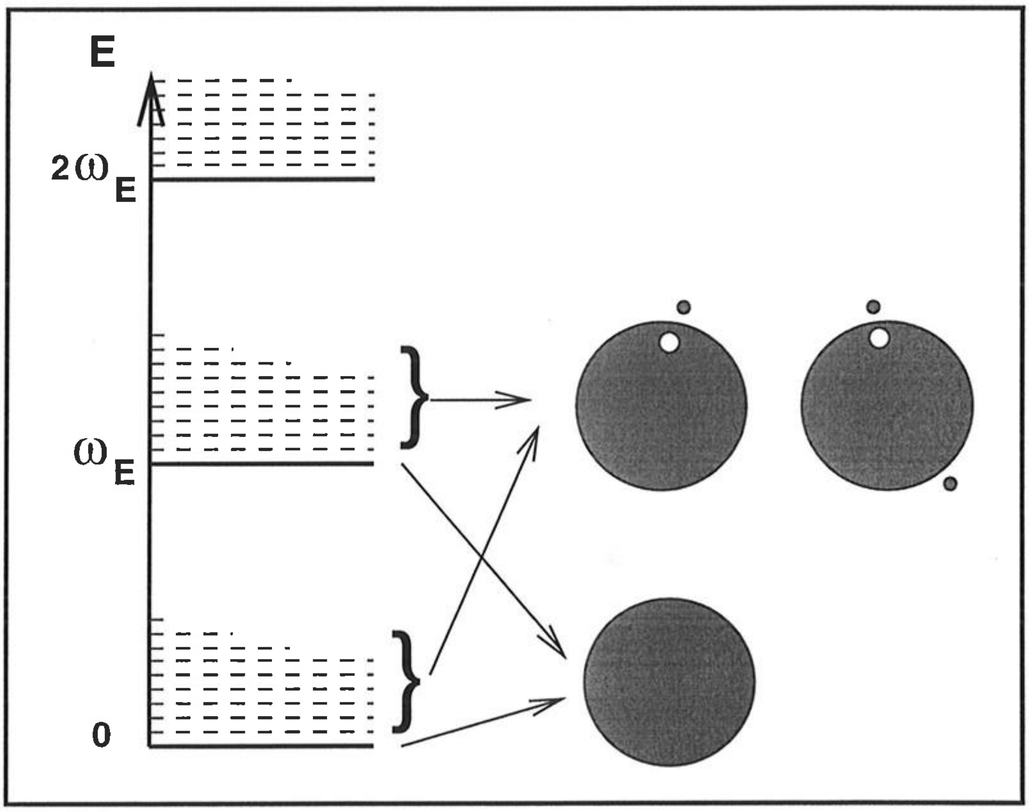

Figure 6.6: *The organization of Hilbert space in the electron-phonon problem (6.40,6.41). It splits up in sectors characterized by the occupancy of the Einstein phonon and every sector consists of the Fermi-sea and its excitations, as for instance a quasiparticle-quasihole pair, two excited quasiparticles and one quasihole, etcetera.*

Notice that the only difference with the problem in section 5.2 (or 6.1) is in the fact that the states described by H_0 live in a different Hilbert space. The ground state of H_0 is the Fermi sea (with energy $E_0 = 0$) and subsequently one can build up configuration space by adding a quasiparticle or hole (at an energy cost $|\varepsilon_k - \mu|$), creating a quasiparticle-quasihole pair (at $|\varepsilon_k - \varepsilon'_k|$), a quasiparticle pair (at $|\varepsilon_k + \varepsilon'_k - 2\mu|$), etcetera. For highly excited quasiparticle configurations, the sectors labelled by phonon occupancy are overlapping, and it is no longer possible to construct a strong coupling perturbation theory. However, if the interest is only in the lowest lying states in the quasiparticle sector with energies $<< \omega_E$, we can directly use the results of the strong coupling theory of section 5.2. The correspondence is as follows (compare (5.12-5.16),

$$\begin{aligned} T_0 &\rightarrow \sum_{\vec{k}\sigma} (\varepsilon_{\vec{k}} - \mu) c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} \quad , && (6.42)\\ V &\rightarrow \omega_E \sum_{\vec{q}} b^\dagger_{\vec{q}} b_{\vec{q}} \quad , && (6.43)\\ T^+ &\rightarrow \mathcal{M} \sum_{\vec{k}\vec{q}\sigma} c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma}\, b^\dagger_{-\vec{q}} \quad , && (6.44)\\ T^- &\rightarrow \mathcal{M} \sum_{\vec{k}\vec{q}\sigma} c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma}\, b_{\vec{q}} \quad . && (6.45) \end{aligned}$$

T^+ and T^- now describe the processes involving the creation- and annihilation of a phonon, respectively. The strong coupling expansion is in the present case controlled by $\mathcal{M}/\omega_E$, assumed to be a small number. We can directly use the central result of section 5.2. Up to second order in $\mathcal{M}/\omega_E$, the low energy states are described by the effective Hamiltonian (see 5.30-5.31),

$$H^2_{eff} = T_0 + H_{int} \tag{6.46}$$

where T^0 describes the free quasiparticles (6.42) and (ρ_q is the quasiparticle density operator, see 4.80),

$$\begin{aligned} H_{int} &\equiv -\frac{1}{\omega_E} T^- T^+ \\ &= -\frac{\mathcal{M}^2}{\omega_E} \sum_{\vec{k}\vec{q}\sigma} \sum_{\vec{k}'\vec{q}'\sigma'} c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} c^\dagger_{\vec{k}'+\vec{q}',\sigma'} c_{\vec{k}',\sigma'} b_{\vec{q}} b^\dagger_{-\vec{q}'} \quad , \\ &= -\frac{\mathcal{M}^2}{\omega_E} \sum_{\vec{k}\vec{q}\sigma} \sum_{\vec{k}'\vec{q}'\sigma'} c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} c^\dagger_{\vec{k}'+\vec{q}',\sigma'} c_{\vec{k}',\sigma'} \delta_{\vec{q},-\vec{q}'} \quad , \\ &= -\frac{\mathcal{M}^2}{\omega_E} \sum_{\vec{k}\vec{k}'\vec{q}} \sum_{\sigma\sigma'} c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} c^\dagger_{\vec{k}'-\vec{q}',\sigma'} c_{\vec{k}',\sigma'} && (6.47) \\ &= -\frac{\mathcal{M}^2}{\omega_E} \sum_{\vec{q}} \rho_{\vec{q}} \rho_{-\vec{q}} && (6.48) \end{aligned}$$

where we used in the third line the fact that the phonon occupation number has to be zero in the ground state sector. We directly infer from (6.47) or (6.48) that the exchange of virtual (high energy) phonons gives rise to an effective interaction between the quasiparticles. Moreover, these interactions are *attractive* (minus sign!).

This sign is easy to understand. The fluctuations to the high energy states push down the low energy states. In the spin- or Cooper pair problem, the system profits from this energy lowering by aligning the spins in an anti-parallel fashion. In this case, the energy is gained by the attractive interactions between the quasiparticles.

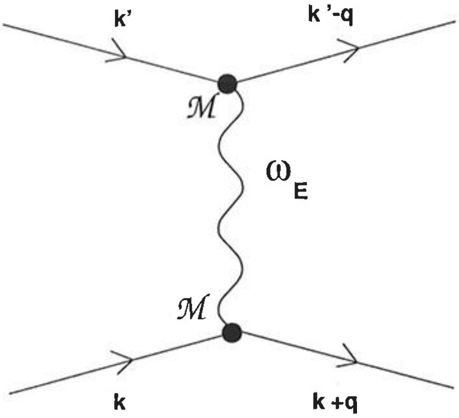

Figure 6.7: *In diagrammatic language, the phonon mediated interaction is represented by merging the phonon lines of two diagrams of the type shown in figure 4.4, to obtain an interaction diagram of the type shown in section 2.4.*

Let us anticipate on the presence of Cooper pairs, and rewrite the interaction term accordingly. After two additional commutations, (6.47) might as well be written as[5],

$$H_{int} \quad = \quad -\frac{\mathcal{M}^2}{\omega_E} \sum_{\vec{k}\vec{k}'\vec{q}} \sum_{\sigma\sigma'} c^\dagger_{\vec{k}+\vec{q},\sigma} c^\dagger_{\vec{k}'-\vec{q},\sigma'} c_{\vec{k}',\sigma'} c_{\vec{k},\sigma} \tag{6.49}$$

Written in this way, the interaction term represents the process where a *pair* of electrons is annihilated (at $\vec{k}$ and $\vec{k}'$), while a new pair is created (at $\vec{k}+\vec{q}$ and $\vec{k}'-\vec{q}$). We have now to recall that theis interaction term applies only to the quasiparticle configurations with an energy, less than the phonon frequency. The energies of the excited pair state $\varepsilon_{\vec{k}+\vec{q}} + \varepsilon_{\vec{k}'-\vec{q}} - \varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'} < \omega_E$. This gives rise to an important kinematic constraint on the allowed momenta as well: the center of mass momentum of the pairs $\vec{K} = \vec{k} + \vec{k}'$ has to vanish if $\omega_E << E_F$. It is easy to see that it is impossible to keep the energy of the pair state within the small shell $\sim \omega_E$ around E_F for a finite center of mass momentum $\vec{K}$. Because $\vec{K} = 0$, $\vec{k} = -\vec{k}'$ and (6.48) simplifies further to

$$H_{int} \quad = \quad -\frac{\mathcal{M}^2}{\omega_E} \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} c^\dagger_{\vec{k}',\sigma} c^\dagger_{-\vec{k}',\sigma'} c_{-\vec{k},\sigma'} c_{\vec{k},\sigma} \tag{6.50}$$

$\Longrightarrow$ Excercise 6.6

Anticipating further on the outcome, we learned in section 6.1 that attractive interactions tend to stabilize Cooper pairs where the electrons have paired up their

---

[5] The anticommutators are only non-zero if the wave numbers of the particles are the same. These contribute $\sim 1/N$ and can be savely neglected in the thermodynamic limit.

spins. We can therefore neglect in (6.49) the terms with parallel spins. Including the kinetic energy of the quasiparticles, this leads to the so-called BCS ('Bardeen-Cooper-Schrieffer') Hamiltonian, the starting point of the discussion of weak coupling superconductivity,

$$H_{BCS} = \sum_{\vec{k}\sigma}(\varepsilon_{\vec{k}} - \mu)c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}\sigma} - V{\sum_{\vec{k}\vec{k}'}}' c^{\dagger}_{\vec{k}',\uparrow}c^{\dagger}_{-\vec{k}',\downarrow}c_{-\vec{k},\downarrow}c_{\vec{k},\uparrow} \tag{6.51}$$

where $V \simeq 2\mathcal{M}^2/\omega_E$, while in the interaction term only quasiparticle states should be taken into account for which $|\varepsilon_{\vec{k}} - \varepsilon_F| < \omega_E$ and $|\varepsilon_{\vec{k}'} - \varepsilon_F| < \omega_E$: only the quasiparticles with an energy less than ω_E are subject to attractive interactions. It is unclear from the above derivation where exactly to place this 'ultraviolet cut-off'. It turns out, however, that the results are in at least in weak coupling rather unsensitive to this choice. If this becomes an issue, as in the so-called 'strong coupling' superconductors like Pb, with small ω_E and large $\mathcal{M}/\omega_E$, one has to consult the full diagrammatic theory.

6.3 Superconductivity in weak coupling: the Bardeen-Cooper-Schrieffer theory.

With the BCS Hamiltonian as a starting point, it becomes particularly easy to construct the weak coupling theory. Initially, this follows the derivation of the spin-density wave in chapter V closely. In analogy with (5.105) we conjecture the existence of vacuum amplitudes,

$$\langle c^{\dagger}_{\vec{k},\uparrow}c^{\dagger}_{-\vec{k},\downarrow}\rangle = O^{*}_{p,\vec{k}} \tag{6.52}$$

$$\langle c_{-\vec{k},\downarrow}c_{\vec{k},\uparrow}\rangle = O_{p,\vec{k}} \tag{6.53}$$

The difference with (5.105) is, that we are now considering an expectation value of a *quasiparticle-quasiparticle pair*, instead of the quasiparticle-quasihole pair of chapter 5 - this we learned to appreciate in section 6.1. In addition, the vacuum expectation values now appear in momentum space, instead of position space. We are forced to do so because only a small fraction of all quasiparticles (which carry momentum as a quantum number) can participate, because of the smallness of the phonon frequency. At the same time, we got already used to momentum space condensation in section 5.5, and the outcome here will be very similar in these regards.

The pair operators are decomposed in a vacuum amplitude and a fluctuation,

$$c^{\dagger}_{\vec{k},\uparrow}c^{\dagger}_{-\vec{k},\downarrow} = O^{*}_{p,\vec{k}} + \delta O^{*}_{p,\vec{k}} \tag{6.54}$$

$$c_{-\vec{k},\downarrow}c_{\vec{k},\uparrow} = O_{p,\vec{k}} + \delta O_{p,\vec{k}} \tag{6.55}$$

and the BCS Hamiltonian (6.51) can be written as

$$\begin{aligned} H_{BCS} = & \sum_{\vec{k}\sigma}(\varepsilon_{\vec{k}} - \mu)c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}\sigma} - V\sum_{\vec{k}\vec{k}'}\Big(O_{p,\vec{k}}c^{\dagger}_{\vec{k}'\uparrow}c^{\dagger}_{-\vec{k}'\downarrow} + O^{*}_{p,\vec{k}}c_{-\vec{k}\downarrow}c_{\vec{k}\uparrow} \\ & -O^{*}_{p,\vec{k}}O_{p,\vec{k}} + \delta O^{*}_{p,\vec{k}}\delta O_{p,\vec{k}}\Big) \end{aligned} \tag{6.56}$$

It is convenient to introduce,

$$\begin{aligned} \Delta_0 &= V \sum_{\vec{k}} O_{p,\vec{k}} \\ \Delta_0^* &= V \sum_{\vec{k}} O^*_{p,\vec{k}} \end{aligned} \tag{6.57}$$

Later on we will learn to appreciate this as the quantity measuring the gap in the single particle spectrum of the superconductor - it is equivalent to the term $U\Omega$, showing up in section 5.5 (e.g., figure 5.6). Neglecting the fluctuation term $\sim \delta O^*_{p,\vec{k}} \delta O_{p,\vec{k}}$ in (6.56) and using (6.57) yields the mean-field Hamiltonian,

$$H^{MF}_{BCS} = \sum_{\vec{k}} \Big((\varepsilon_{\vec{k}} - \mu)(c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}\uparrow} + c^{\dagger}_{\vec{k}\downarrow} c_{\vec{k}\downarrow}) - \Delta_0 c^{\dagger}_{\vec{k}\uparrow} c^{\dagger}_{-\vec{k}\downarrow} - \Delta_0^* c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} \Big) + \frac{|\Delta_0|^2}{V} \tag{6.58}$$

This has the same status as (5.114): we have first to integrate out the electrons, to subsequently minimize the classical energy to obtain the orderparameter Δ_0/V. From (6.58) it follows that the first step involves a diagonalization of the Bogoliubov type, as discussed in section 2.4.

Before we proceed with the calculation, let us first seek for further simplifications. From (6.57) it is inferred that the orderparameter is a complex quantity. Writing $\Delta_0/V = |\Delta_0|/V \exp(i\phi)$ it is easy to see from the strong coupling limit that ϕ corresponds with the phase angles ϕ of the strong-coupling XY pseudo-spins. Although spatial uniformity has been imposed, the order parameter as a whole still respects the $O(2)$ rotational invariance when the orderparameter is taken to be a complex quantity.

$\Longrightarrow$ Excercise 6.7

At the same time, we have implicitely assumed that $\vec{A} = 0$ in (6.51) and we learned in section 5.1 that the vector potential is an integral part of the order parameter. It is difficult to construct a manifest gauge invariant weak coupling theory. Since we should be convinced in the mean time that the symmetries of the problem cannot get lost in the continuation from strong coupling to weak coupling, we might as well simplify the weak coupling theory as much as we can: we fix $\phi = 0$ such that the order parameter becomes real $\Delta_0 = \Delta_0^* = \Delta$. The mean-field Hamiltonian simplifies further,

$$H^{MF}_{BCS} = \sum_{\vec{k}} \Big((\varepsilon_{\vec{k}} - \mu)(c^{\dagger}_{\vec{k}\uparrow} c_{\vec{k}\uparrow} + c^{\dagger}_{\vec{k}\downarrow} c_{\vec{k}\downarrow}) - \Delta (c^{\dagger}_{\vec{k}\uparrow} c^{\dagger}_{-\vec{k}\downarrow} + c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow}) \Big) + \frac{\Delta^2}{V} \tag{6.59}$$

The Bogoliubov transformation, diagonalizing a 'particle-particle' problem like (6.59), works differently from the usual 'particle-hole' diagonalizations. This causes a somewhat different appearance of the present mean-field theory, as compared to the one discussed in chapter V. (6.59) amounts to a 'two-level' Bogoliubov problem for every pair of $\vec{k}\uparrow, -\vec{k}\downarrow$ electrons. Recalling the results in section 2.4, this problem is diagonalized by,

$$\begin{aligned} c_{\vec{k}\uparrow} &= u_{\vec{k}}\,\gamma_{\vec{k}0} + v_{\vec{k}}\,\gamma^{\dagger}_{\vec{k}1} \quad , \\ c^{\dagger}_{-\vec{k}\downarrow} &= -v_{\vec{k}}\,\gamma_{\vec{k}0} + u_{\vec{k}}\,\gamma^{\dagger}_{\vec{k}1} \quad . \end{aligned} \tag{6.60}$$

with the condition that

$$u^2_{\vec{k}} + v^2_{\vec{k}} = 1 \tag{6.61}$$

The inverse of (6.60) is,

$$\begin{aligned} \gamma_{\vec{k}0} &= u_{\vec{k}}\,c_{\vec{k}\uparrow} - v_{\vec{k}}\,c^{\dagger}_{-\vec{k}\downarrow} \quad , \\ \gamma^{\dagger}_{\vec{k}1} &= v_{\vec{k}}\,c_{\vec{k}\uparrow} + u_{\vec{k}}\,c^{\dagger}_{-\vec{k}\downarrow} \quad . \end{aligned} \tag{6.62}$$

and the $\gamma^{\dagger}$'s describe fermions,

$$\begin{aligned} \left\{\gamma_{\vec{k}\sigma}\,,\,\gamma^{\dagger}_{\vec{k}'\sigma'}\right\} &= \delta_{\vec{k}\vec{k}'}\,\delta_{\sigma\sigma'} \quad , & (\sigma,\sigma'=0,1) \quad , \\ \left\{\gamma_{\vec{k}\sigma}\,,\,\gamma_{\vec{k}'\sigma'}\right\} &= \left\{\gamma^{\dagger}_{\vec{k}\sigma}\,,\,\gamma^{\dagger}_{\vec{k}'\sigma'}\right\} = 0 \quad , & (\sigma,\sigma'=0,1) \quad . \end{aligned} \tag{6.63}$$

Substituting (6.60) in the mean-field Hamiltonian (6.59) and ordering the operators yields,

$$\begin{aligned} H^{MF}_{BCS} = \sum_{\vec{k}} \Big[&\Big((\varepsilon_{\vec{k}}-\mu)(u^2_{\vec{k}}-v^2_{\vec{k}}) + 2\Delta u_{\vec{k}}v_{\vec{k}}\Big)\left(\gamma^{\dagger}_{\vec{k}0}\gamma_{\vec{k}0} + \gamma^{\dagger}_{\vec{k}1}\gamma_{\vec{k}1}\right) \\ &+ 2\left((\varepsilon_{\vec{k}}-\mu)v^2_{\vec{k}} - \Delta u_{\vec{k}}v_{\vec{k}}\right) \\ &+ \left(2(\varepsilon_{\vec{k}}-\mu)u_{\vec{k}}v_{\vec{k}} + \Delta(v^2_{\vec{k}}-u^2_{\vec{k}})\right)\left(\gamma_{\vec{k}1}\gamma_{\vec{k}_0} + \gamma^{\dagger}_{\vec{k}0}\gamma^{\dagger}_{\vec{k}_1}\right)\Big] + \frac{\Delta^2}{V} \end{aligned} \tag{6.64}$$

It follows that the Hamiltonian becomes diagonal in the $\gamma^{\dagger}$'s if we impose the condition,

$$2(\varepsilon_{\vec{k}}-\mu)u_{\vec{k}}v_{\vec{k}} + \Delta(v^2_{\vec{k}}-u^2_{\vec{k}}) = 0 \quad . \tag{6.65}$$

Multiplying (6.65) with $\Delta/u^2_{\vec{k}}$ we obtain,

$$\left(\frac{\Delta v_{\vec{k}}}{u_{\vec{k}}}\right)^2 + 2(\varepsilon_{\vec{k}}-\mu)\left(\frac{\Delta v_{\vec{k}}}{u_{\vec{k}}}\right) - \Delta^2 = 0 \tag{6.66}$$

with the solution,

$$\frac{\Delta v_{\vec{k}}}{u_{\vec{k}}} = E_{\vec{k}} - (\varepsilon_{\vec{k}}-\mu) \tag{6.67}$$

$$E_{\vec{k}} = \sqrt{(\varepsilon_{\vec{k}}-\mu)^2 + \Delta^2} \tag{6.68}$$

Together with the normalization condition (6.61), we have two equations for the unknowns $u_{\vec{k}}, v_{\vec{k}}$, and it follows that,

$$v^2_{\vec{k}} = 1 - u^2_{\vec{k}} = \frac{1}{2}\left(1 - \frac{(\varepsilon_{\vec{k}}-\mu)}{E_{\vec{k}}}\right) \quad . \tag{6.69}$$

Substituting (6.69) yields the mean-field Hamiltonian in diagonal form,

$$
\begin{aligned}
H &= \sum_{\vec{k}} \left((\varepsilon_{\vec{k}} - \mu) - E_{\vec{k}} \right) + \frac{\Delta^2}{V} \\
&\quad + \sum_{\vec{k}} E_{\vec{k}} (\gamma^\dagger_{\vec{k}0} \gamma_{\vec{k}0} + \gamma^\dagger_{\vec{k}1} \gamma_{\vec{k}1}) \quad .
\end{aligned} \tag{6.70}
$$

$\Longrightarrow$ Excercise 6.8

Being used to particle-hole problems like (5.120), one could be tempted to fill up the new fermion state $\gamma^\dagger$ up to k_F. In this regard, the Bogoliubov transformation works quite differently. The normal (Fermi-liquid) state should be recovered by setting $\Delta = 0$ in (6.70). Because we counted from the unperturbed Fermi sea, the ground state energy should be in this case $E_0(\Delta = 0) = 0$, and together with (6.62, 6.68) this implies that in this case the $\gamma^\dagger$ describe quasiparticle/hole excitations *on top* of the Fermi sea. For finite Δ, the first term in (6.70) becomes negative, indicating a lowering of the electronic contribution to the vacuum energy, and apparently the $\gamma^\dagger$'s describe the fermionic *excitations* of the superconducting condensate. This observation can be used to deduce the wavefunction, describing the classical state in weak coupling. Because the $\gamma^\dagger$'s describe excitations,

$$
\begin{aligned}
\gamma_{\vec{k}0} | \Phi^0_{Cl} \rangle &= 0 \ , \ \ \forall \vec{k} \quad , \\
\gamma_{\vec{k}1} | \Phi^0_{Cl} \rangle &= 0 \ , \ \ \forall \vec{k} \quad .
\end{aligned} \tag{6.71}
$$

Combining this with (6.62)

$$
\begin{aligned}
u_{\vec{k}}\, c_{\vec{k}\uparrow} | \Phi^0_{Cl} \rangle &= v_{\vec{k}}\, c^\dagger_{-\vec{k}\downarrow} | \Phi^0_{Cl} \rangle \quad , \\
v_{\vec{k}}\, c^\dagger_{\vec{k}\uparrow} | \Phi^0_{Cl} \rangle &= -\, u_{\vec{k}}\, c^\dagger_{-\vec{k}\downarrow} | \Phi^0_{Cl} \rangle \quad .
\end{aligned} \tag{6.72}
$$

It is easy to verify that the condensate wave function has to be

$$
| \Phi^0_{Cl} \rangle = \Pi_{\vec{k}} \left(u_{\vec{k}} + v_{\vec{k}} c^\dagger_{\vec{k}\uparrow} c^\dagger_{-\vec{k}\downarrow} \right) | vac. \rangle \tag{6.73}
$$

This is the famous BCS wavefunction. Notice that the product in (6.73) has to be taken over all possible wavevectors, not only those satisfying $k \leq k_F$.

$\Longrightarrow$ Excercise 6.9

$\Longrightarrow$ Excercise 6.10

(6.73) is nothing else than a straightforward $\vec{k}$ space generalization of the real space condensate wave function encountered in section 6.1. For instance, if the kinematic constraint on the wavevectors coming from $\omega_E / E_F << 1$ would be absent, and we would make V large compared to the bandwidth, the $u_{\vec{k}}$ and $v_{\vec{k}}$'s would become $\vec{k}$ independent and transforming the fermions back to real space one would find $| \Phi^0_{Cl} \rangle = \Pi_{\vec{i}} \left(u + v c^\dagger_{\vec{i}\uparrow} c^\dagger_{\vec{i}\downarrow} \right) | vac. \rangle$: (6.9) with $\phi_i = 0$ and $\cos(\theta/2) = u$.

Historically, (6.73) was the starting point of the development of the theory of superconductivity. In the original paper, (6.73) was presented as a variational wavefunction and in 1957 it was not realized that wavefunctions of the same general structure (single determinant, non exact, implying rigidity) describe classical objects, including crystals and antiferromagnets. The mere fact that (6.73) is a wavefunction has misled generations of physicists to believe that superconductivity is about macroscopic quantum-mechanics, while crystals and antiferromagnets are not. These misunderstandings persist up to the present day - it is not hard to find eminent physicist claiming that superconductivity is different *because* (6.73) is a wavefunction. The remedy: teach them section 6.1 and chapter 5.

As in magnetism, the problem in weak coupling is to establish whether the constituents of the order parameter (in this case the pairs) can exist. In strong coupling, the pair amplitude $\sin^2(\theta/2)$ is finite at all energies $< |U|$, while in weak-coupling it is not a-priori clear if Δ will be finite under all circumstances. To determine Δ we have to minimize the classical ground state energy,

$$E_{Cl} = \sum_{\vec{k}} \left((\varepsilon_{\vec{k}} - \mu) - E_{\vec{k}} \right) + \frac{\Delta^2}{V} \tag{6.74}$$

Minimizing to Δ by $\delta E_{Cl}/\delta\Delta = 0$ yields the saddle point equation (compare (5.123)-(5.127))

$$\frac{1}{2} {\sum_{\vec{k}}}' \frac{1}{\sqrt{(\varepsilon_{\vec{k}} - \mu)^2 + \Delta^2}} = \frac{1}{V} \tag{6.75}$$

Recall that the (primed) summation over wavenumbers has to be taken such that only wavenumbers satisfying $|\varepsilon_k - \mu| < \omega_E$ are taken into account. Only one quasiparticle energy appears in (6.75), and it is now directly possible to evaluate (6.75) in terms of the quasiparticle density of states $N(E)$. Taking into account the constraint on the allowed quasiparticle energies as well, (6.75) can be written as,

$$1 = \frac{V}{2} \int_{-\omega_E}^{\omega_E} d\tilde{\varepsilon} \frac{N(\tilde{\varepsilon})}{\sqrt{\tilde{\varepsilon}^2 + \Delta^2}} \tag{6.76}$$

where $\tilde{\varepsilon} = \varepsilon - \mu$. Let us now consider the weak coupling limit, $V/W \sim VN(0) << 1$ ($N(0)$ is the density of states at E_F). $N(\varepsilon)$ will barely vary on the scale of V and therefore,

$$1 \simeq VN(0) \int_0^{\omega_E} \frac{d\tilde{\varepsilon}}{\sqrt{\tilde{\varepsilon}^2 + \Delta^2}} \tag{6.77}$$

$$= VN(0) arcsinh \frac{\omega_E}{\Delta} \tag{6.78}$$

Inverting this expression,

$$\Delta = \frac{\omega_E}{sinh \frac{1}{VN(0)}} \simeq 2\omega_E e^{-1/VN(0)} \tag{6.79}$$

This expression for the gap/orderparameter is in fact quite similar to what we found in the context of spin density waves, Eq. (5.134): Regardless its smallness, every attractive interaction will give rise to a finite superconducting orderparameter! As in the case of the spin density waves, the magnitude of the orderparameter becomes very small for small $VN(0)$. Comparing (6.79) and (5.134), they are also numerically similar. $2\pi t/U$ is equivalent to $1/VN(0)$. The difference is in the prefactors: the full bandwidth in the case of spin density waves and only the phonon frequency in the case of the superconductors. This is the reason that we were allowed to be rather sloppy in our choice of ω_E as the upper energy bound for the attractive interactions: small numerical errors in the factor $VN(0)$ in the exponent will outnumber imprecisions in the choice of the cut-off energy.

The truely remarkable feature of (6.79) is that it holds *regardless the electron density or dimensionality.* This is quite different from the 'particle-hole' instabilities, like the spin density wave discussed in section 5.5. There we found *nesting* to be a necessary condition for the instability to occur in the weak coupling limit, which limited the phenomenon basically to one dimension. Nesting meant that the spatial structure of the order parameter is such, that the new Brillouin zone boundary precisely spans the Fermi-surface. Superconducting order, on the other hand, is characterized by an 'automatic' nesting: the pair amplitude Δ/V maps the Fermi-surface on itself (see figure 6.8). The pair potentials Δ lead to an Umklapp, folding the hole states at $-\vec{k}, -\sigma$ onto the electron states at $\vec{k}, \sigma$. The fundamentals are most easily recognized in strong coupling, where we found that the low energy Hilbert space of the attractive problem is spin-like, regardless the particle density. This property cannot get lost in the continuation to weak coupling.

$\Longrightarrow$ Excercise 6.11

$\Longrightarrow$ Excercise 6.12

It was already announced that Δ actually relates to the gap in the single fermion spectrum of the superconductors. This follows immediately from (6.70). We learned that the $\gamma^{\dagger}$'s represent fermionic *excitations* of the superconductor. According to (6.70) and (6.68), these excitations cost an energy of at least $E_{\vec{k}=\vec{k}_F} = |\Delta|$. To find out the nature of these excitations, it is interesting to consider their effect on the condensate wavefunction (6.73),

$$\begin{aligned} \gamma^{\dagger}_{\vec{k}0} |\Phi^0_{Cl}> &= \left(u_{\vec{k}} c^{\dagger}_{\vec{k}\uparrow} - v_{\vec{k}} c_{-\vec{k}\downarrow}\right) \left(u_{\vec{k}} + v_{\vec{k}} c^{\dagger}_{\vec{k}\uparrow} c^{\dagger}_{-\vec{k}\downarrow}\right) \prod_{\vec{k}_1 \neq \vec{k}} (\cdots)|vac\rangle \\ &= c^{\dagger}_{\vec{k}\uparrow} \prod_{\vec{k}_1 \neq \vec{k}} \left(u_{\vec{k}_1} + v_{\vec{k}_1} c^{\dagger}_{\vec{k}_1\uparrow} c^{\dagger}_{-\vec{k}_1\downarrow}\right) |vac\rangle \quad , \qquad (6.80) \\ \gamma^{\dagger}_{\vec{k}1} |\Phi^0_{Cl}> &= c^{\dagger}_{-\vec{k}\downarrow} \prod_{\vec{k}_1 \neq \vec{k}} \left(u_{\vec{k}_1} + v_{\vec{k}_1} c^{\dagger}_{\vec{k}_1\uparrow} c^{\dagger}_{-\vec{k}_1\downarrow}\right) |vac\rangle \quad , \qquad (6.81) \end{aligned}$$

It is seen from these expressions that the $\gamma^{\dagger}$'s break up a $\vec{k}$ space Cooper pair, to leave behind an unpaired electron. In addition, it is easy to see that these final states are hole like when $k << k_F$ and electron like when $k >> k_F$. Consider high energy states such that $|\varepsilon_{\vec{k}} - \mu| \sim |v_F k| >> \Delta$. (6.69) simplifies to

$$v^2_{\vec{k}} = 1 - u^2_{\vec{k}} \simeq \frac{1}{2}\left(1 - \frac{(\varepsilon_{\vec{k}} - \mu)}{|\varepsilon_{\vec{k}} - \mu|}\right) \qquad (6.82)$$

and it follows that for $k << k_F$, $v^2_{\vec{k}} = 1$ and $u^2_{\vec{k}} = 0$, while for $k >> k_F$, $v^2_{\vec{k}} = 0$ and $u^2_{\vec{k}} = 1$. For states far below the Fermi-energy ($|v_F k| > \omega_E$), $\gamma^\dagger_{\vec{k}0} \sim c_{-\vec{k}\downarrow}$, acting on a component in the BCS wavefunction $\sim c^\dagger_{\vec{k}\uparrow} c^\dagger_{-\vec{k}\downarrow}$: $\gamma^\dagger_{\vec{k}0}$ creates just a quasihole. In the same way, the $\gamma^\dagger$'s create quasiparticles when $\vec{k} >> \vec{k_F}$. What happens when $k = k_F$? $u^2_{k_F} = v^2_{k_F} = 1/2$ and apparently the $\gamma^\dagger$'s create 'half an electron' and 'half a hole'. This is not as mysterious as it sounds. Imagine an experiment where one measures the *probability* to add- or remove an electron at a given energy or momentum. As will be further explained in the next chapter, this experiment actually exist: (inverse) photoemission. The result of such a measurement is indicated in figure 6.8. At momenta $k << k_F$ ($k >> k_F$) one finds the hole (electron) in the quasiparicle state at $-v_F k$ ($v_F k$). Approaching k_F from below, one finds both below and above the Fermi-energy a finite probability to annihilate- and create an electron at energies $\pm E_{\vec{k}}$. The weight above E_F increases untill the probability distribution becomes equal at both sides of E_F at $k = k_F$, while the weight above E_F start to grow if k is further increased.

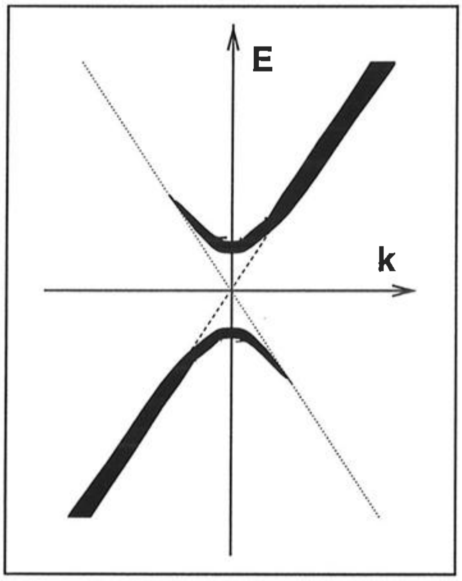

Figure 6.8: *The dispersion of the electron $\vec{k}, \sigma$ (dashed line) and the hole at $-\vec{k}, \bar{\sigma}$ (dotted line) are crossing each other at the Fermi-energy: the automatic nesting characteristic for a superconductor. In the presence of a finite pair amplitude Δ/V these states mix, and instead one finds the Bogoliubov dispersion $E_{\vec{k}}$ (Eq. 6.68). The thick line illustrates what is seen in the (inverse) photoemission experiment: the thickness of the lines is proportional to the* probability *to either annihilate- or create an electron in the system, as function of energy and momentum.*

$\Longrightarrow$ Excercise 6.13

Next to these fermionic excitations one can also address the nature of the charge and spin excitations, described in terms of pairs of fermion creation- and annihilation operators. We already discussed the supercurrent in section 6.1, which is the most interesting property of the superconductor in the charge sector[6]. The spin sector deserves some special attention as well. Although the condensate wavefunctions (6.9) or (6.73) are not eigenstates of total spin, they are linear superpositions of the vacuum and pairs of electrons in singlet states. One anticipates that, next to the Meissner contributions, the spin response of the superconductor is also diamagnetic. This is easy to see. Acting *twice* with $\gamma^\dagger_{\vec{k},0}$ on the condensate,

$$\gamma^\dagger_{\vec{k}0}\gamma^\dagger_{\vec{k}'0}|\Phi^0_{Cl}> \; = \; c^\dagger_{\vec{k}\uparrow}c^\dagger_{\vec{k}'\uparrow}\prod_{\vec{k}''\neq\vec{k},\vec{k}'}\left(u_{\vec{k}''}+v_{\vec{k}''}c^\dagger_{\vec{k}''\uparrow}c^\dagger_{-\vec{k}''\downarrow}\right)|vac.\rangle \; \left(\vec{k}\neq\vec{k}'\right) \quad .(6.83)$$

breaks up singlet pairs at $\vec{k},\vec{k}'$, to produce a state which is a triplet. When $\vec{k}=\vec{k}_F$, this is the lowest energy spin excitation one can make and this costs and energy 2Δ. Hence, at energies less than 2Δ, spin has disappeared from the universe as defined by the ('singlet') superconducting vacuum[7].

Let us finally consider the temperature dependence of the order parameter and gap in the weak coupling case. 2Δ is in conventional superconductors quite small, typically like $1-100$ K in temperature units. If temperature becomes of order of the gap one expects gross changes to occur. In principle one should work oneself through the fluctuation theory, to address the influence of temperature, as we did in section 4.6. For *very special reasons* these fluctuations are utterly unimportant in the weak coupling limit, and a complete account of the temperature dependences follows directly from the mean-field theory. How to take into account finite temperature on the mean-field level? In taking the average of the diagonal mean field Hamiltonian (6.70) to obtain the classical energy, we have to realize that the excited states ($\gamma^\dagger$'s) become populated if temperature is finite (F_{Cl} is the mean-field free energy),

$$\begin{aligned} F_{Cl} &= \sum_{\vec{k}}\left((\varepsilon_{\vec{k}}-\mu)-E_{\vec{k}}\right)+\frac{\Delta^2}{V} \\ &\quad +\sum_{\vec{k}}E_{\vec{k}}(\langle\gamma^\dagger_{\vec{k}0}\gamma_{\vec{k}0}\rangle+\langle\gamma^\dagger_{\vec{k}1}\gamma_{\vec{k}1}\rangle) \quad . \end{aligned} \tag{6.84}$$

because the $\gamma^\dagger$'s are genuine fermions,

$$\langle\gamma^\dagger_{\vec{k}0,1}\gamma_{\vec{k}0,1}\rangle = n_F(\beta E_{\vec{k}}) \tag{6.85}$$

where n_F is the Fermi-factor Eq. (2.53). Using

$$1-2n_F(\beta E_{\vec{k}}) \; = \; 1-2\frac{1}{e^{\beta E_{\vec{k}}}+1} \; = \; \frac{e^{\beta E_{\vec{k}}}-1}{e^{\beta E_{\vec{k}}}+1} \; = \; \tanh\frac{\beta E_{\vec{k}}}{2} \quad . \tag{6.86}$$

the saddle-point equation becomes,

$$\frac{1}{2N}\sum_{\vec{k}}{}' \frac{1}{E_{\vec{k}}}\tanh(\frac{\beta E_{\vec{k}}}{2}) \; = \; \frac{1}{V} \tag{6.87}$$

---

[6] In addition a plasmon is found at long wavelength, which is not different from the plasmon in the normal state, which is discussed in chapter VII.

[7] For special forms of the attractive interaction (see excercise 6.13) it is possible to construct a pair wave function which carries even angular momentum, while the spins in the pair are aligned in a triplet state. This actually happens in ^3He.

similar to (6.75) except for the thermal factor $\tanh(\frac{\beta E_{\vec{k}}}{2})$. This becomes in the continuum limit,

$$\frac{1}{V} = \mathcal{N}(0) \int_0^{\omega_E} d\tilde{\varepsilon} \, \frac{\tanh \frac{1}{2}\beta\sqrt{\tilde{\varepsilon}^2 + \Delta^2}}{\sqrt{\tilde{\varepsilon}^2 + \Delta^2}} \quad . \tag{6.88}$$

$\Longrightarrow$ Excercise 6.14

The integral in (6.88) cannot be evaluated analytically. One expects, however, that the population of the excited states will weaken the superconducting order, and eventually the order parameter should disappear. The temperature where this happens (the transition temperature T_c) can be derived analytically. T_c is the temperature where $\Delta \to 0$. This happens according to (6.88) when ($\beta_c = 1/k_B T_c$)

$$\frac{1}{\mathcal{N}(0)V} = \int_0^{\omega_E} dx \frac{\tanh(\frac{1}{2}\beta_c x)}{x} = \int_{x=0}^{x=\beta_c\omega_E} d(\ln x) \, \tanh(\frac{1}{2}x) \quad , \tag{6.89}$$

$$= \ln(\beta_c \omega_E) \, \tanh(\beta_c\omega_E/2) - \int_0^{\beta_c\omega_E} dx \, \ln x \, \frac{d \, \tanh(\frac{1}{2}\,x)}{dx} \quad . \tag{6.90}$$

Because of the derivative of the tanh, the integrand can be neglected except for $x \leq 1$. Because $\hbar\omega_E/k_B T_c \gg 1$, the second term is independent of T_c and it turns out to be ln(1.13). The answer for T_c is

$$\beta_c^{-1} \simeq 1.13\omega_E e^{-\frac{1}{\mathcal{N}(0)V}} \quad . \tag{6.91}$$

Interestingly, in weak coupling the gap to T_c ratio becomes a universal number,

$$\frac{2\Delta(0)}{k_B T_c} = 3.53 \tag{6.92}$$

and this relation is quite well obeyed in superconductors of this type.

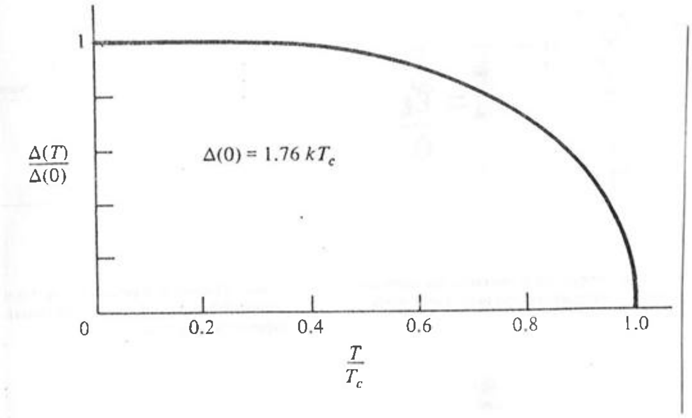

Figure 6.9: *The superconducting gap as function of temperature in weak coupling as calculated from Eq. (6.88).*

The integral in (6.88) can be evaluated numerically for arbitrary temperatures and the result is shown in figure 6.9. At low temperatures, nearly nothing happens with

Δ: in order to excite the pair breaking excitations one has to overcome the energy gap 2Δ and intitially the density of these excitations is exponentially small $\sim \exp(-\beta 2\Delta)$. Raising the temperature this density increases, and this decreases the gap magnitude, such that the density increases further. T_c signals the temperature where this feed back process gets out of control, with the result that the order parameter disappears alltogether. Close to the transition $\Delta(T)/\Delta(0) \sim ((T_c - T)/T_c)^{1/2}$. The reader familiar with statistical mechanics will recognize the generic mean-field phase transition.

I emphasize that the disappearance of the superconductivity in the weak coupling case is driven by the disappearance of the Cooper pairs themselves. This is quite different in strong coupling where the number of Cooper pairs is fixed at energies $< |U|$. Instead, the phase transition in the strongly coupled system would be driven by the long-wavelength phase fluctuations, in precise analogy with the thermal melting of crystals as discussed in section 4.6. Because in weak coupling the Cooper pair density itself lives on an energy scale of $k_B T$, it is reasonable to take this into account discussing the temperature dependence. What right do we have, however, to neglect the long wavelength $O(2)$ fluctations alltogether? The resolution is elegant, and special to the weak coupling limit. Recall the discussion towards the end of section 5.6. We argued there that the spin density wave gap implied a length scale ξ, the 'coherence length'. In the context of superconductivity this is not different and the coherence length $\xi(T)/a \sim E_F/(2\Delta(T))$. We learned in the context of spin density waves that the order parameter fluctuation is frozen out on length scales smaller than ξ. This is the same here: the order parameter is composed of large numbers of overlapping Cooper pairs and this mimics long range interactions, quenching fluctuations (see section 5.4). When temperature increases, the gap thereby decreases, but the coherence length increases. Although one would expect more thermal fluctuations at higher temperatures, these are 'eaten' by the increasing coherence length. At the transition itself, the coherence length diverges to infinity and no order parameter fluctuation is possible at all! In strong coupling this is quite different; the coherence length equals the lattice constant at all relevant temperatures, and in order to adress, e.g., the behaviour of the order parameter near T_c one has work him/herself through the full critical theory which is not an easy task. In this way, the smallness of the interaction causes a tremendous simplification of the theory: *mean-field theory becomes exact.* The curve in figure 6.9 reproduces precisely the behaviour of the order parameter in many real superconductors.

This ends the discussion of the fundamental nature of the superconducting state. There are many more stories to tell. The physics of superconductors is actually a rather large and entertaining subfield in condensed matter physics. From the theoretical side, the above weak coupling theory can be further extended to the case that the coupling strength $VN(0)$ is large, while ω_E/E_F is still a small number. This is the so-called 'strong coupling'[8] or 'Eliashberg-Migdal' theory. Some quantitative

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[8] Notice again a semantic ambiguity. True strong coupling is the local pair limit as discussed in section 6.1, where both parameters in the theory (V/W and ω_E/E_F) are large. In the present context, only V/W is large. ω_E/E_F is the more important control parameter. As long as this number is small, the pairing occurs in $\vec{k}$ space and the coherence length is large. For these reasons,

aspects change, but it turns out that this theory exhibits the same level of control as the weak coupling theory. This 'high quality' theory makes detailed comparisons possible with a large variety of experiments with many surprising outcomes. I refer the interested student to the specialized literature[9].

6.4 Excercises

6.1 Verify that (6.2,6.3,6.5) form a $su(2)$ algebra. Consider a two site model $H = \vec{T}_1 \cdot \vec{T}_2$ and discuss the physical nature of the various eigenstates.

6.2 Derive (6.6-6.8) explicitely using the results of section 5.2. Specifically, (5.30) can be directly used after reinterpreting the various operators in this expression, in order for them to apply in the present context.

6.3 Derive (6.11) explicitely, using the results of section 5.3.

6.4 Proof that (6.15) is invariant under the gauge transformation (6.14,6.16,6.17).

6.5 Show that (6.30) follows from (6.9) and (6.25,6.26).

6.6 Consider a spherical Fermi-surface and demonstrate graphically that the scattering processes of a pair of particles with $\vec{K} \neq 0$ can be neglected, compared with those involving a vanishing center of mass momentum, if all particles have an energy $|\varepsilon_{\vec{k}} - E_F| < \omega_E$, while $\omega_E << E_F$.

6.7 Mean-field theory of the attractive Hubbard model (6.1). Since all electrons can participate in the condensate ($\omega_E \rightarrow \infty$) we can directly use the recipy of section 5.5. Consider now the order parameter amplitudes in *real space* and keep track of the phase freedom: $c_{\vec{i}\downarrow} c_{\vec{i}\uparrow} = \Delta^0_{\vec{i}} + \delta\Delta^0_{\vec{i}}$, and its hermitian conjugate, while $\Delta^0_{\vec{i}} = \Delta_{\vec{i}} \exp(i\phi_{\vec{i}})$ (Δ is real). Show that for arbitrary U/W one recovers (6.58) when Δ_0 is taken to be uniform in space. The only difference is that the $\vec{k}$ summations are no longer restricted.

6.8 Verify (6.64-6.70).

6.9 Check that (6.73) satisfies (6.71).

6.10 A specialty of the BCS wavefunction is that the total particle number $N = \sum_{\vec{k}\sigma} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma}$ is a fluctuating quantity. $\bar{N}$ is the average particle number.

   a. Show that $\langle \Phi^0_{Cl} | (N - \bar{N})^2 | \Phi^0_{Cl} \rangle = 4 \sum_{\vec{k}} u^2_{\vec{k}} v^2_{\vec{k}}$.

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the outcomes of Eliashberg-Migdal theory are qualitatively quite similar to weak coupling BCS, although there are substantial quantitative differences.

[9] See M. Tinkham, 'Introduction to Superconductivity' (McGraw-Hill, New York, 1975); J. R. Schrieffer, 'Theory of superconductivity' (Addison-Wesley, 1988); G. Rickayzen, 'Theory of Superconductivity' (Wiley, New York, 1965).

b. Show that the result under (a.) implies that the root mean square number fluctuation $\delta N_{rms} = \sqrt{\langle \Phi^0_{Cl} | (N - \bar{N})^2 | \Phi^0_{Cl} \rangle} \sim \sqrt{\bar{N}}$ for a fixed density, changing the volume. Hence, the number fluctuation is unimportant in the thermodynamic limit.

6.11 Although the direct quasiparticle-quasiparticle interactions vanish in the low energy limit, they are in principle still finite at an energy scale ω_E. An explicit calculation of these residual repulsive interactions is very complicated and in practice impossible. It can nevertheless be argued that the strongest residual interaction will be in the local (hard-core, s-wave) channel. This suggest an additional term in the quasiparticle Hamiltonian,

$$H_{\mu^*} = V_{Cps} \sum_{\vec{q}} \rho_{\vec{q}} \rho_{-\vec{q}} \tag{6.93}$$

where the (repulsive) 'Coulomb pseudo potential' V_{Cps} enters as a free parameter which can be determined experimentally. Show that the gap equation of the superconductor becomes in the presence of this term,

$$\Delta \simeq 2\omega_E e^{-1/(VN(0)-\mu^*)} \tag{6.94}$$

with $\mu^* \equiv V_{Cps} N(0)$. It is believed that metals like Cu or the alkali's do not undergo a superconducting transition because the phonon-mediated attraction is smaller than the residual Coulomb interaction: $VN(0) - \mu^* < 0$.

6.12 Strongly $\vec{k}$ dependent interactions. It is believed that the 'isotropic' superconductor with a momentum independent order parameter, which is explained in the text, is unavoidable if the effective interactions are phonon mediated - the locality wired into eq. (6.40,6.41) is unavoidable. This turns out to be different in unconventional superconductors. It can for instance be argued that spin wave like excitations tend to mediate strongly $\vec{k}$ dependent effective interactions.

a. Consider an interaction term of the BCS kind, keeping the momentum dependence explicit:

$$H = \sum_{\vec{k}} \varepsilon_{\vec{k}\sigma} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \sum_{\vec{k},\vec{k}'} V_{\vec{k},\vec{k}'} c^\dagger_{\vec{k}'\uparrow} c^\dagger_{-\vec{k}'\downarrow} c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} \tag{6.95}$$

show that the gap equation becomes,

$$\Delta_{\vec{k}'} = -\frac{1}{2N} \sum_{\vec{k}} V_{\vec{k}'\vec{k}} \frac{\Delta_{\vec{k}}}{\sqrt{(\varepsilon_{\vec{k}} - \mu)^2 + \Delta^2_{\vec{k}}}} \tag{6.96}$$

with $\Delta_{\vec{k}} = \sum_{\vec{k}'} V_{\vec{k}\vec{k}'} O_{p,\vec{k}'}$.

b. Recall the Fermi surface of the square lattice tight binding problem at half-filling (e.g. Fig. 5.8). Assume an interaction which is strongly attractive along the (1,0) and (0,1) directions in the Brillouin zone while it is repulsive along the (1,1) and (1,-1) directions. Sketch how the gap function $\Delta_{\vec{k}}$

evolves around the Fermi-surface, assuming (i) $\Delta_{\vec{k}}$ has the same symmetry as the Fermi surface ('anisotropic s'), (ii) $\Delta_{\vec{k}}$ has a lower symmetry than the Fermi-surface but it is still even parity. The latter 'd-wave' superconductor is believed to be realized in high T_c superconductors.

6.13 Show that the total quasiparticle density of states at zero temperature is given by (ε measured from μ)

$$\rho(\varepsilon) \sim \frac{N(0)\varepsilon}{\sqrt{\varepsilon^2 - \Delta^2}} \tag{6.97}$$

For $\varepsilon \geq \Delta$, and $\rho(\varepsilon) = 0$ otherwise. Why is a square root singularity present at $\varepsilon = \Delta$?

6.14 Derive (6.88) from (6.84,6.85).

7 Electrons in normal metals: the Fermi-liquid condensate.

One of the few notions of condensed matter physics which are taught in high schools is that electrical current in metals is due to moving electrons. Freshmen in physics are offered a more complete explanation. The metallic state is used to illustrate the workings of plane wave electrons and Fermi-Dirac statistics: the Sommerfeld model. It is said that one should not worry about interactions between the electrons. Instead, one should apply Fermi-Dirac statistics to fill up the plane wave dispersions, to find a Fermi-energy and a Fermi-surface. This construction yields an amazingly succesful description of the metallic state: it explains why the specific heat and the thermopower are so small while the magnetic response is of the Pauli-type. Taking into account in addition the band structure effects of chapter 3, it explains transport phenomena like the de Haas-van Alphen oscillations. Last but not least, the modern technique of photoemission allows for a direct observation of these band electrons. Obviously, there is truth to these non-interacting fermions.

There is one problem: real electrons interact! The logical implication is that the stuff doing the hard work in the Sommerfeld/band model cannot be 'just' electrons. In order to be non-interacting, the charge of the electron has somehow vanished. In fact, it can also be seen in a different manner that the non-interacting fermions of the Sommerfeld model have to be fundamentally different from electrons. The most important scale parameter in metals is the Fermi-energy which can be translated into a fermion mass. In all metals, the mass of the low energy fermions is larger than the bare electron mass (including band corrections). In some systems, this 'mass enhancement' takes a spectacular form: the effective fermions in ^3He are ten times as heavy as ^3He atoms, while in some actinide and rare earth systems the fermions can be as much as 1000 times as heavy as bare electrons (the 'heavy fermion' systems). It is well established that in these systems density and inhomogeneity conspire to cause strong correlations between the real electrons. Hence, it seems that there is a one-to-one relationship between the strength of the microscopic interactions and the mass of the free fermion showing up in the effective theory describing the macroscopic physics.

We have excercised the notion of 'low energy effective theory': strongly interacting bare particles can act cooperatively to create a low energy universe which is characterized by weakly interacting, particle like excitations. Up to this point we have only encountered bosonic Goldstone modes: given that the system is a classical condensate, the physics at the lowest energies is completely described in terms of non-interacting bosons. This is the key to the nature of the non-interacting Sommerfeld fermions: *the non-interacting fermions found in metals are the fermionic counterparts of the bosonic Goldstone modes.* We learned that Goldstone type excitations only exist because of the presence of a condensate. The central question is therefore: what is the macroscopic, classical object in a metal? The answer is: *the Fermi-sphere* itself. The classical aspect is that at zero temperature the Fermi-surface is localized in single particle momentum space. This is actually a property of a system of non-interacting Fermions. However, at the moment that the interactions are finite the exact quantum-mechanical states would not posses the property Fermi-surface: single particle momentum is *not* a quantum number of the interacting system. Only in the thermodynamic limit the Fermi-surface reappears, but now as the product of a classical condensation process.

The single determinant wavefunction describing the condensate ('$|\Phi^0_{Cl}\rangle$') is of a deceptive simplicity: the $Y^\dagger$'s are nothing else than the simple one electron momentum eigenstates. As we needed real space wavepackets to describe the crystalline state, or spin-coherent states to describe antiferromagnets, we now need single particle states which imply the classical object Fermi surface and the only choice available are the one particle momentum states. Different from the other condensates, this wavefunction reduces to the exact wavefunction of the non-interacting system when the interactions vanish. This has caused much confusion in the history of this subject: one is tempted to think that one is dealing with non-interacting electrons plus some quantitative corrections due to the interactions. This perspective is, however, quite misleading. The rigid nature of the Fermi-surface is a genuine collective phenomenon of the classical kind, well comparable with the rigidity of a superconductor or an antiferromagnet. This rigidity controls the existence of the non-interacting excitations, including the fermions. For instance, the Fermi-surface and the independent fermions do not exist in one dimension, for the same reasons as that crystals and phonons do not exist in this dimension. Also the phenomenology of this state is richer than the litteral Sommerfeld state of non-interacting electrons. This was first realized by Landau who called this state the 'Fermi-liquid'.

Next to the independent fermion excitations, the Fermi-liquid condensate also carries *bosonic* excitations: the zero-sound of the neutral system (^3He) which becomes the plasmon in electron systems. This is the straightforward way to convince oneself that one is dealing with the familiar classical condensate. These modes fall in the Goldstone-class and they correspond with a breathing vibration of the Fermi-surface: in an interacting system, the Fermi surface behaves as an elastic membrane. As will be demonstrated in sections 7.2 (zero-sound) and 7.3 (plasmon), these modes follow from the same kind of reasoning as was used to explain phonons and magnons. Because of the presence of the low energy fermionic modes, the calculation becomes technically more complicated. In order to organize these calculations, it appears necessary to first learn to ask precise questions. For these purposes, the powerful linear response formalism with its spectral- and response functions is introduced in section 7.1.

Although the outcomes might surprise the reader, the conceptual content of this bosonic (zero-sound/plasmons) part of the story is close to the previous chapters. The novelty is in the 'non-interacting fermions' or 'quasiparticles'. It is impossible to address those without the help of a minimum of field-theoretic formalism (Greens functions, diagrams). This formalism serves the purpose of both neatly organizing complex perturbative calculations, as well as a mathematical enrichment of the physicist' view on the world. In section 7.4, I have deliberately sacrified the first aspect to optimize the exposure of the physics part. The reader is warned: do not use this section to do calculations yourself! This is the point where traditionally theory and experiment start to bifurcate and section 7.4 is meant to (a) give experimentalists some clue about the meaning of discussions during theory seminars, (b) give theoreticians some physical intuition which might be helpful in the study of the real thing[1]. Using the Greens function language some key aspects of the Fermi-liquid theory will be shortly discussed: the quasiparticle mass, the overlap between the quasiparticle and the bare electron, as well as the vanishing quasiparticle-quasiparticle interactions. I emphasize that this discipline is not quite a closed subject and recent advancements indicate that there might be another way of looking at the fermionic modes which appears as more fundamental. However, this is a very novel development and I refer the interested reader to the research literature[2].

7.1 Spectral- and Response Functions.

Up to this point in this text, the focus has been on the general properties of the condensed state and we did not worry much about how to precisely measure these properties. In order to address the rather complicated excitation spectrum of the Fermi-liquid, it appears necessary to organize the theory using the same questions as experimentalists would ask. In order to learn anything from a system, one has to perturb it from the outside. Most experiments in condensed matter physics are designed in such a way that the external perturbation is infinitisimally weak compared to the intrinsic energy scales of the system under investigation. As a consequence, the system itself does not change due to the perturbation, and perturbation theory can be applied rigorously. This leads to a mathematically precise description of the outcomes of the measurement process, in terms of the eigenstates of the system. This is the so called *linear response theory.* There are two central objects in this theory:

(i) Spectral functions, describing what kind of information can be obtained by perturbing the system by a single test particle. When the particle is a fermion this is called a *one particle spectral function.* When it does not relate to the fermionic sector, it is called a *dynamic form factor.*

(ii) The response to an external field is described in terms of a *dynamical susceptibility.* For the special case of a charge density perturbation one also defines the

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[1] The theory is most easily formulated in the language of functional integrals: J. W. Negele and H. Orland, 'quantum many particle systems' (Addison-Wesley, 1987). In addition, it is useful as well to study the conventional (Brueckner) formulation as well: 'AGD' ('Methods of quantum field theory in statistical mechanics', A. A. Abrikosov, L. P. Gorkov and I. E. Dzyaloshinskii, Dover) supported by G. D. Mahan's 'Many Particle Physics' (Plenum). For further background reading on sections 7.1-7.3, the classic 'the theory of quantum liquids' by D. Pines and P. Nozieres (Benjamin, New York, 1966) is recommended.

[2] This is the subject of bosonization. The basic idea is that the fundamental excitations of the Fermi-liquid are the bosonic modes describing the vibrations of the Fermi-surface. The fermions appear as the kink-like excitations (disorder operators) of the fundamental bosonic fields. See J. Fröhlich, R. Götschmann and P. A. Marchetti, J. Phys. A, **28**, 1169 (1995) and references therein.

related *dielectric function.*

In this chapter we only consider density responses. The current response functions, underlying transport theory, deserve a separate, in depth treatment.

The simplest linear response object is the dynamical form factor. Imagine an experiment of the inelastic neutron scattering variety. A test particle is located at $\vec{R}_e$ in a system of particles i at positions $\vec{r}_i$. the interaction potential

$$H_{\text{int}} = \sum_i \mathcal{V}\left(\vec{r}_i - \vec{R}_e\right) \tag{7.1}$$

is weak. In momentum space,

$$H_{\text{int}} = \sum_{\vec{q}} \left(\mathcal{V}_{\vec{q}}\, \rho^*_{\vec{q}}\, e^{-i\,\vec{q}\cdot\vec{R}_e} + h.c.\right) \tag{7.2}$$

where $\rho_{\vec{q}}$ is the Fourier transform of the fluctuation in the particle density (compare (4.80)),

$$\begin{aligned} \rho_{\vec{q}} &= \int d^d r\, \rho(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} = \sum_i \int d^d r\, \delta(\vec{r} - \vec{r}_i) e^{-i\vec{q}\cdot\vec{r}} \\ &= \sum_i e^{-i\vec{q}\cdot\vec{r}_i} \end{aligned} \tag{7.3}$$

One could read here as well the charge- or spin density, dependent on the details of the experiment. For instance, neutrons communicate with the density of nucleons and the spin density of the electrons. Energetic electrons and photons see in first instance the charge density of the electrons.

Because of the weakness of H_{int}, the Hilbert space can be build from product states $|n, \vec{P}_e\rangle$ of the plane-wave test particle states $\sim \exp(i\vec{P}\cdot\vec{R}_e)$ and the *exact* eigenstates $|n\rangle$ of the system, with energy eigenvalues E_n. The exact groundstate of the system is $|0\rangle$. We now use Fermi's golden rule: the probability that the test particle exchanges a momentum $\vec{q}$ and an energy ω with the system per unit time is given by the second order in H_{int},

$$P(\vec{q}, \omega) = 2\pi \sum_n \left|\langle n, \vec{P}_e - \vec{q}| H_{\text{int}} |0, \vec{P}_e\rangle\right|^2 \delta(\omega - E_n + E_0) \tag{7.4}$$

with $\omega = \frac{\hbar^2}{2m}((P_e - q)^2 - P_e^2)$. Because the testparticle is described by a plane wave,

$$\langle n,\, \vec{P}_e - \vec{q}| H_{\text{int}} |0,\, \vec{P}_e\rangle = V_{\vec{q}} \langle n|\rho^*_{\vec{q}}|0\rangle \tag{7.5}$$

We define

$$P(\vec{q}, \omega) = 2\pi |V_{\vec{q}}|^2\, S(\vec{q}, \omega) \tag{7.6}$$

It follows that all system specific information is contained in the function,

$$S(\vec{q}, \omega) = \sum_n |\langle 0\, |\rho_{\vec{q}}| n\rangle|^2\, \delta(\omega - E_n + E_0) \tag{7.7}$$

$S(\vec{q},\omega)$ is the *dynamical form factor.* S is simply a density of states, weighted by the (transition) probability $|\langle 0|\rho_{\vec{q}}|n\rangle|^2$ for the system to be excited to a state $|n\rangle$ by a density fluctuation with momentum $\vec{q}$.

The dynamical form factor contains information about the collective 'bosonic' response of the system. For instance, in a crystal the neutron form factor would be dominated by peaks corresponding with the phonons. In electron systems, an even simpler quantity can be measured by photoemission experiments: the *one electron spectral function.* $|0\rangle$ is the exact ground state with energy E_0 of the system containing N electrons. In addition, we define the exact states of the system with $N+1$ electrons as $|N+1,i\rangle$ and energies E_i^{N+1}, as well as the eigenstates of the $N-1$ electron system $|N-1,j\rangle$ at E_j^{N-1}. Starting from the N electron ground state, a single electron in a plane wave state $\vec{k},\sigma$ is created or annihilated. The one electron spectral function is defined as,

$$\begin{aligned} A_{k\sigma}(\omega) &= \sum_i |\langle N+1,i|c^\dagger_{k\sigma}|0\rangle|^2\ \delta(\omega - E_i^{N+1} + E_0) \\ &+ \sum_j |\langle N-1,j|c_{k\sigma}|0\rangle|^2\ \delta(\omega + E_j^{N-1} - E_0) \end{aligned} \tag{7.8}$$

which is the density of states of the $|N\pm 1\rangle$ many electron states, weighted by the probability to arrive in these states, starting from the N particle ground state with one additional electron/hole carrying momentum $\vec{k}$ and σ. Notice that in a non-interacting system this spectral function would consist of delta-functions at the band-dispersions $\omega_{\vec{k}}$. This is also the reason for the sign convention of the energies in (7.8): upon the addition of an electron (unoccupied states), the energy cost is a positive number. However, upon the creation of the hole (occupied states) the energy cost becomes a negative number, the more negative when the excitation energy increases. This is just a convention to draw the electron addition- and electron removal spectra in one picture, with the added advantage that one uses the same convention as in independent electron problems where this convention is natural because of the Pauli principle. As we will see, in interacting problems A has a much richer structure than in the independent particle limit. A is roughly measured in the combination of photoemission (occupied states, $N-1$) and inverse photoemission (unoccupied states, $N+1$) experiments. Since A is a central quantity in the theory, this experimental technique has become quite popular recently.

$\Longrightarrow$ Excercise 7.1

The system can also be perturbed by an external magnetic- or electric field. The (linear) response of the system on the presence of the field can be expressed in terms of the dynamical (spin or charge) susceptibility $\chi(\vec{q},\omega)$. This quantity can also be expressed in terms of the exact quantum mechanical states of the many particle system. This derivation is more laborious. We consider a scalar, time dependent field with potential $\varphi(\vec{r},t)$ coupling to one of the densities (spin-, charge-, number) $\rho(\vec{r},t)$ of the system, described again by (7.1-7.3). First, a choice has to be made regarding the temporal boundary conditions. A natural choice is to switch on the external field at $t=-\infty$, to let it grow as $\sim e^{\eta t}$, with a rate η which is small compared to any response time of the system, so that the system can adjust adiabatically to the field. At the end of the calculation, the limit $\eta \rightarrow 0$ is taken[3]. The time dependent perturbation becomes,

$$\mathcal{H}_e = \sum_{\vec{q}} \int \frac{d\omega}{2\pi} \left(\rho^*_{\vec{q}} \varphi(\vec{q}, \omega) e^{(-i\omega+\eta)t} + h.c. \right) \tag{7.9}$$

where $\phi(\vec{q}, \omega)$ corresponds with the Fourier component of the potential at frequency ω and momentum $\vec{q}$.

Assume that the *exact* wavefunction of the system at time t (Schrödinger picture) can be determined in the presence of the external field. The mean density fluctuation at time t is,

$$\langle \rho(\vec{q}, t) \rangle = \langle \psi(\vec{r}, t) | \rho_{\vec{q}} | \psi(\vec{r}, t) \rangle \tag{7.10}$$

The perturbation is taken to be periodic in time, and because the system can follow the growth of the oscillating field adiabatically,

$$\langle \rho(\vec{q}, t) = \langle \rho(\vec{q}, \omega) \rangle e^{(-i\omega+\eta)t} \tag{7.11}$$

with

$$\langle \rho(\vec{q}, \omega) \rangle = \langle \psi(r, t) | \rho_{\vec{q}} | \psi(r, t) \rangle e^{(i\omega-\eta)t} \tag{7.12}$$

$\langle \rho(\vec{q}, \omega) \rangle$ is the response of the system. This quantity is normalized with regard to the magnitude of the external potential,

$$\chi(\vec{q}, \omega) = \frac{\langle \rho(\vec{q}, \omega) \rangle}{\varphi(\vec{q}, \omega)} \tag{7.13}$$

$\chi(\vec{q}, \omega)$ is the *dynamical* (spin, charge, $\cdots$) *susceptibility*.

χ only depends on the intrinsic properties of the system if the field is choosen to be weak enough such that the response is linear ($\langle \rho \rangle \sim \varphi$). Different from the scattering experiment (7.4-7.7), the external field already shows up in the first order of the perturbation expansion of (7.13). The time development of the exact wavefunction is given by,

$$i \frac{\partial}{\partial t} | \Psi(t) \rangle = (\mathcal{H} + \mathcal{H}_e) | \Psi(t) \rangle \tag{7.14}$$

with the boundary condition that at time $t \rightarrow -\infty$ the system was in the groundstate $|0\rangle$. $|\Psi(t)\rangle$ is expanded in the complete set of eigenstates of H ($|n\rangle$),

$$|\Psi(t)\rangle = \sum_n a_n(t) e^{-iE_n t} |n\rangle \tag{7.15}$$

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[3] A subtlety: in order to prevent heating, one should first let the strength of the potential go to zero, before $\eta \rightarrow 0$. This is automatically taken care off by the perturbation theory.

while at $t \to -\infty$ all $a_n = 0$'s, except $a_0(t = -\infty) = 1$. Up to first order in ϕ ($n \neq 0$),

$$a_n(t) = \Bigg\{ \frac{\langle n|\rho^*_{\vec{q}}|0\rangle \varphi(q,\omega)}{\omega - E_n + E_0 + i\eta} \, e^{\left(i(-\omega+E_n-E_0)+\eta\right)t} - \frac{\langle n|\rho_{\vec{q}}|0\rangle \varphi^*(q,\omega)}{\omega + E_n - E_0 - i\eta} \, e^{\left(i(\omega+E_n-E_0)+\eta\right)t} \Bigg\} \tag{7.16}$$

⟹ Excercise 7.2

In addition, the average charge fluctuation is to first order,

$$\langle \rho(\vec{q},t)\rangle = \sum_n \left\{ \langle 0|\rho_{\vec{q}}|n\rangle \; a_n(t) \; e^{-i(E_n-E_0)t} + \langle n|\rho_{\vec{q}}|0\rangle \; a^*_n(t) \; e^{i(E_n-E_0)t} \right\} \tag{7.17}$$

combining (7.16,7.17),

$$\langle \rho(\vec{q},t)\rangle = \varphi(q,\omega) \, e^{(-i\omega+\eta)t} \sum_n \left\{ \frac{|\langle n|\rho^*_q|0\rangle|^2}{\omega - E_n + E_0 + i\eta} - \frac{|\langle n|\rho_q|0\rangle|^2}{\omega + E_n - E_0 + i\eta} \right\} \tag{7.18}$$

⟹ Excercise 7.3

The susceptibility follows by comparing (7.18) with (7.12,7.13),

$$\chi(q,\omega) = \sum_n \; \langle 0|\rho_q|n\rangle \langle n|\rho^*_q|0\rangle \left\{ \frac{1}{\omega - E_n + E_0 + i\eta} - \frac{1}{\omega + E_n - E_0 + i\eta} \right\} \tag{7.19}$$

Comparing (7.19) with the expression for the dynamical form factor (7.7) shows that this quantity and the dynamical susceptibility are related,

$$\chi(\vec{q},\omega) = \int_0^\infty d\omega' \; S(\vec{q},\omega') \left\{ \frac{1}{\omega - \omega' + i\eta} - \frac{1}{\omega + \omega' + i\eta} \right\} \tag{7.20}$$

The susceptibility is a complex quantity. As will become clear, the in-phase (reactive) real part of χ (χ') relates to the reversible response of the system, while the imaginary part (χ'') corresponds with the irreversible, dissipative respons (the losses). Given that $f(z)$ is analytic on the complex plane (P is the principal part),

$$\lim_{\eta \to 0} \int \frac{f(x)}{x - a \mp i\eta} = P \int \frac{f(x)}{x - a} \pm i\pi f(a) \tag{7.21}$$

or symbolically (the Dirac relation),

$$\lim_{\eta \to 0} \frac{1}{x - a \mp i\eta} = P \, \frac{1}{x - a} \pm i\pi\delta(x - a) \tag{7.22}$$

which will turn out to be a very useful relation: it links the delta function, relating to a density of states, to a complex function. This is a main reason that much of what follows will appear as an excercise in complex analysis. Using (7.22), the real- and imaginary part of χ can be written as,,

$$\chi'(\vec{q},\omega) = \int_0^\infty d\omega'\ S(\vec{q},\omega')P\left(\frac{2\omega'}{\omega^2-\omega'^2}\right) \tag{7.23}$$

$$\chi''(\vec{q},\omega) = -\pi\left\{S(\vec{q},\omega)-S(\vec{q},-\omega)\right\} \tag{7.24}$$

$\Longrightarrow$ Excercise 7.4

The relations (7.23) and (7.24) give a clear insight in the nature of the dynamical susceptibility. The meaning of the dynamical form factor S is immediately clear: it is a measure of the number of real (not virtual) transitions with energy ω and momentum $\vec{q}$ in the system, caused by the presence of the test particle. Although it is obvious that the dissipative response of the system to the external field (χ'') has to relate to these real excitations as well, the precise form (7.24) is not obvious at all, let alone that the reactive part relates to S by (7.23). Because the above derivation is rigorous, (7.24) has a mathematical status: it is called the *fluctuation-dissipation theorem* - χ'' is the dissipation and S the fluctuation[4]

Many experiments relate to the 'twin' dynamical form factor - dynamical susceptibility. Let us consider a simple example. Imagine a magnetic system with a singlet ground state. In the presence of spin-orbital coupling, a magnetic field can couple this singlet to excited states, carrying a spin (triplets, quintuplets, etcetera). The potential ϕ becomes $\varphi \sim BS^z$ and B is an external magnetic field. Neutrons carry spin and they can loose energy by exciting magnetic states. We assume that only one triplet state is important (all other states are at very high energy), while this state is nearly decoupled from the rest of the world so that it lives for a nearly infinite time. The energy-loss spectrum of the neutron is directly proportional to the dynamical formfactor, and the latter corresponds with a single delta function peak (infinite life-time) at the triplet energy ε_0 (figure 7.1),

$$S(\vec{q},\omega) = A\delta(\omega-\varepsilon_0) \tag{7.26}$$

Using (7.23,7.24), the dynamical susceptibility follows directly (figure 7.1),

$$\begin{aligned}\chi'(\vec{q},\omega) &= A\,\frac{2\varepsilon_0}{\omega^2-\varepsilon_0^2}\\ \chi''(\vec{q},\omega) &= -\pi A\Big(\delta(\omega-\varepsilon_0)-\delta(\omega+\varepsilon_0)\Big)\end{aligned} \tag{7.27}$$

By applying the external field one can attempt to measure the dynamical susceptibility directly. This is in practice not so easy. It is impossible to construct a magnet, producing a field with a modulation in space ($\vec{q}$) or time (ω) which is anywhere close

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[4] It is straightforward to generalize this to finite temperature. Among others,

$$NS(\vec{q},\omega=0) = -\int\frac{d\omega}{2\pi}\chi''(\vec{q},\omega)coth(\frac{\beta\omega}{2}) \tag{7.25}$$

$S(\vec{q},\omega=0)$ is the mean quadratic density fluctuation $\langle\rho^*_{\vec{q}}\rho_{\vec{q}}\rangle$.

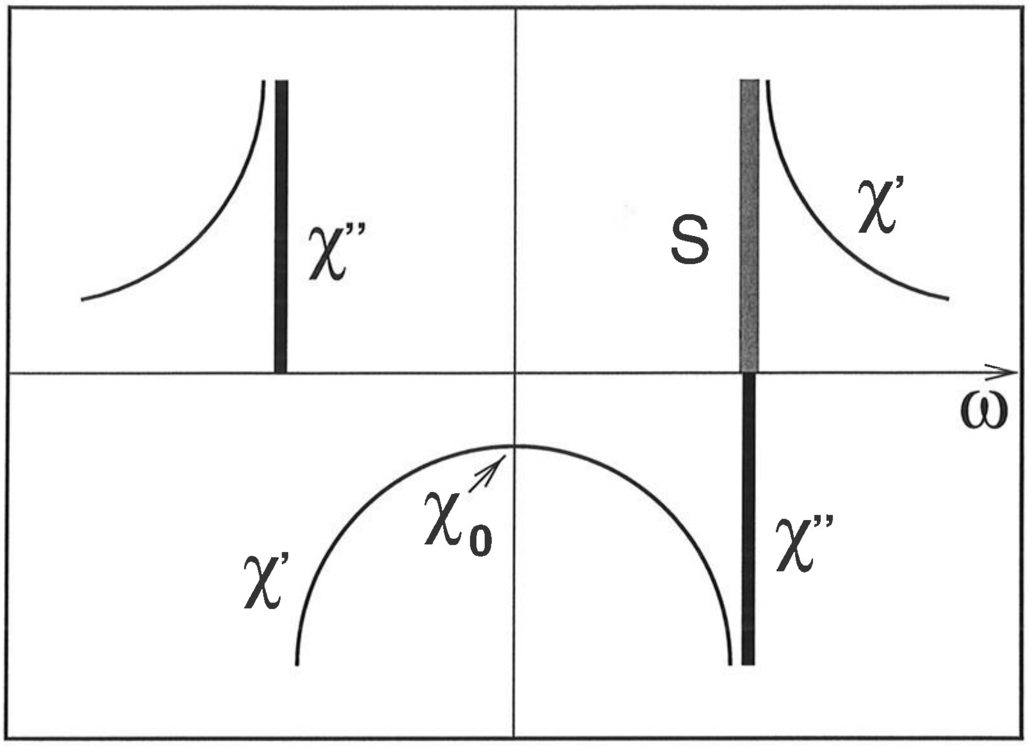

Figure 7.1:*the toy-linear response experiment. The magnetic state would show up as a peak in an inelastic neutron scattering experiment (S).* χ'' *is also characterized by peaks, but now at positive and negative frequencies, while* χ' *(including the bulk susceptibility* χ_0*) follows from causality.*

to the microscopic scales, and therefore the measurement is limited to $\vec{q} \rightarrow 0$ (not important in this local system) and $\omega \rightarrow 0$. In a magnetometer the reactive response is measured and according to (7.26) the 'bulk susceptibility' is,

$$\chi_0 \equiv \chi'(q = 0, \omega = 0) = -\frac{2A}{\varepsilon_0} \qquad (7.28)$$

Because of the definition of χ, the negative sign of χ_0 implies a paramagnetic response and this kind of paramagnetism is called 'van Vleck paramagnetism'.

This example illustrates in a realistic manner how linear response is used in practice to let different kinds of experiment cooperate. The inelastic scattering experiments (neutron scattering for spins and nuclei; electron energy loss and X-ray scattering for charge) have the great advantage that they give access to large regions in frequency and momentum space. At the same time, they are technically difficult and by their very nature not very accurate. For instance, it might be quite difficult to obtain the matrix elements, coupling the neutron spin to the spin of the electron system. On the other hand, the bulk experiments (magnetic susceptibility, resistivity, specific heat) are very limited in their $\vec{q}$ and $\vec{\omega}$ range, but are highly accurate and can be used to 'gauge' the dynamical information[5]. This 'orchestrated' experimentation has been

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[5] In addition, there are experiments which cover a larger part of $\vec{q}, \omega$ space. Optical experiments (optical conductivity/reflectivity) in the linear response regime cover the charge (current) response

the true driving force behind the progress in condensed matter physics.

7.2 The Fermi-surface: statistics or condensation?

As I already announced in the introduction, the independent particle picture for metals is quite misleading. Instead, one can better view the Fermi-liquid state as a classical condensate, albeit one which carries a richer physics than the condensates we have encountered in the previous chapters. Next to the usual bosonic Goldstone excitations, it carries fermionic 'modes' as well, and the latter are harder to understand than the former. In this section, we will focus on the nature of the rigidity of this state, as well as on the bosonic excitations as implied by this rigidity, to find that this part of the story fits quite well in the paradigm of section 1.2. In this section, the focus is on fermion systems without long range interactions: the neutral Fermi-fluid. The results as obtained in this section apply directly to ^3He and the theory is easily extended to include the charged (electron) Fermi-liquid, which will be discussed in the next section.

Let us in first instance neglect the ion potentials and consider the homogeneous fermion-gas or 'jellium': we imagine that the particles move in a flat background potential. This simplifies the discussion appreciably while the physics does not change qualitatively by the presence of a more interesting background potential. The essence of the Fermi-liquid is of a deceptive simplicity: the single determinant wave function defining the classical state (Eq. 1.1) is the simplest possibility one can imagine for fermions,

$$|\Phi^0_{Cl}\rangle_{FL} = \Pi_{\vec{k}\sigma} c^\dagger_{\vec{k}\sigma} \mid \text{vac.} \rangle \tag{7.29}$$

the ground state wavefunction of a system of non-interacting fermions! At first sight, it might sound odd to identify this wavefunction with something classical. One should keep in mind, however, that: (a) in the presence of interactions, (7.29) is not an eigenstate of the system; (b) the true eigenstates would look like coherent superpositions of large numbers of single determinant states, and in this regard (7.29) is neither better, nor worse than the other condensate wavefunctions we learned to appreciate; (c) there is nothing arguing against constructing condensate wavefunctions in momentum space, as we learned to appreciate in the context of weak-coupling magnetism and superconductivity - the only novelty is that we can no longer continue to a strong coupling, real space picture. The coherence length is infinite, because there is no gap. (d) As will be explained, (7.29) implies rigidity and Goldstone modes when the interactions are finite, and these properties make the condensate qualitatively different from the non-interacting system. This looks quite similar to the other condensates. For instance, in one dimension the Fermi-liquid cannot exist, for the same reasons that the crystal cannot exist.

Since (7.29) describes non-interacting electrons, one can easily confuse oneself with

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on the ω axis, but are limited to $\vec{q} \rightarrow 0$ because of the small momentum of the phonon. NMR yields information on the $\vec{q}$ behaviour of χ away from $\vec{q} = 0$ but measures at very low frequency (typically MHz).

the thought that this is all controlled by interaction strength: the non-interacting system has to be *corrected* quantitatively by perturbation theory for the effects of interactions and when these are weak, the corrections are small. This viewpoint is abundant in the older literature. Unfortunately, it is severely flawed. *Interaction strength is in first instance irrelevant for the (non)existence of the Fermi-liquid.* The existence of the Fermi-liquid is controlled by the same parameters which control the existence of the other classical condensates (crystals, antiferromagnets, superconductors): dimensionality and microscopic quantum fluctuation. For instance, despite the gigantic interaction strengths, Fermi-liquids are realized in the three dimensional heavy fermion systems. At the same time, it can be *proven* that the Fermi-liquid disappears in a one dimensional system at the very moment that the interactions become finite. Although the books are not yet closed on the subject, it seems that the Fermi-liquid state is *always* realized in *infinite dimensions*, at least if no competing classical condensations intervene[6].

This confusion was partly based on the fact that a limit can be identified where the effects of the interactions litterally vanish: the high density limit. This is a peculiarity of the fermion system. For classical objects or bosons, the effects of the interactions become more severe if the density increases; recall the discussion in section 5.1. In fermion systems, however, the average kinetic energy of the particles increases faster with density than the average interaction energy, and it is the ratio of these two which determines the coupling strength. r_s is the radius of the sphere containing precisely one electron charge ($r_s^3 \sim 1/n_0$, n_0 is the density). The Fermi-energy is a measure of the kinetic energy and this increases as $E_F \sim 1/r_s^2$ with decreasing r_s, while the Coulomb energy increases slower, $E_{ww} \sim 1/r_s$, and the ratio $E_{ww}/E_F \to 0$ when $n_0 \to \infty$. The perturbation expansion around (7.29) could then be interpreted as a high density expansion. Although it is true that the numerical effects of the interactions become less important when the density increases[7], it is equally true that this perturbation theory is singular if the dimensionality does not allow the condensate to form, regardless the density of the system.

The next question is: given (7.29), what is the order parameter and the associated ridigidity of the Fermi-liquid state? This is equivalent to: which symmetry is spontaneously broken? The only physical feature carried by the state (7.29) is the *expectation value of the number operator for all single particle momenta $\vec{k}$ and spin σ*,

$$\langle n_{\vec{k}\sigma} \rangle = \theta(\vec{k} - \vec{k}_F) \tag{7.30}$$

The specialty of the non-interacting state is that this average shows a *discontinuity*, and this discontinuity actually defines the Fermi-surface. Since for every $\vec{k}$ the locus of the discontinuity can be determined ($\vec{k}_F$) we can establish a surface in *single particle* momentum space on which the discontinuities lie: the Fermi surface. We need all

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[6] For the 'dynamical mean-field theory' becoming exact in $d \to \infty$, see Vollhard et al, Rev. Mod. Phys., in press.

[7] This explains the success of independent fermion theory in astrophysics; the cores of heavy stars, neutron stars, etcetera, are all very high density objects.

fermions to accomplish this, and the Fermi-surface is a collective property of the system, albeit a simple one in the non-interacting limit. *Single particle* momentum does not commute with the interaction term in the Hamiltonian and the exact ground state of the interacting system does not carry single particle momentum as a quantum number. Because the single particle momenta are fluctuating quantities, it is not possible to construct a precisely determined object out of these fluctuating states: the exact ground state of the interacting Fermi system does not allow for the existence of a Fermi-surface! *The localization of the Fermi-sphere in single particle momentum space involves a symmetry breaking and this is the classical aspect of the Fermi-liquid.*

Hence, the problem is that according to exact quantum mechanics it is not possible to localize the Fermi-sphere in single particle momentum space. It is again interesting to consider the situation where the symmetry restoring fluctuation gets out of hand: one dimension. As we will see in a moment, it is not hard to identify modes which describe the motions of the Fermi-surface around its average position, and it is the admixing of these modes in the classical (Fermi-liquid) ground state, describing a 'wobbling' of the Fermi-surface in k space, which renders the perturbation theory around (7.29) unstable. Recall the discussion towards the end of section 6.3, where I argued that coupling strength tunes the magnitude of the quantum fluctuations. These fluctuations show up in the ultraviolet of the Fermi-surface wandering problem and by approaching the weak coupling limit, the dimensionless coupling constant measuring the microscopic fluctuation becomes quite small. The charge and spin density modes describing the Fermi-surface motions are much like phonons and the classical state is always killed by the longest wavelength modes. The net result is that the one dimensional interacting fermion system becomes a floating solid in the weak coupling limit, in terms of the collective modes describing the Fermi-surface motions. Accordingly, the Fermi-surface becomes 'fuzzy' in k-space and the state which is realized instead is called the 'Luttinger liquid'.

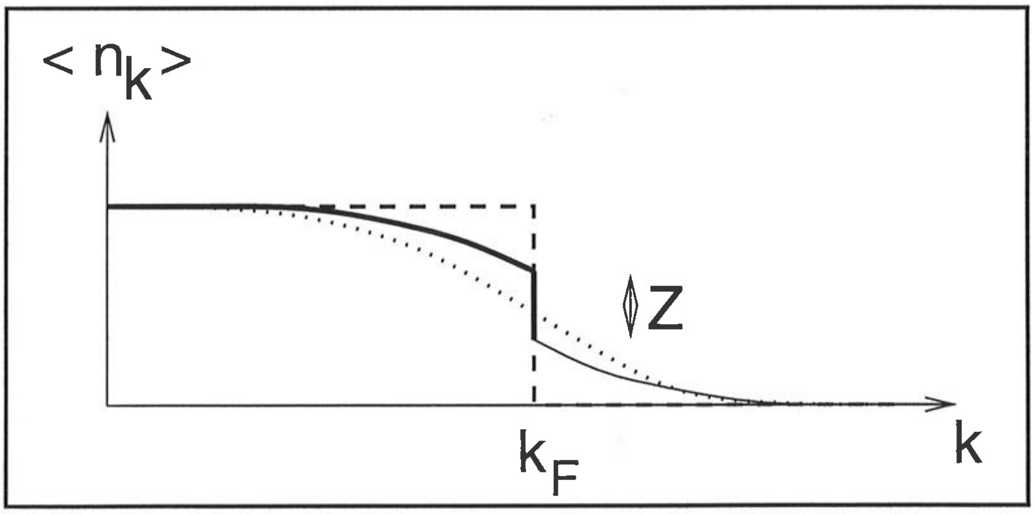

Figure 7.2:*momentum distribution of a Fermi-liquid (full line), which is a superposition of the discontinuous independent electron distribution (dashed line) and a continuous contribution due to the vacuum fluctuations (dotted line).*

We find a repetition of a now familiar pattern: a single determinant wavefunction defining an order (the location of the Fermi-surface), which is violating quantum mechanical symmetry requirements. Apparently, this state is carrying as well order parameter modes which are capable of disordering the state when the dimensionality becomes too low. What happens in higher dimensions? At least in $d = 3$ ($d = 2$ is not completely clear), this condensate is very often realized. As for the other condensates, this does not mean that (7.29) becomes exact: there are still quantum fluctuations reducing the magnitude of the order parameter. I already stated that the localization of the Fermi-surface is in a one-to-one correspondence with the *discontinuity* in the momentum distribution function $\langle n_{\vec{k}} \rangle$ and the *height* of this discontinuity can actually be used as the order parameter. The real ground state wavefunction of the Fermi-liquid, including the fluctuations, is of the same form as Eq. (1.1),

$$|\Phi_{FL}\rangle \;=\; A\,\Pi_{\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma} \mid \text{vac.}\rangle + \sum_i a_i |\Phi_i\rangle \tag{7.31}$$

and the states $|\Phi_i\rangle$ will correspond with excited states of the independent particle problem. At the moment something is excited on top of the Fermi-sea, the discontinuity in the momentum distribution disappears - for instance, recall the Fermi-Dirac distribution at finite temperature. As a consequence,

$$\langle \Phi_{FL} | n_{\vec{k}} | \Phi_{FL} \rangle \;=\; A^2\, \theta(\vec{k} - \vec{k}_F) + f(\vec{k}) \tag{7.32}$$

where $f(\vec{k})$ has to be continuous at $\vec{k}_F$ because this contribution originates in the Φ's which are characterized by the absence of a discontinuity in their momentum distributions. The real momentum distribution is indicated in figure 6.2. Hence, the fluctuations decrease the magnitude of the discontinuity, but as long as the discontinuity exists, the Fermi-surface is localized and the state is of a classical nature.

The added difficulty encountered in the Fermi-liquid is that this state is also characterized by fermionic excitations at arbitrarily low energies, and the structure of the theory underlying these 'modes' is quite different from that of the Goldstone bosons. This will be the subject of section 7.4, where it will be shown that the finiteness of the discontuinity implies (a) that these fermions become non-interacting in the low energy limit, (b) the overlap with the bare fermion, as measured by the one particle spectral function (7.8), is *finite* and this overlap (the 'pole strength', Z) is actually directly related to the weight of the classical component in the ground state wavefunction A^2, (c) it is demonstrated that this pole strength is actually inversely proportional to the enhancement of the effective mass of the quasiparticle. In the indepent electron limit ($A^2 = 1$) the mass of the quasiparticle equals the mass of the electron. However, when the weight of (7.29) decreases in (7.31), the mass of the quasiparticle *increases*: a quasiparticle mass of $1000 m_e$, as found in the heavy fermion systems, means that the probability that the vacuum is in the classical state is as small as 1/1000. Despite this small weight, this classical component is still in full control of the macroscopic properties of these systems!

Next to this fermionic sector, the Fermi-liquid also carries a sector of bosonic excitations. This looks much more familiar: it amounts to a variation on the now familiar theme of classical order. For finite interactions, the *Fermi-surface becomes a rigid object.* Accordingly, it carries modes describing coherent (propagating) vibrations of the Fermi-sphere and at long wavelengths these obey the Goldstone theorem (linear dispersion, infinite life-time). Let us first consider the case of short range interactions: the neutral Fermi-liquid which is realized at low temperatures in ^3He.

In contrast to the other condensates, the Fermi-liquid can only be formulated in momentum space and we are forced to set up the fluctuation theory in momentum space as well. This is technically more demanding, but the principles are the same as in real space, as we already explained in section 5.6. The present problem is in fact easier than the problem addressed in section 5.6, because the classical state (7.29) is easier than the spin density wave, and we will here pursue the full 'Random phase approximation' (RPA). The simplification comes from the fact that the classical state is also the ground state of the independent particle problem. Let us therefore first study the excitation spectrum of the non-interacting system, using the linear response formalism of section 7.1. The Hamiltonian of a system of non-interacting fermions is,

$$\mathcal{H}^0 = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} \tag{7.33}$$

The fermion density fluctuation at wavelength $\vec{q}$ is described by the operator (eq, (4.80)),

$$\rho_{\vec{q}} = \sum_{\vec{k}\sigma} \rho_{\vec{k}\vec{q}\sigma} \tag{7.34}$$

with,

$$\rho_{\vec{k}\vec{q}\sigma} = c^\dagger_{\vec{k}\sigma} c_{\vec{k}+\vec{q}\sigma} \tag{7.35}$$

describing an electron-hole pair excitation with center of mass momentum $\vec{q}$.

$\Longrightarrow$ Excercise 7.5

An external scalar field is switched on, which couples to the fermion density according to (7.9). In the presence of this field, the equation of motion for the electron-hole pair operator becomes,

$$\begin{aligned} i\dot{\rho}_{\vec{k}\vec{q}\sigma} &= \left[\rho_{\vec{k}\vec{q}\sigma}, \mathcal{H}^0 + \mathcal{H}_{\text{ext}}\right] && (7.36) \\ &= \left(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}}\right) \rho_{\vec{k}\vec{q}\sigma} + \left\{ c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} - c^\dagger_{\vec{k}+\vec{q}\sigma} c_{\vec{k}+\vec{q}\sigma} \right\} e\, \varphi_{\text{ext}}(\vec{q}, \omega)\, e^{-i\omega t}\, e^{\eta t} + \\ &\quad \left\{ c^\dagger_{\vec{k}\sigma} c_{\vec{k}+2\vec{q}\sigma} - c^\dagger_{\vec{k}-\vec{q}\sigma} c_{\vec{k}+\vec{q}\sigma} \right\} e\, \varphi^*_{\text{ext}}(\vec{q}, \omega)\, e^{i\omega t}\, e^{\eta t} && (7.37) \end{aligned}$$

In the regime of linear response, the external field does not change the system of fermions and since (7.30) is exact in the absence of interactions, we can set $n^0_k = \langle c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} \rangle = \theta(k - k_F)$ and $\langle c^\dagger_{\vec{k}\sigma} c_{\vec{k}+2\vec{q}\sigma} \rangle = 0$. The time-dependent electron-hole operator is expressed as,

$$\rho_{\vec{k}\vec{q}\sigma}(t) = \rho_{\vec{k}\vec{q}\sigma}(\omega) e^{-i\omega t} \cdot e^{\eta t} \tag{7.38}$$

Filling in (7.38) in (7.37) and taking the expectation values yields for the density susceptibility (7.13),

$$\begin{aligned}\chi^0(\vec{q},\omega) &= \frac{\sum_{\vec{k}}\langle\rho_{\vec{k}\vec{q}\sigma}(\omega)\rangle}{\varphi_{\mathrm{ext}}(\vec{q},\omega)} && (7.39)\\ &= \sum_{\vec{k}} \frac{n^0_k - n^0_{k+q}}{\omega - \varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{q}} + i\eta} && (7.40)\end{aligned}$$

which can also be written as,

$$\chi^0(\vec{q},\omega) = \sum_{\vec{k}} n^0_k(1-n^0_{k+q}) \left\{\frac{1}{\omega - \varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{q}} + i\eta} - \frac{1}{\omega + \varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}} + i\eta}\right\} \quad (7.41)$$

by relabeling: $\vec{k} \to -\vec{k} - \vec{q}, \varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}} \to -\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{q}}$. In (7.41), the form $\chi'' \sim S(\omega) - S(-\omega)$ is recognized.

$\Longrightarrow$ Excercise 7.6

Let us now switch on the fermion-fermion interactions. A pair interaction in a Galilean-invariant system, like the jellium, can be written in terms of the Fourier components of the particle density as,

$$\mathcal{H}_1 = \sum_{\vec{q}} \frac{\mathcal{V}_q}{2}\rho_{\vec{q}}\rho_{-\vec{q}} = \sum_{\vec{k}\vec{k}'\vec{q}\sigma\sigma'} \frac{\mathcal{V}_q}{2}\, c^\dagger_{\vec{k}+\vec{q}\sigma} c^\dagger_{\vec{k}'-\vec{q}\sigma'} c_{\vec{k}'\sigma} c_{\vec{k}\sigma} \quad (7.42)$$

with

$$\mathcal{V}_q = \frac{1}{\sqrt{N}} \sum_{\vec{R}} \mathcal{V}(|\vec{R}|)\, e^{i\vec{q}\cdot\vec{R}} \quad (7.43)$$

In the interacting system, the time development of the electron-hole pair operator also relates to the commutator of $\rho_{\vec{k}\vec{q}\sigma}$ with H_1,

$$\left[\rho_{\vec{k}\vec{q}\sigma}, \mathcal{H}_1\right] = \sum_{\vec{p}} \left(\frac{\mathcal{V}_p}{2}\right) \left\{\rho_{\vec{p}}\left(c^\dagger_{\vec{k}\sigma}c_{\vec{k}+\vec{q}-\vec{p}\sigma} - c^\dagger_{\vec{k}+\vec{p}\sigma}c_{\vec{k}+\vec{q}\sigma}\right) + \left(c^\dagger_{\vec{k}\sigma}c_{\vec{k}+\vec{q}-\vec{p}\sigma} - c^\dagger_{\vec{k}+\vec{p}\sigma}c_{\vec{k}+\vec{q}\sigma}\right)\rho_{\vec{p}}\right\} \quad (7.44)$$

Together with (7.37), this equation has the same status as the exact expressions (5.56) or (5.148), which were encountered in the context of magnetism. It is no longer possible to solve the equations of motion exactly. At this moment we need the notion of the Fermi-liquid order parameter, to decouple (7.44). In *precise analogy* with (5.106), we assume that the operators describing an electron-hole fluctuation can be decomposed in a scalar, 'vacuum amplitude' part corresponding with (7.30) and a 'harmless' fluctuation,

$$c^\dagger_{\vec{k}\sigma}c_{\vec{k}+\vec{q}-\vec{p}\sigma} = \delta_{\vec{k},\vec{q}}n^0_k + \delta n_{\vec{k}\sigma} \quad (7.45)$$

to neglect the effects of the quantum fluctuations $\delta n_{\vec{k}\sigma}$ in first instance[8]. Consistency with (7.45) requires $c^{\dagger}_{\vec{k}+\vec{p}\sigma} c_{\vec{k}+\vec{q}\sigma} = n^0_{k+q} + \delta n_{\vec{k}+\vec{q}\sigma}$, and together with (7.43) the equation of motion, describing the classical linearized dynamics of the electron-hole pairs, becomes

$$i \langle \dot{\rho}_{\vec{k}\vec{q}\sigma} \rangle = (\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}}) \langle \rho_{\vec{k}\vec{q}\sigma} \rangle + \left(n^0_k - n^0_{k+q} \right) \left(e\varphi_{\text{ext}}(\vec{q},\omega) e^{-i\omega t} e^{\eta t} + \mathcal{V}_q \langle \rho_{\vec{q}} \rangle \right) \quad (7.46)$$

This equation has the same status as (4.22) in the context of crystals, or (5.60) in the context of the Néel state. Summing over $\vec{k}$, using (7.40),

$$\langle \rho_{\vec{q}}(\omega) \rangle = \chi_0(\vec{q},\omega) \Big(\varphi_{\text{ext}}(\vec{q},\omega) + \mathcal{V}_q \langle \rho_{\vec{q}}(\omega) \rangle \Big) \quad (7.47)$$

and it follows that,

$$\chi(\vec{q},\omega) = \frac{\langle \rho_{\vec{q}}(\omega) \rangle}{\varphi_{\text{ext}}(\vec{q},\omega)} \quad (7.48)$$

$$= \frac{\chi_0(\vec{q},\omega)}{1 - \mathcal{V}_q \chi_0(\vec{q},\omega)} \quad (7.49)$$

(7.49) is an important result. Although the fluctuations give rise to large quantitative corrections, the form of (7.49) survives in the fully renormalized low energy theory.

Despite its simple form, (7.49) has a rich physical content. The reason is that the susceptibility of the non-interacting system, χ_0, is a rather complicated function. For the $d = 3$ jellium, the integral appearing in (7.40) was for the first time solved by Lindhard. The imaginary part of this so-called Lindhard function is relatively simple,

$$\chi''_0(\vec{q},\omega) = \frac{m}{4\pi q} \left[\theta(k_F - k_-)(k_F^2 - k_-^2) - \theta(k_F - k_+) \cdot (k_F^2 - k_+^2) \right] \quad (7.50)$$

with ($\varepsilon_{\vec{q}} = q^2/2m$, as usual $\hbar = 1$),

$$k_{\pm} = \frac{m}{q} \left| \varepsilon_{\vec{q}} \pm \omega \right| \quad (7.51)$$

$\Longrightarrow$ Excercise 7.7

The real part is more complicated (In a d=3 jellium, the density of states at E_F is $N_0 = 3n_0/2E_F$),

$$\chi'_0(\vec{q},\omega) = -\frac{3n_0}{2E_F} \Bigg\{ 1 + \frac{m^2}{2k_F q^3} \left(4E_F \varepsilon_{\vec{q}} - (\varepsilon_{\vec{q}} + \omega)^2 \right) \ln \left| \frac{\varepsilon_{\vec{q}} + q v_F + \omega}{\varepsilon_{\vec{q}} - q v_F + \omega} \right|$$

$$+ \frac{m^2}{2k_F q^3} \left(4E_F \varepsilon_{\vec{q}} - (\varepsilon_{\vec{q}} - \omega)^2 \right) \ln \left| \frac{\varepsilon_{\vec{q}} + q v_F - \omega}{\varepsilon_{\vec{q}} + q v_F + \omega} \right| \Bigg\} \quad (7.52)$$

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[8] This is the origin of the vocabulary 'random phase approximation'. When this theory was invented the 'approximation' was rationalized by referring to the cancellation of the contributions coming from $\vec{q} \neq \vec{p}$ because of their rapidly varying phases. See D. Pines and P. Nozieres, 'The theory of quantum liquids' (W. A. Benjamins, 1966).

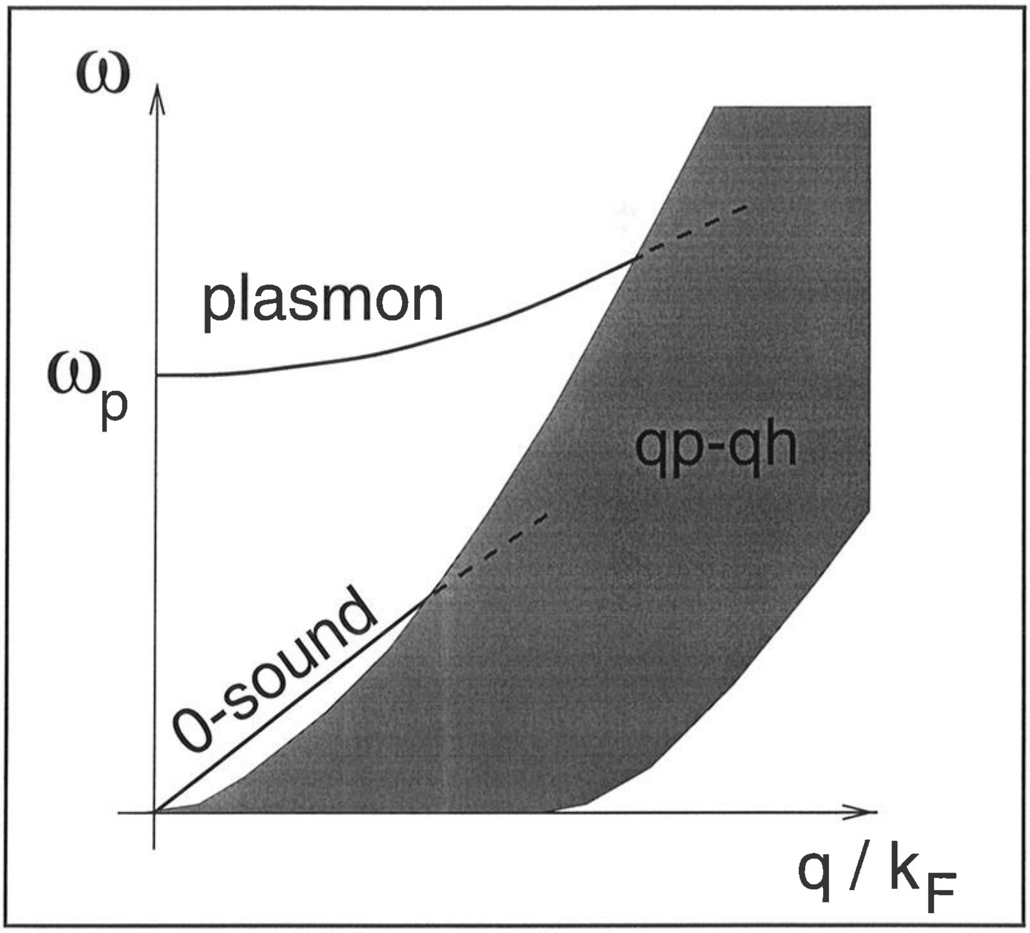

Figure 7.3: *general appearance of the imaginary part of the RPA dynamical susceptibility. In the grey area in momentum/frequency space, incoherent quasiparticle-quasihole excitations are found. In addition, the zero-sound mode of the neutral Fermi-liquid and the plasmon of the charged Fermi-liquid are indicated as well.*

In order to interpret χ_0, we first focus on the imaginary part: we learned from linear response theory that the positive frequency part is a measure for the density of real excitations at momentum $\vec{q}$ and energy ω. *In the absence of interactions, the spectrum of density excitations is exhausted by the particle-hole excitations of a given center of mass momentum $\vec{q}$ and energy ω.* χ_0'' is nothing else than the particle-hole density of states. In figure (7.3) it is indicated where χ_0'' is non-zero in momentum-energy space by the grey area, as follows directly from the kinematics.

$\Longrightarrow$ Excercise 7.8

In the non-interacting limit, the response of the Fermi-gas to a density perturbation is *incoherent.* The system adjusts to the density perturbation by exciting *independent* particle-hole excitations, and there is no sense of rigidity: its response is like the response of a gas. This changes qualitatively at the moment that the interactions become finite. Although there are still independent fermion excitations (now described in terms of the quasiparticles), collective propagating excitations are found as well which actually dominate in the long-wavelength limit. These have the same status as the other Goldstone modes we already encountered. These modes vividly illustrate the *rigid* nature of the Fermi-surface in the interacting system: the Fermi surface vibrates as an overinflated balloon! The mode where the sphere vibrates uniformly (s-wave) is the most important one, and this mode has been observed in ^3He, where it is called 'zero-sound'.

In the long wavelength limit, the detail of the (short range) interactions becomes unimportant and we assume a hard-core interaction: $\mathcal{V}_{\vec{q}} \to \mathcal{V}$. (7.49) simplifies to,

$$\chi(\vec{q},\omega) = \frac{\chi_0(\vec{q},\omega)}{1 - \mathcal{V}\chi_0(\vec{q},\omega)} \tag{7.53}$$

In first instance, we are interested in the imaginary part of (7.53) to find out about the excitations of the system. It follows directly from (7.53),

$$\chi''(\vec{q},\omega) = \frac{\chi_0''(\vec{q},\omega)}{\left(1 - \mathcal{V}\chi_0'(\vec{q},\omega)\right)^2 + (\mathcal{V}\chi_0''(\vec{q},\omega))^2} \tag{7.54}$$

There are two possibilities:
(i) $\vec{q}$ and ω are outside the grey area of figure 7.3, such that $\chi_0''(\vec{q},\omega) = 0$. The imaginary part of χ is only non-zero if the denominator vanishes. When this happens, a pole is found in the spectrum

$$\chi''(\vec{q},\omega) = 2\pi\delta\left(1 - \mathcal{V}\chi_0'(\vec{q},\omega)\right), \quad \chi_0''(\vec{q},\omega) = 0\ . \tag{7.55}$$

The condition to find the pole is,

$$\chi_0'(\vec{q}_s,\omega_q) = \frac{1}{\mathcal{V}}, \quad \chi_0''(\vec{q}_s,\omega_q) = 0 \tag{7.56}$$

Hence, a sharp, isolated excitation is found at $\vec{q}_s$ and $\omega_{\vec{q}}$. This is the signature of a mode - also phonons and magnons would show up in this way in the dynamical susceptibility. The condition (7.56) can only be satisfied if the interaction is finite ($\mathcal{V} \neq 0$) and this is the zero-sound mode.
(ii) The condition for the real part in (7.56) is satisfied but $\chi_0''(\vec{q}_s,\omega_q) \neq 0$ (inside the grey area of figure 7.3). Choosing $\mathcal{V}\chi_0''$ to be small compared with $\omega_{\vec{q}}$, this would correspond according to (7.54) with a Lorentzian peak which is centered at $\vec{q}_s, \omega_{\vec{q}}$, with a width $\sim \mathcal{V}\chi_0''(\vec{q}_s,\omega_{\vec{q}})$. The collective excitation has now a lifetime $\tau \sim \hbar/\mathcal{V}\chi_0''(\vec{q}_s,\omega_{\vec{q}})$: *the zero-sound mode is damped because it can decay into the continuum of incoherent particle-hole excitations.* This process is called Landau damping. Notice that this is a different process than the damping coming from mode-mode interactions, as discussed in section 4.4. The present theory is still on the Gaussian level, and the Landau damping is an additional decay channel, caused by the presence of the quasiparticle excitations. It actually turns out that the decay rate is rapidly increasing when the zero-sound mode penetrates the particle-hole spectrum and very quickly the mode

becomes overdamped and the excitation spectrum start again to look like that of independent quasiparticles (χ_0'').

When are the conditions (7.56) satisfied? Let us focus on the Goldstone regime of low frequencies and large wavelengths, where the Gaussian theory is expected to work best. (7.52) is expanded for small q and (7.56) becomes,

$$\frac{\omega_q}{q_s v_F} \ln \left| \frac{\omega_q + q_s v_F}{\omega_q - q_s v_F} \right| = 1 + \frac{1}{N_0 \mathcal{V}} \tag{7.57}$$

$\Longrightarrow$ Excercise 7.9

For arbitrary coupling strength $N_0 V$ there is one solution,

$$\omega_q = c q_s \tag{7.58}$$

We recover the usual linear Goldstone spectrum! The zero-sound velocity depends strongly on the coupling strength, and is given by the solution of the implicit equation,

$$c = v_F \left(1 + \frac{1}{N_0 \mathcal{V}} \right) \frac{1}{\ln \left| \frac{c + v_F}{c - v_F} \right|} \tag{7.59}$$

This has an interesting behaviour in the weak coupling limit. For $N_0 \mathcal{V} \to 0$, $c \to v_F$. For small q, the upper bound in energy of the particle-hole continuum behaves as $\omega_q^{max} = v_F q + q^2/2m \to v_F q$ and it is found that the zero-sound mode has disappeared completely in the continuum when the interaction is zero: zero-sound does not exist in the non-interacting system. For *every* finite interaction strength, the propagating mode however exists, as long as the wavelength is large enough. (7.59) reduces in weak coupling ($N_0 \mathcal{V} << 1$) to,

$$c = v_F \left(1 + 2 e^{-\frac{1}{N_0 \mathcal{V}}} \right) \tag{7.60}$$

$\Longrightarrow$ Excercise 7.10

This behaves in a way analogous to a weak coupling instability: for every finite coupling strength the mode exists because $c > v_F$, although the mode is exponentially close to the onset of the continuum initially - the mode exists always, because the upper bound of energy of the continuum increases quadratically for small energies (figure 7.3).

For increasing coupling strength, the Fermi velocity becomes a smaller and smaller fraction of the zero-sound velocity: the rigidity of the Fermi surface increases. According to (7.59), the zero sound velocity should diverge at $N_0 \mathcal{V} \to 1$, or $\mathcal{V} \sim E_F$. This is unphysical. In order to treat the strong coupling regime, one has to pursue the perturbation theory (treating the fluctuations δn) to find, among others, an upward renormalization of the density of states and a downward renormalization of the effective interactions. The resulting effective 'Landau Fermi-liquid theory' has nevertheless the same basic structure as the bare theory presented here, which is

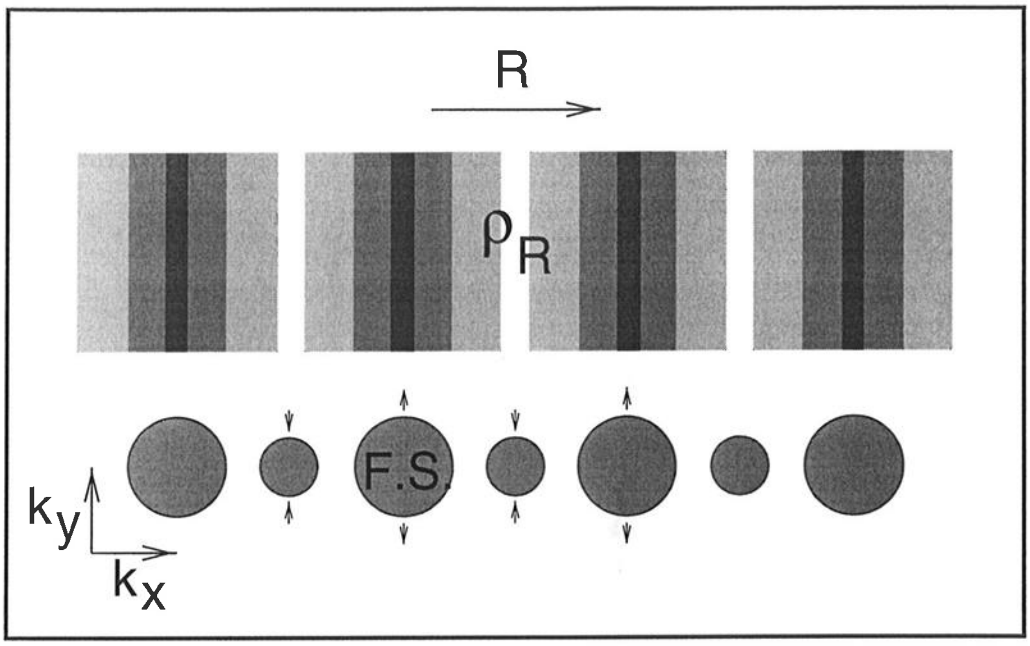

Figure 7.4: *zero-sound corresponds with a density mode, which in the Fermi-liquid should be thought off as an s-wave (breathing) vibration of the Fermi-sphere.*

only quantitatively accurate in the weak-coupling limit. It is again the principle of adiabatic continuation at work.

How to interpret zero-sound? The external potential excites a density oscillation in the Fermi-liquid. This means that the Fermi-sphere shrinks in the regions with a depleted density and expands in regions with an enhanced density, as indicated in figure 7.4. Because the Fermi surface behaves as an elastic membrane, the medium can support a propagating Fermi-sphere breathing mode. In addition, at a lower frequency it is also possible for the system to respond to a density perturbation by exciting independent electron-hole pairs. This gives rise to a gaseous response, because these excitations do not relate to the rigidity of the system.

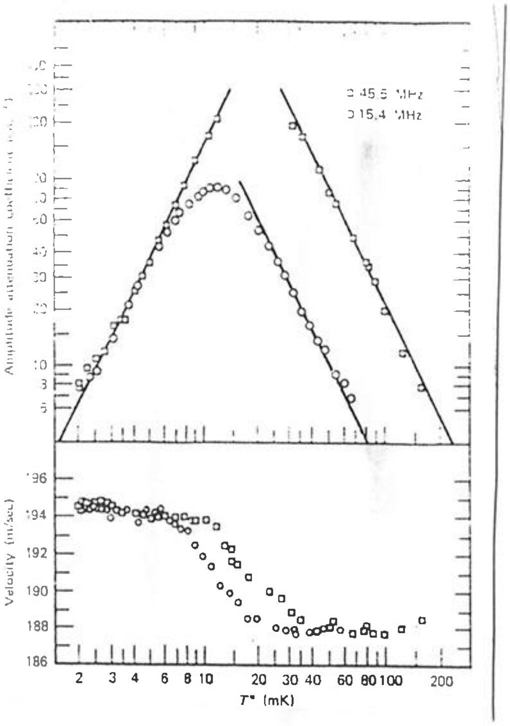

Figure 7.5: *experimental results for the damping of sound (upper panel), and the sound velocity (lower panel) in ^3He at millikelvin temperatures.*

I find zero-sound the most counterintuitive manifestation of rigidity. To honor this, I will make an exception to the set up of this text by showing experimental data. Although zero-sound has not yet directly been detected in ^3He by inelastic neutron scattering, it clearly shows up in experiments studying the propagation of sound. Zero sound is a mode fluctuating the density and it therefore looks quite like ordinary ('first') sound. In figure 7.5, the *damping* ('attenuation') of longitudinal acoustic density waves in ^3He is shown as function of temperature. It is seen that the decay rate initially *increases* as function of temperature, to turn over at $\sim$ 10 mK to decrease again. This is accompanied by a change in sound velocity. What is going on? The crucial observation is that, regardless the dimensionality of space, the Fermi-liquid condensate disappears at any finite temperature: *the Fermi-liquid undergoes a zero temperature phase transition.* At finite temperature, the discontinuity disappears because of the thermal smearing, as described by the Fermi-factor, and the Fermi-surface is fuzzy[9]. Hence, only at zero temperature the decay rate of zero sound vanishes (see figure 7.5). At any finite temperature, the Fermi-surface has lost its rigidity and, as a consequence, the Goldstone theorem no longer applies. Zero sound still exists as a transient at a finite temperature, to get however quickly overdamped. At the same time, the thermal fluctuations release quasiparticle excitations from the condensate and at energies less than $k_B T$ these behave as a gas of classical particles. When the density of this classical gas becomes large enough, normal ('first') sound

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[9] Notice that the rule that a quantum-mechanical problem looks like a similar classical thermal problem in one higher dimension is not obeyed at all in the context of Fermion systems.

starts to propagate, and this is the mode which is found at high temperature. The big difference is that first sound is a hydrodynamic mode, finding its origin in a dissipative dynamics and hydrodynamic conservation laws, while zero-sound is a consequence of the rigidity carried by the Fermi-liquid condensate.

7.3 The charged Fermi liquid.

In the preceding section, we dealt with fermion systems with short range interactions and these are not found in great abundance in nature: ^3He is the only example. Metallic electron systems are of course abundant, but these are characterized by interactions with a long range: Coulomb interactions. These long range interactions have an important effect: they cause the Golstone mode to live at a finite frequency in the long wavelength limit. In a metal, the 'massive' Goldstone modes are called plasmons.

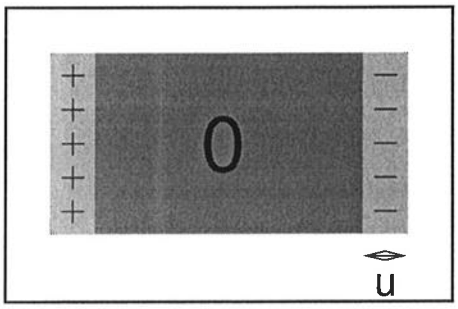

Figure 7.6

It is actually quite easy to understand the origin of the plasmon gap. In order to avoid the $\vec{q} = 0$ Coulomb divergency, one should consider the charged fermion system always in conjunction with a compensating positive background. The discussion of zero sound in the previous section implied that the Fermi-liquid responds as a rigid object to a density fluctuation. In the charged Fermi-liquid, this (number) density fluctuation is at the same time a fluctuation in the charge density. How does the $\vec{q} \to 0$ Goldstone mode look like in such a system? This is indicated in figure 7.6: the Fermi-liquid vibrates as a rigid charged object against the compensating, oppositely charged background. Because the interactions are now long ranged, we have to care for a *boundary* effect. Displacing the Fermi-liquid by an amount u, the resulting charge accumulating at the left (right) boundary is $-n_0 eu$ ($n_0 eu$) per surface unit. This causes an electric field of magnitude $4\pi\times$ the surface charge $= 4\pi n_0 eu$. The equation of motion becomes $m\ddot{u} = -4\pi n_0 e^2 u$, where the electric field acts as a restoring force. The solution is $u \sim exp(i\omega_p t)$, where the 'plasma frequency' $\omega_p^2 = 4\pi n_o e^2/m$[10].

Let us now consider the problem with long range interactions in RPA. In a jellium,

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[10] A similar mode is also found in thermal plasmas. This should be looked at as massive first sound.

the Coulomb interaction becomes,

$$\mathcal{H}^c = \frac{1}{2} \sum_{\vec{R}_1, \vec{R}_2} \frac{e^2}{|\vec{R}_1 - \vec{R}_2|} n(\vec{R}_1) n(\vec{R}_2) \tag{7.61}$$

$n(\vec{R})$ measuring the density at position $\vec{R}$,

$$n(\vec{R}) = \sum_{\sigma} \psi^\dagger_{\vec{R}\sigma} \psi_{\vec{R}\sigma} \tag{7.62}$$

with the fermion operators in position representation. Because the jellium is Galilean invariant,

$$\mathcal{H} = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \frac{1}{2N} \sum_{\vec{q} \neq 0} \mathcal{V}_q \rho_{\vec{q}} \rho_{-\vec{q}} \tag{7.63}$$

with $\varepsilon_{\vec{k}} = \hbar^2 k^2 / 2m$. The density operator is in momentum space,

$$\rho_{\vec{q}} = \sum_{\vec{k}\sigma} c^\dagger_{\vec{k}\sigma} c_{\vec{k}+\vec{q}\sigma} \tag{7.64}$$

and $V_{\vec{q}}$ is the Fourier-transform of the Coulomb interaction,

$$\mathcal{V}_q = \frac{4\pi e^2}{q^2} \tag{7.65}$$

Notice that one should neglect $\vec{q} = 0$ in the interaction term. This contribution is exactly cancelled by the potential of the stabilizing positively charged background.

All we have to do is to repeat the zero sound calculation of the previous section with the modified interaction potential. It follows directly from (7.56),

$$\begin{aligned} \mathcal{V}_q \, \chi_0'(\vec{q}, \omega_q) &= \frac{4\pi e^2}{q^2} \chi_0'(\vec{q}, \omega_q) & (7.66) \\ &= \frac{4\pi e^2}{q^2} \sum_{\vec{k}} \frac{n^0_k (1 - n^0_{k+q}) \, 2(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}})}{\omega_q^2 - (\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}})^2} \\ &= 1 & (7.67) \end{aligned}$$

Anticipating on the outcome that $\omega_q \neq 0$ when $\vec{q} \to 0$, the imaginary part of $\chi_0(0, \omega_{q=0})$ can be neglected. By expanding χ_0' (7.52) for small q one finds,

$$\omega_q = \omega_p \left\{ 1 + \frac{3}{10} \left(\frac{q v_F}{\omega_p} \right)^2 + 0(q^4) \right\} \tag{7.68}$$

with the plasmafrequency ($\omega_p = \omega_{q=0}$),

$$\omega_p^2 = \frac{4\pi n_0 e^2}{m} \tag{7.69}$$

recovering the outcome from the simple argument given at the beginning of this section. The outcome for the full χ'' is also indicated in figure 7.4. Except for the different frequency behaviour of the plasmon, it looks very similar to zero-sound, including the Landau damping setting in when the plasmon hits the particle-hole continuum at large momenta. The plasma frequencies in good metals are typically quite large (~ 10 eV) and plasmons are easy to observe directly, using electron energy loss spectroscopy (EELS).

$\Longrightarrow$ Excercise 7.11

What are the physical consequences of the plasmon gap? In section 5.4 we learned that long range interactions tend to help classical condensation. This is also the case in the present context and it is interesting to consider the effect of this energy scale on the quasiparticle sector. I already argued that the quasiparticle-quasiparticle interactions have to vanish in order for the Fermi-liquid to exist. The 'screening' processes, giving rise to the disappearance of the interactions, are in fact much easier to understand for long range interactions than for short range interactions. The reason is that the plasma frequency represents an energy scale and one can control the low energy theory using ω/ω_p as a small parameter. In contrast to the short range case, the screening of the long range electron-electron interaction is already accurately described on the present Gaussian level. However, Green's functions are needed and this will be discussed in more detail in the next section. On the other hand, the essence of the screening mechanism can already be seen using the simple device of an external test charge. We consider a (longitudinal) external potential $\varphi_{ext}(\vec{q}, \omega)$, caused by an external charge density $\rho_{ext}(\vec{q}, \omega)$,

$$\varphi_{\text{ext}}(\vec{q}, \omega) = \mathcal{V}_q \rho_{ext}(\vec{q}, \omega) \tag{7.70}$$

In response to the presence of the test charge, the electron system will adjust its charge distribution. The dielectric function $\varepsilon(\vec{q}, \omega)$ is defined by the ratio of the external potential to the total potential ($\varphi_{tot}(\vec{q}, \omega)$), which includes the contribution of the electron system as well,

$$\varphi_{\text{tot}}(\vec{q}, \omega) = \frac{1}{\varepsilon(\vec{q}, \omega)} \, \varphi_{\text{ext}}(\vec{q}, \omega) \tag{7.71}$$

The total potential is ,

$$\varphi_{\text{tot}}(\vec{q}, \omega) = \varphi_{\text{ext}}(\vec{q}, \omega) + \mathcal{V}_q \langle \rho(\vec{q}, \omega) \rangle \tag{7.72}$$

$\langle \rho(\vec{q}, \omega) \rangle$ is the induced charge density in the electron system. This is the charge density appearing in the definition of the charge susceptibility: $\chi(\vec{q}, \omega) = \langle \rho(\vec{q}, \omega) \rangle / \varphi_{ext}(\vec{q}, \omega)$ (7.13). It follows that,

$$\frac{1}{\varepsilon(\vec{q}, \omega)} = 1 + \frac{4\pi e^2}{q^2} \, \chi(\vec{q}, \omega) \tag{7.73}$$

Using the RPA form for χ (7.49),

$$\varepsilon_{\text{RPA}}(\vec{q}, \omega) = 1 - \frac{4\pi e^2}{q^2} \, \chi_0(\vec{q}, \omega) \tag{7.74}$$

Recall figure 7.1; big peaks are expected in in χ'' centered at the plasma frequency and this implies that χ' has to be negative when $|\omega| < \omega_p$ and therefore $Re(1/\varepsilon(\vec{q}, \omega)) < 1$ when $\omega < \omega_p$. Hence, the real potential which is dressed (screened) by the electron system will be *smaller* than the bare external potential φ_{ext} when the energy is *smaller* than the plasma frequency. We will find in the next section that this motive is also responsible for the diminishing of the quasiparticle-quasiparticle interactions.

We can limit the discussion to the case $\omega = 0$ - little will change untill the energy approaches the plasma frequency. This limit is of a direct empirical relevance, because it adresses the penetration of a static electric field in a metal, as well as the screening of the field of a charged impurity. The interest is in the static limit of (7.52) with the Coulomb potential (7.65),

$$\begin{aligned} \varepsilon_{\mathrm{RPA}}(q) &= 1 + \frac{1}{2}\frac{q_{\mathrm{TF}}^2}{q^2}\left[1 + \frac{1}{2x}(1-x^2)\ell n\left|\frac{1+x}{1-x}\right|\right] && (7.75) \\ x &= q/2k_F && (7.76) \end{aligned}$$

The so-called Thomas-Fermi wavenumber is defined by

$$q_{\mathrm{TF}}^2 = \frac{6\pi e^2 n_0}{E_F} \tag{7.77}$$

Let us first consider the long-wavelength limit, such that $q << 2k_F$. We specialize on a point-like impurity with charge z. The screened impurity potential becomes,

$$\varphi_{scr}(q, \omega) = \frac{4\pi z}{q^2 + \frac{1}{2} q_{\mathrm{TF}}^2} \tag{7.78}$$

This is nothing else than a Yukawa potential. Transforming to real space,

$$\varphi_{scr}(r, \omega) = \frac{z}{r}\, e^{-q_{\mathrm{TF}} r/2} \tag{7.79}$$

The impurity potential falls of exponentially in space with a characteristic length scale $\sim 1/q_{TF}$, which is called the 'metallic screening length'. This behaviour is only correct at large length scales. For shorter lengths, one picks up in addition the length scale $\sim 1/2k_F$. By doing the integrals, one finds small amplitude oscillations, superimposed on the decaying potential (7.78) with a wavelength $\pi/2k_F$: the Friedel oscillations. The response of the electron system in the spin-sector is very similar to the above charge response. The spin density induced in the system by a magnetic impurity also shows these $2k_F$ ('RKKY') oscillations. The difference is now that the spin density of the unperturbed Fermi-liquid is zero, and therefore the induced spin density changes sign repeatedly before it has decayed. As a consequence, the magnetic interactions between different impurities can be both ferromagnetic and anti-ferromagnetic, depending on their precise distance. When the impurities are distributed randomly, the spin system becomes fully frustrated and this is the origin of the spin-glass behaviour, as found in metals containing magnetic impurities.

7.4 The fluctuations around the Fermi-liquid: kindergarten Greens functions.

Up to this point we have dealt with the classical limit of the Fermi-liquid, having the same status as the theory of the classical crystal with its classical lattice vibrations, etcetera. The next step is to study the quantum order parameter fluctuations. In view of the past experiences, we could argue that a Goldstone mode is present, which can be quantized to yield an order parameter fluctuation which is expected to be similar to the one in crystals: the Fermi-liquid can exist in $d \geq 2$. This is part of the truth. However, it is not all: *next to the collective modes, also the quasiparticle excitations appear at low energies and it has to be checked if these do not give rise to dangerous terms in the perturbation theory.* These fermionic 'modes' or quasiparticles render the Fermi-liquid to be a richer subject than the condensates of the previous chapters..

What is the implication of the order parameter stability in the quasiparticle sector? I argued that the discontinuity in $\langle n_{\vec{p}\sigma} \rangle$ is the measure of the order in the Fermi-liquid, and the discontinuity has to be *finite*. This implies for the limit $\omega \rightarrow 0$ and $\vec{k} \rightarrow \vec{k}_F$:

(i) Fermionic quasiparticles have to be present carrying the quantum numbers of the bare electrons ($\vec{k}$, σ, -e). *The lowest lying states of the system with one quasiparticle removed (or added) have a finite overlap with the states of the system where a bare particle carrying the same quantum numbers has been removed (added).* This is a necessary condition to find the discontinuity. The aforementioned overlap is called the quasi-particle pole strength, $Z_{\vec{k}}$.

(ii) The quasiparticles become infinitely long lived when $\omega \rightarrow 0$. Otherwise, the discontinuity could not exist because the quasiparticles themselved are ill-defined. This is equivalent to: *the quasiparticle-quasiparticle interactions have to vanish if the excitation energy goes to zero.* In addition, the quasiparticles should decouple from the zero-sound mode/plasmon, but this is usually not a problem.

There is a proof available that the Fermi-liquid *can exist* - it is unproven that the Fermi-liquid *has* to exist. This proof is quite complex, and needs the full machinery of diagrammatic perturbation theory which is beyond the scope of this text. At the same time, Greens functions and diagrams do enrich your physical view on the world and it is possible to learn some of the principles with relatively little effort. What follows is optimized to help your physical intuition. Although some basic features are shared with the standard diagrammatic perturbation theory, the latter is derived in a different way. It takes more formal effort to derive the full size diagrams, with the reward that the formalism is more efficient than the minimal version presented here. When you plan to do calculations yourself, consult first the specialized books like Mahan, AGD, and Negele and Orland.

The mathematical object 'Greens function' or 'propagator' plays a central role in the formalism. The essence is that it is in more than one regard beneficial to attempt to *invert* the Hamiltonian, instead of to diagonalize the Hamiltonian. This has a physical reason: the inverse of the Hamiltonian relates directly to the measurable quantities introduced in section 7.1, the response- and spectral functions. There is also a technical advantage. Perturbation theory is formulated in a more natural way when the inverse of the Hamiltonian is asked for. As you will see in a moment, this makes it possible to pursue the perturbation expansion up to infinite order with little effort.

The empirical relevance of Greens functions follows directly from the work done in section 7.1. Consider the dynamical form factor (7.7). From the Dirac relation (7.22) it follows directly that,

$$\begin{aligned} S(\vec{q},\omega) &= \langle 0|\rho^*_{\vec{q}} \left[\sum_n |n\rangle \delta(\omega - E_n + E_0)\langle n|\right] \rho_{\vec{q}}|0\rangle & (7.80)\\ &= \frac{1}{\pi} \lim_{\eta\to 0} Im \langle 0|\rho^*_{\vec{q}} \left[\sum_n |n\rangle \frac{1}{\omega - i\eta - E_n + E_0}\langle n|\right] \rho_{\vec{q}}|0\rangle & (7.81)\\ &= \frac{1}{\pi} \lim_{\eta\to 0} Im \langle 0|\rho^*_{\vec{q}} \hat{G}(\omega - i\eta + E_0) \rho_{\vec{q}}|0\rangle & (7.82) \end{aligned}$$

Defining the so-called 'resolvent' operator,

$$\begin{aligned} \hat{G}(z) &= \sum_n |n\rangle \frac{1}{z - E_n}\langle n| & (7.83)\\ &\equiv \frac{1}{z - H} & (7.84) \end{aligned}$$

Hence, the Hamiltonian has to be inverted in order to calculate the form factor! The matrix elements of the resolvent operator with regard to one or the other prepared state is 'the' Greens function. Also the susceptibility (7.19) can be written in a Greens function form,

$$\chi(\vec{q},\omega) = \lim_{\eta\to 0} \langle 0|\rho^*_{\vec{q}} \left(\hat{G}(\omega + i\eta + E_0) + \hat{G}(-\omega - i\eta + E_0)\right) \rho_{\vec{q}}|0\rangle \qquad (7.85)$$

The reactive part of χ relates to the *real* part of the Greens function. Also the single particle spectral function (7.8) can be written as the imaginary part of a Greens function,

$$G_1(\vec{k}, z) = \langle 0|c_{\vec{k}\sigma} \hat{G}(z + E_0) c^\dagger_{\vec{k}\sigma}|0\rangle - \langle 0|c^\dagger_{\vec{k}\sigma} \hat{G}(-z + E_0) c_{\vec{k}\sigma}|0\rangle \qquad (7.86)$$

The first term represents the unoccupied- and the second term the occupied states (check the signs !). This 'one particle Greens function' plays a central role in Fermi-liquid theory.

It is also easy to see why perturbation theory simplifies, using Greens functions. The main advantage of diagrammatic perturbation theory is, that it becomes possible to handle classes of perturbative processes up to infinite order. This is called 'resummation'. The key to this is the so-called Dyson equation. We assume a basis which diagonalizes H_0 and consider a perturbation H_1. The diagonal resolvent is

$$\hat{G}_0 = \frac{1}{z - H_0} \qquad (7.87)$$

By straightforward operator manipulation,

$$\begin{aligned}\hat{G} &= \frac{1}{z - H_0 - H_1} && (7.88)\\ &= \hat{G}_0 \frac{1}{1 - H_1 \hat{G}_0} && (7.89)\\ &= \hat{G}_0 + \hat{G}_0 H_1 \hat{G}_0 + \hat{G}_0 H_1 \hat{G}_0 H_1 \hat{G}_0 + \cdots && (7.90)\end{aligned}$$

We derive in two lines a perturbative expansion for G which runs up to arbitrary high order - 'only' the expectation values have to be calculated. (7.90) can also be written in a recursive form,

$$\hat{G} = \hat{G}_0 + \hat{G}_0 H_1 \hat{G} \tag{7.91}$$

and this is the Dyson equation, the working horse of the formalism. It expresses that a perturbation series like (7.90) can be summed up to infinite order by reformulating it in the form of a *self-consistency* (recursive) equation: G is guessed and filled in on the right hand side of (7.91), to calculate the left hand side, which is inserted on the right hand side again, repeating this untill self consistency is reached. This is the resummation principle, which can be regarded as a dynamical generalization of the saddle-point equations encountered in mean-field theory.

The method is general and it applies as well to single particle problems, as to the more difficult many particle problems. The formalism is especially suited to deal with single particle *impurity* problems. A simple example is the Clogston-Wolff impurity model,

$$\begin{aligned}H_0 &= \sum_k c_k^\dagger c_k && (7.92)\\ H_1 &= \frac{V}{N} \sum_{k,q} c_k^\dagger c_{k+q} && (7.93)\end{aligned}$$

descibing a point scatterer (H_1) at the origin, embedded in an electron gas (H_0, the spin of the electrons is neglected). The interest is in the local impurity density of states. This model can be diagonalized, and subsequently this density of states can be calculated. This is, however, a rather lengthy calculation and using Greens functions instead, it is a matter of a few lines. Define the Greens functions,

$$\begin{aligned}G_{k,k'}(z) &= \langle k|\hat{G}(z)|k'\rangle && (7.94)\\ G_k^0(z)\delta_{kk'} &= \langle k|\hat{G}_0(z)|k'\rangle && (7.95)\\ &= \frac{1}{z - \varepsilon_k}\delta_{k,k'} && (7.96)\end{aligned}$$

and the impurity density of states is calculated from the imaginary part of (7.94) by,

$$\begin{aligned}A_{loc}(\omega) &= \frac{1}{\pi} \lim_{\eta \to 0} Im G_{loc}(\omega - i\eta) && (7.97)\\ G_{loc}(z) &= \frac{1}{N} \sum_{k,k'} G_{k,k'}(z) && (7.98)\end{aligned}$$

because $|R_{i=0}\rangle = (1/\sqrt{N})\sum_k |k\rangle$. $G_{k,k'}$ is given in terms of the expectation value of the Dyson equation (7.91),

$$G_{k,k'}(z) = G_k^0(z)\delta_{k,k'} + G_k^0(z)\frac{V}{N}\sum_q G_{k+q,k'}(z) \tag{7.99}$$

Because the interest is in (7.98) we sum both sides over k, k' to find

$$G_{loc}(z) = G_{loc}^0(z) + G_{loc}^0(z)VG_{loc}(z) \tag{7.100}$$

with

$$G_{loc}^0(z) = \sum_k \frac{1}{z - \varepsilon_k} \tag{7.101}$$

having an imaginary part, corresponding with the density of states of the unperturbed electron gas. Solving (7.100),

$$G_{loc}(z) = \frac{G_{loc}^0(z)}{1 - VG_{loc}^0(z)} \tag{7.102}$$

The right hand side of this expression contains only known quantities and, together with (7.97), the impurity density of states can be calculated.

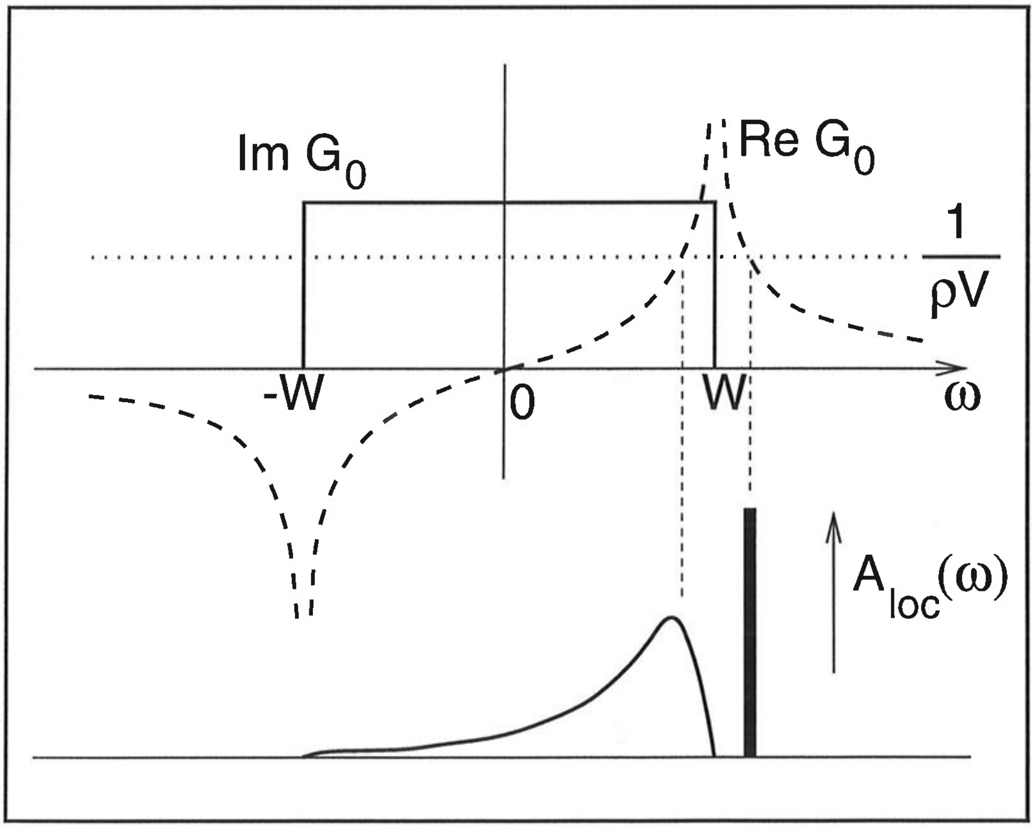

Figure 7.7: *the various ingredients (upper panel), needed to calculate the density of states (lower panel) of the Clogston-Wolff impurity*

In the Greens function formalism, physics seems often to reduce to an excercise in complex function theory and (7.102) is a typical example. To simplify matters, let us assume that the density of states of the unperturbed electron gas corresponds with a rectangular box with height ρ and upper/lower bound $\pm W$ ($2W$ is the bandwidth, figure 7.7),

$$\begin{aligned} A^0_{loc}(\omega) &= \frac{1}{\pi}\lim_{\eta\to 0} ImG^0_{loc}(\omega - i\eta) && (7.103)\\ &= \rho\theta(W - |\omega|) && (7.104)\end{aligned}$$

Using the Dirac relation (7.22), it follows directly that the real part of G^0 can be expressed in terms of the imaginary part by[11],

$$\begin{aligned} ReG^0_{loc}(\omega) &= P\int d\omega' \frac{A^0_{loc}}{\omega - \omega'} && (7.105)\\ &= \rho\ln|\frac{W+\omega}{W-\omega}| && (7.106)\end{aligned}$$

When is the imaginary part of the full Green's function G_{loc} unequal to zero? This we have seen before in the context of zero sound, (7.54-7.56) - this is not an accident, as will become clear soon! The first possibility is that $ImG^0_{loc} \neq 0$: this means that the band electrons have a finite probability to be present on the impurity site. In terms of wavefunctions localized on the impurity site, one can consider this as the impurity wave function leaking out into the remainder of space. Hence, the impurity of states is always non-zero when the host density of states is non-zero. The second possibility is that the *denominator* of (7.102) becomes zero, while $ImG_0 = 0$ - this corresponds with an isolated pole, a delta function peak located outside the band (recall the zero-sound pole). This corresponds with a state where the electron is *bound* to the impurity. The condition for this to happen is,

$$\ln|\frac{W+\omega}{W-\omega}| = \frac{1}{\rho V} \qquad (7.107)$$

This looks much like a weak-coupling saddle point equation. For arbitrary coupling, this is most easily solved graphically. In figure 7.7, the real part of G_0 is sketched and the pole condition is met when this intersects with the straight line given by $1/\rho V$. For a repulsive potential ($V > 0$) a bound state can be found above the top of the band and for an attractive potential ($V < 0$) the bound state will be found below the bottom of the band. When the potential is large, the $1/\rho V$ line is close to the x-axis and the intersection will occur for large positive or negative energy: the impurity (anti) bound state will have a large (anti) binding energy. Reducing V, the (anti) bound state will move in the direction of the bottom (top) of the band. The specialty of this host density of states is, that the real part of the Greens function is logarithmically divergent at the band edges, and regardless the smallness of the

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[11] This is actually a general (Kramers-Kronig) relation between the real and imaginary parts of Greens functions.

interaction, a bound state will always exist! For very small ρV the binding energy has a weak coupling form $\Delta \sim \exp(-1/(\rho V))$ - it turns out that when one casts mean field calculations in the Greens function formalism, one finds precisely the same logarithm in the real part of the appropriate G_0 in nested problems. The logarithm in the real part is caused by the *discontinuity* in the imaginary part of G^0, because of (7.106). Discontinuities in one particle density of states are only found in one dimensional systems. In higher dimension, the density of states goes continuously to zero, and the real part of G_0 is therefore finite everywhere. As a result, these weak-coupling impurity bound states only occur in one dimension.

This is not yet the whole story. As can be seen from the figure, (7.107) can also be satisfied when ImG_0 is finite. When this is the case, the impurity density of states will get enhanced at the energy where this happens (ω_r), and this tends to produce a peak as well. The difference is that the peak now has a *width* $\sim VImG_0(\omega_r)$. This is a resonance (also called 'virtual bound state' in the impurity context): the electron tends to localize in the neighbourhood of the impurity, but after a time $\sim 1/VImG_0$ it leaves the impurity again. In the many-particle context, the same happens and the width of the peak corresponds with a decay rate.

Summarizing, in this simple impurity example one obtains already a clear view on some central aspects of the 'Greens function search light': by resummation, (7.100), one is able to treat non-perturbative aspects of the problem (like bound states). *Real* excitations are counted by the *imaginary* part of the Greens functions, and the *real* part of the Greens function is keeping track of the *virtual* fluctuations. The real parts of the zero-th order Greens functions relate to *shifts* of the energy levels, and are also doing the hard work leading to bound states. The imaginary parts of those relate to decay rates or, more generally, *dissipation.*

Let us return to the many-particle context. I just mentioned the striking mathematical similarity between the impurity problem and the RPA calculation of section 7.2. This is no accident, as can be seen directly. We have only to realize that both χ and χ^0 correspond with a sum of two Greens functions and the Dyson equation also holds for a sum of Greens functions. (7.49) can be rewritten as,

$$\begin{aligned}
\chi(\vec{q},\omega) &= \chi_0(\vec{q},\omega) + \chi_0(\vec{q},\omega) V_q \chi(\vec{q},\omega) && (7.108)\\
&= \chi_0(\vec{q},\omega) + \chi_0(\vec{q},\omega) V_q \chi_0(\vec{q},\omega) \\
&\quad + \chi_0(q,\omega) V_q \chi_0(\vec{q},\omega) V_q \chi_0(\vec{q},\omega) + \cdots && (7.109)
\end{aligned}$$

and we directly recognize the perturbation series (7.90) and the resummed series (7.91). In contrast to the impurity resummation (7.100), the resummation (7.108) does *not* represent the exact solution. At the same time, we realize that the zero-sound pole does not show up in any finite order in the resummation (7.109): only if this is summed up to infinite order, one recovers (7.108) and (7.49) which do describe zero-sound. I stressed that zero-sound is not present in the non-interacting electron gas and only exists in the Fermi-liquid *condensate*, which is qualitatively different from the electron gas. Using equations of motions, zero-sound showed up because of our insistence on the existence of the vacuum amplitude. (7.108) and (7.109) exhibit the structure of the perturbation theory around the non-interacting electron-gas. Because the summation has to be carried through up to infinite order, the Fermi-liquid cannot be reached by any *finite* order perturbation theory, starting from the non-interacting limit. This infinity is the cause for the qualitatively different nature of the Fermi-liquid.

Despite the fact that the RPA resummation takes into account infinite order corrections, it includes only a very small subset of all possible perturbative corrections. The reason that RPA is nevertheless qualitatively correct is, that it keeps track of the processes which are 'dangerous' for the non-interacting electron gas, namely those which are responsible for the rigidity of the Fermi-surface. The administration of all possible perturbative processes is a task of great complexity. To help the mind to keep track of this accountancy problem, diagrams are introduced. Diagrams are nothing else than a pictorial representation of expansions like (7.90), helping the mind to sort the information. Pictures are more ergonomic than integrals! Crudely speaking, the recipy is as follows[12]: the electrons (fermions) are coded by full lines, with an arrow pointing from left to right. The holes are also represented by a full line, but with an arrow pointing from the right to the left ('time runs from left to right': do not take this too litteral !). The (instanteneous) Coulomb interaction is represented by a vertical dashed line. The external field is already fully integrated out (section 7.1) and is indicated with a cross: on 'time $-\infty$' an electron-hole pair is created at the cross and this pair has to be annihilated at a second cross located at 'time $+\infty$'. Many things can happen in between to these two 'times', which are in first instance unknown, and this we indicate with a hatched area. The diagram corresponding with the susceptibility χ is indicated in figure 7.8.

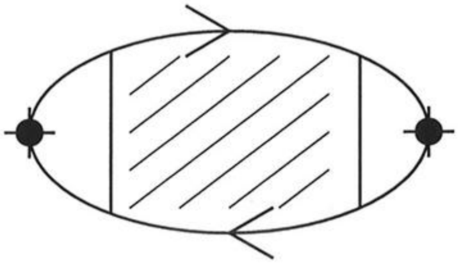

Figure 7.8

This becomes simple in the non-interacting limit. Nothing can happen with the electron-hole pair and the hatched region disappears. χ_0 now corresponds with the 'bare bubble' (or 'loop'), figure 7.9. The diagram for the Coulomb interaction $V_{\vec{q}}$ was already introduced in chapter 2, and is shown once more in figure 7.10. It is directly seen that the graphical representation of the RPA expansion (7.109) becomes the sum of bubble 'chains', as indicated in figure 7.11. For obvious reasons, RPA is also called 'the bare bubble resummation'. The diagram pictures offer a convenient vocabulary to

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[12] In order to get the prefactors right, related to the multiplicities of the various terms, one has to work onself through the perturbation theory more carefully. I refer to the book by Mahan for a transparent derivation of the Feyman rules. This book contains also a useful discussion of the finite temperature (Matsubara) formalism.

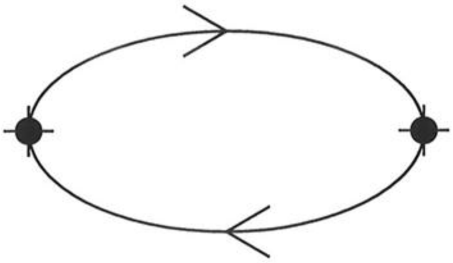

Figure 7.9

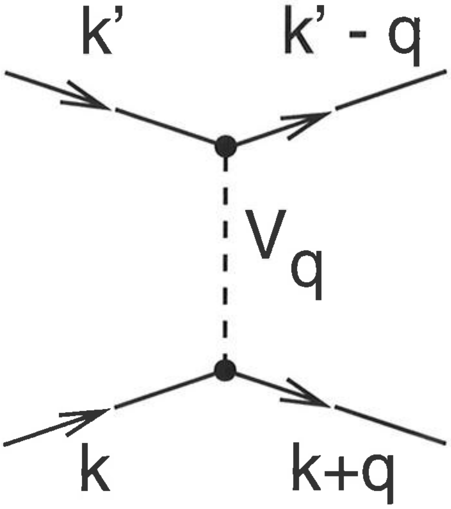

Figure 7.10

discuss further improvements. For instance, from the picture one infers that in RPA it is assumed that the bubbles involve bare (non-interacting) electrons. This is actually quite unreasonable, because I argued before that also the fermions are affected by the interactions. Instead of thinking electrons, one should think quasiparticles which are well defined only because of the condensate. Hence, one would like to replace the bare fermion lines in figure 7.11 by something else which relates to the proper objects, and it could be that one again needs resummations to get these objects right. Fot this purpose we have to investigate the single particle Greens function G_1 (7.86), relating to the spectral function of the electrons themselves.

The specialty of the Fermi-liquid is that the quasiparticles still carry the same quantum-numbers as the bare electrons and one can continue from the latter to the former by perturbation theory: the rigidity of the Fermi-liquid is consequential only in the sector of collective excitations (zero-sound etcetera). I already argued that this has to be the case in order for the discontinuity in the single particle momentum to exist: the quasiparticles have to be ('non-exact') *eigenstates* of the single particle Fermi momentum k_F. Assuming that the discontinuity exist, a non-trivial consequence follows for the form of G_1. As long as the discontinuity is finite, G_1 can be written in the form,

$$G_1(\vec{k}, \omega) = \frac{1}{\omega - \varepsilon_{\vec{k}} - \Sigma(\vec{k}, \omega)} \tag{7.110}$$

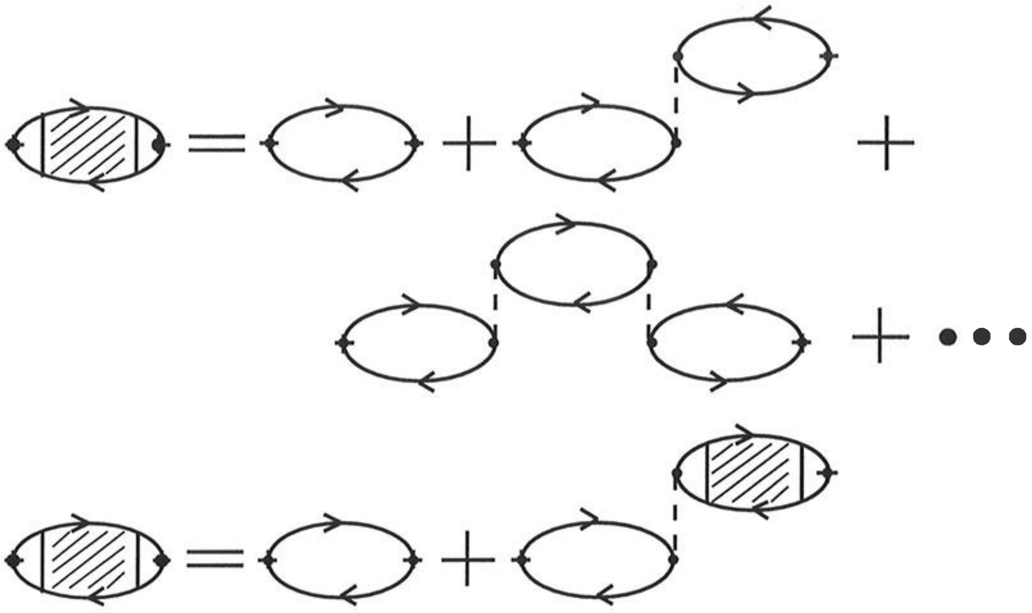

Figure 7.11

$\varepsilon_{\vec{k}}$ is the band kinetic energy of the non-interacting electron. The so-called self-energy Σ is a complex function,

$$\Sigma(\vec{k},\omega) = \Sigma'(\vec{k},\omega) + i\Sigma''(\vec{k},\omega) \tag{7.111}$$

which collects *all* the effects of the interactions. Σ itself is obtained by resumming the perturbation expansion for G_1 in a particular way (Σ is in the denominator !), and this defines a perturbation expansion for Σ as well. The expansion for the self-energy is truely perturbative in a Fermi-liquid and can be carried out order by order. Let us consider one additional electron with $k > k_F$, added to the Fermi-liquid (except for a nasty minus sign, the argument is the same for an added hole). We can define a classical (single determinant) state which now relates to an excited state of the Fermi-liquid with one extra electron at $\vec{k}$ and spin σ,

$$|\Phi^0_{Cl};\vec{k}\sigma\rangle = c^\dagger_{\vec{k}\sigma}\Pi^{k_F}_{\vec{k}',\sigma'}c^\dagger_{\vec{k}'\sigma'}|vac> \tag{7.112}$$

Recall the definition of the single particle Greens function (7.86). The first term on the right hand side describes the unoccupied states ("$G_1^>$"), and assuming that the fully renormalized Fermi-liquid condensate ($|\Phi_{Cl}\rangle$) exists,

$$G_1^>(k,z) = \langle\Phi_{Cl}|c_{\vec{k}\sigma}\frac{1}{z-H}c^\dagger_{\vec{k}\sigma}|\Phi_{Cl}\rangle \tag{7.113}$$

counting from the ground state energy. Because $|\Phi^0_{Cl};\vec{k}\sigma\rangle \equiv c^\dagger_{\vec{k}\sigma}|\Phi^0_{Cl}\rangle$ and using $1 = \sum_{\vec{k}\sigma}|\Phi^0_{Cl};\vec{k}\sigma\rangle\langle\Phi^0_{Cl};\vec{k}|$,

$$G_1^>(k,z) = |\langle\Phi^0_{Cl}|\Phi_{Cl}\rangle|^2\langle\Phi^0_{Cl};\vec{k}\sigma|\frac{1}{z-H}|\Phi^0_{Cl};\vec{k}\sigma\rangle \tag{7.114}$$

Clearly, the Greens function can only relate to the bare electrons, when the overlap factor $|\langle\Phi^0_{Cl}|\Phi_{Cl}\rangle|^2$ is finite - if this would not be the case, it would become impossible to find back single electron quantum numbers in the system. By definition, this overlap factor is finite in the Fermi-liquid (height of the discontinuity). However, this overlap factor would become precisely zero in a non-Fermi liquid and in such a system the notion of electron would loose its meaning, which is actually the case in one dimensional metals. It should not come as a surprise that in such cases the self-energy expansion itself becomes singular, as will be discussed later on.

It is now demanded that,

$$\langle \Phi^0_{Cl}; \vec{k}\sigma | \frac{1}{z-H} | \Phi^0_{Cl}; \vec{k}\sigma \rangle = \frac{1}{z - \varepsilon_k - \Sigma_{red}(k,z)} \tag{7.115}$$

The self-energy Σ_{red} is the 'reducible' self-energy which is different from the 'irreducible' self-energy Σ appearing in (7.110). The Hilbert space is explored by letting H_1 operate repeatedly on (7.112). For instance, doing this once we obtain states (dropping the label Φ^0_{Cl}),

$$\begin{aligned} H_1 |k\rangle &\sim c^\dagger_{k'-q} c_{k'} c^\dagger_{k+q} |\Phi^0_{Cl}\rangle \\ &= |l\rangle \end{aligned} \tag{7.116}$$

The electron scatters off the Fermi-sea, liberating an electron-hole pair. Letting H_1 operate twice, one finds two electron-hole pairs, etcetera. Later on this will be disentangled using diagrams, and for the time being we only need an abstract definition for the states and matrix elements in this basis,

$$\begin{aligned} \langle l | \frac{1}{z-H_0} | m \rangle &= G^0_l(z) \delta_{l,m} \\ &= \frac{\delta_{l,m}}{z - \xi_l} \qquad (7.117) \\ \langle l | H_1 | m \rangle &= V_{lm} \qquad (7.118) \end{aligned}$$

ξ_l is the sum of all one-particle energies of the excited electrons and holes. Let us now expand the left hand side of (7.115) using the Dyson equation (7.91), extracting every time the term from the summation which leads back to the initial state $|k\rangle$. After one iteration,

$$\langle k|\hat{G}(z)|k\rangle = G^0_k(z) + G^0_k(z)\Sigma^{(1)}\langle k|\hat{G}(z)|k\rangle + G^0_k(z)\sum_{l\neq k} V_{kl}\langle l|\hat{G}(z)|k\rangle \tag{7.119}$$

and we read off the first order contribution to Σ_{red},

$$\Sigma^{(1)}_k = \langle k|H^1|k\rangle \tag{7.120}$$

corresponding with the expectation value of the interaction in the non-interacting vacuum. This is repeated, to find up to second order,

$$\begin{aligned} \langle k|\hat{G}(z)|k\rangle &= G^0_k(z) + G^0_k(z)\left(\Sigma^{(1)}(k) + \Sigma^{(2)}(k,z)\right)\langle k|\hat{G}(z)|k\rangle \\ &\quad + G^0_k(z)\sum_{l,l'\neq k} V_{kl} G^0_l(z) V_{ll'} \langle l'|\hat{G}(z)|k\rangle \end{aligned} \tag{7.121}$$

defining the second order contribution to the self-energy,

$$\Sigma^{(2)} = \sum_{l \neq k} V_{kl} G_l^0(z) V_{lk} \tag{7.122}$$

Carrying on, a third order contribution is found

$$\Sigma^{(3)} = \sum_{l,l' \neq k} V_{kl} G_l^0(z) V_{ll'} G_{l'}^0(z) V_{l'k} \tag{7.123}$$

and so on. By induction, one finds the self-energy resummation up to infinite order,

$$\begin{aligned} \langle k;0|\hat{G}(z)|k;0\rangle &= G_k^0(z) + G_k^0(z)\Sigma_{red}(k,z)\langle k;0|\hat{G}(z)|k;0\rangle & (7.124) \\ &= \frac{1}{z - \varepsilon_k - \Sigma_{red}(k,z)} & (7.125) \end{aligned}$$

with

$$\Sigma_{red}(k,z) = \sum_{i=1}^{\infty} \Sigma^{(i)}(k,z) \tag{7.126}$$

while the i-th order self-energy is given by,

$$\Sigma^{(i)}(k,z) = \sum_{l,l_1 \cdots \neq k} V_{kl} G_l^0(z) V_{ll_1} G_{l_1}^0(z) \cdots G_{l_{i-1}}^0 V_{l_{i-1}k} \tag{7.127}$$

containing in total i interaction matrix elements. One already anticipates that calculating an arbitrary high order contribution to the self-energy is a daunting task: it might well involve an integral over $\sim i-1$ internal momenta. Fortunately, this self-energy expansion tends to converge rather rapidly, at least in 'good' Fermi-liquids characterized by large discontinuities.

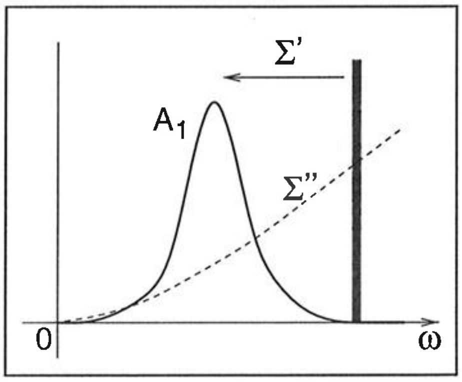

Figure 7.12: *illustration of the meaning of the self-energy* Σ. *The real part shifts the bare state, while the imaginary part gives rise to a lifetime broadening.*

The self-energy (or 'complex mass' as it is called in relativistic field theory) is a very useful concept. Let us consider a simple example. If the interactions are weak and we are sure that the Fermi-liquid exists, we might stop the expansion of Σ at second order. The first order contribution (7.120) is not so interesting; it just amounts to a number shifting the energy of the 'quasiparticle pole': $\varepsilon_{\vec{k}} \to \varepsilon_{\vec{k}} + \Sigma^{(1)}$. The second order contribution (7.120) is more interesting: it is an integral over two interaction matrix elements and the Greens function describing the scattered electron and the excited electron hole pair $G_l^0(z) \sim 1/(z - \varepsilon_1 + \varepsilon_2 - \varepsilon_3)$, having an imaginary part $ImG_l^0 \sim \delta(\omega - \varepsilon_1 + \varepsilon_2 - \varepsilon_3)$. Hence, because we have to integrate over the internal momenta, the imaginary part of $\Sigma^{(2)}$ will correspond with a three-particle density of states, weighted by the interaction matrix elements: $\Sigma''(\omega) \sim V^2 \rho(\omega)$. A detailed calculation of this integral is not straightforward and this will be kept for later. All what we need is that $\rho(\omega)$ is a smooth function. The real part of Σ can again be obtained using the Kramers-Kronig relation (compare with 7.106). Summarizing,

$$\begin{aligned}
\Sigma(k,\omega) &= \Sigma'(k,\omega) + i\Sigma''(k,\omega) \\
\Sigma''(k,\omega) &= \pi V_k^2 \rho(\omega) \\
\Sigma'(k,\omega) &= P\int d\omega' \frac{\Sigma''(k,\omega')}{\omega - \omega'}
\end{aligned} \tag{7.128}$$

The real interest is in the spectral function of the electron,

$$A_1(k,\omega) = \frac{1}{\pi} ImG_x(k,\omega) \tag{7.129}$$

$$= \frac{1}{\pi}\frac{\Sigma''(k,\omega)}{(\omega - \varepsilon_k - \Sigma'(k,\omega))^2 + (\Sigma''(k,\omega))^2} \tag{7.130}$$

The condition for finding a pole at E_k is that $E_k = \varepsilon_k + \Sigma'(k, E_k)$: the energy of the electron state changes due to the interaction and this is called 'mass-renormalization'. Notice that one has to solve an implicit equation to find E_k. This reflects the resummation behind the self-energy, and although this does not produce novel behaviour, it allows for large quantitative changes. At the same time, $\Sigma''(k, E_k) \neq 0$ always in the present context, and as long as ρ is smoothly varying on the scale of E_k, (7.130) will be close to a Lorentzian peak: the imaginary part of the self-energy represents the decay rate (or inverse life time) of the electron-like state at E_k (Figure 7.12). Hence, the self-energy is a powerful mathematical object which allows for a unified description of both the 'reactive' (energy shifts) and 'dissipative' (lifetime broadenings) aspects of particle-like excitations. The concept of self-energy is not restricted to fermionic excitations. One can as well define self-energies for bosonic excitations like phonons, magnons, etcetera, with imaginary parts describing the decay rates (e.g., section 4.4), while the real part gives rise to for instance a renormalization of the velocities.

$\Longrightarrow$ Excercise 7.12

Let us now consider the self-energy expansion for the electron in a Fermi-liquid in more detail. The first order term, (7.120), is not particularly interesting. Writing it explicitely in terms of the basis (7.112) and the interaction (7.93),

$$\Sigma^{(1)}(\vec{k}) \equiv \sum_{\vec{q}} V_{\vec{q}} \langle \Phi_{Cl}^0; \vec{k} | \rho_{\vec{q}} \rho_{-\vec{q}} | \Phi_{Cl}^0; \vec{k} \rangle \tag{7.131}$$

This contribution is ω independent and amounts to the expectation value of the interaction with regard to zero-th order state. Since the expectation value has to be calculated with regard to all electrons, the extra electron at $\vec{k}$ can be neglected,

$$\Sigma^{(1)}(\vec{k}) = \Sigma^{(1)} = \sum_{\vec{q}} V_{\vec{q}} \langle \Phi^0_{Cl} | \rho_{\vec{q}} \rho_{-\vec{q}} | \Phi^0_{Cl} \rangle \tag{7.132}$$

This is nothing else than the expectation value of the interaction Hamiltonian with regard to the condensate state. We should now recall section 1.2: the energy of the classical condensate itself (E_0) is given by the expectation value of the *whole* Hamiltonian with respect to this state: $E_0 = \sum_{\vec{k}}^{\vec{k}_F} \varepsilon_{\vec{k}} + \langle \Phi^0_{Cl} | \sum_{\vec{q}} V_{\vec{q}} \rho_{\vec{q}} \rho_{-\vec{q}} | \Phi^0_{Cl} \rangle$. All what $\Sigma^{(1)}$ does, is to let the electron addition spectrum start at the thermodynamic potential of the classical state, which is different from the thermodynamic potential of the non-interacting system.

$\Sigma^{(1)}$ thus coincidizes with the interaction correction to the classical vacuum energy, and it is interesting to consider this contribution in more detail. The only averages which exists in the Fermi liquid are the momentum distributions $\langle n_{\vec{k}} \rangle = \theta(\vec{k} - \vec{k}_F)$. The interaction term can be decoupled in two ways. The first one is straightforward (the 'Hartree' contribution),

$$\langle 0;0 | \sum_q V_q \rho_q \rho_{-q} | 0;0 \rangle = V_{q=0} n_0^2 \tag{7.133}$$

where n_0 is the uniform charge density $\sim \sum_{\vec{k}} \langle n_{\vec{k}} \rangle = \sum_{\vec{k}} \theta(\vec{k} - \vec{k}_F)$. This is equivalent to the charge density dependency of the mean-field energy as we encountered in section (5.5). In the jellium, this term is supposed to be cancelled precisely by the interaction with the positive background charge. This is different in an *inhomogeneous* electron gas where these terms in general lead to a *smoothing* of the charge distribution: it removes self-consistently charge from high density regions where an excess Hartree energy has to be paid, and moves this charge to regions of low charge density. Together with a special potential, approximating the effects of exchange and correlation in terms of a function depending on the local charge density as will be discussed in a moment, this is the way the interactions are treated in the standard 'local density approximation' band structure theory. Next to (7.133), there is a second way to decouple (7.132) which should therefore also be taken into account. Consider $\sigma = \sigma'$, the electrons which interact have the same spin,

$$\begin{aligned} \langle \Phi^0_{Cl} | \sum_{k,k',q,\sigma} c^\dagger_{k\sigma} c_{k+q\sigma} c^\dagger_{k'\sigma} c_{k'-q\sigma} | \Phi^0_{Cl} \rangle &= -\langle \Phi^0_{Cl} | \sum_{k,k',q,\sigma} c^\dagger_{k\sigma} c_{k'-q\sigma} c^\dagger_{k'\sigma} c_{k+q\sigma} | \Phi^0_{Cl} \rangle \\ &= -\langle \Phi^0_{Cl} | \sum_{k,q\sigma} n_{k\sigma} n_{k+q\sigma} | \Phi^0_{Cl} \rangle \\ &= -\sum_{\vec{p},\vec{k}} V_{\vec{p}-\vec{k}} \theta(\vec{k} - \vec{k}_F) \theta(\vec{p} - \vec{k}_F) \qquad (7.134) \end{aligned}$$

using $k = k' - q$ to get from he first to the second line, and $p = k + q$ to recognize the third line in the second line. This is called a Fock term, and it reflects that the electrons with parallel spins in $|\Phi^0_{Cl}\rangle$ tend to avoid each other because of the Pauli principle, thereby paying less interaction energy.

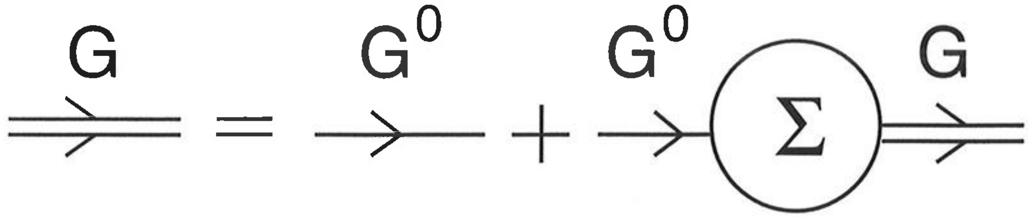

Figure 7.13

Let us return to the self-energy expansion. The second order contribution (7.122) is far more interesting. To keep track of the meaning of the various processes described by this term, it becomes now very convenient to do the accountancy using diagrams. Following the diagram rules, the defining equation for the self-energy (7.124) has the graphical representation as indicated in figure 7.13. The double line now represents the full Greens function G_1 which represents the 'renormalized' electron 'dressed up' with the self-energy: its energy has changed, it has acquired a life-time, etcetera.

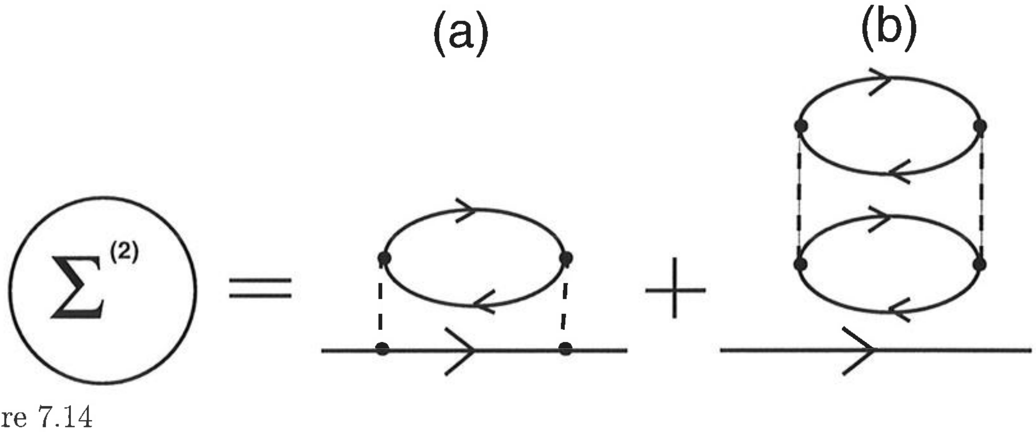

Figure 7.14

Let us now consider the second order self-energy. Given that the interaction term acts twice, and using the interaction graph we deduce the two possibilities shown in figure 7.14. The diagram for $\Sigma^{(2a)}$ represents the process we already discussed: the external electron scatters against the Fermi-sea, exciting an electron-hole pair. This diagram therefore describes the dressing of the electron, giving rise to a finite life-time, energy shift, etcetera. The diagram for $\Sigma^{(2b)}$ describes actually the renormalization of the vacuum: the external electron does not interact at all with the Fermi-sea. Instead two electron-hole pairs are excited because of the interaction acting on the Fermi-sea itself! Accordingly, diagrams like the one for $\Sigma^{(2b)}$, with the external electron-line omitted, are called 'vacuum polarization diagrams' and summing these together amounts to bringing the classical state $|\Phi^0_{Cl}\rangle$ to the dressed vacuum $|\Phi_{Cl}\rangle$. At the same time, it is obvious that the vacuum polarization diagrams have nothing to do with the properties of the extra electron. Although it is not easy to see from the present formalism, it turns out that all disconnected diagrams (the ones containing vacuum polarization diagrams) as show up in the self-energy expansion, add up to precisely cancel the overlap factor $|\langle\Phi^0_{Cl}|\Phi_{Cl}\rangle|^2$ in (7.114). Hence, when we neglect all disconnected diagrams we can neglect this overlap factor as well. One can now define an 'irreducible' (or 'proper') self-energy $\Sigma = \Sigma_{red} - (\textit{disconnected diagrams})$ and this is the self-energy appearing in (7.110), describing exclusively the fate of the extra electron.

Although there are many more diagrams to be discussed, the RPA resummation and the concept of self-energy actually suffice to discuss a class of theories which are technically managable while they work quite well at the same time. The basic strategy is to search for particular diagrams which show up in all orders of perturbation theory, while they can be resummed using the Dyson equation. At the same time, one has to neglect an infinity of other diagrams and picking the important diagrams is a matter of physical intuition, as well as opportunism: generic high order diagrams correspond with high dimensional integrals which cannot be solved by the fastest computer. Fortunately, these diagrams have the habit to be quite unimportant as long as the vacuum is the proper (classical) one. Let me illustrate this with the so-called 'GW' approximation, which turns out to yield a rather accurate quantitative description of 'simple' electron systems, like weakly correlated metals and semiconductors. At the same time, GW offers a rational for the success of the local density approximation underlying band-structure theory. In essence, GW amounts to saying that only the bubble summation (RPA, fig. 7.11) and the second order irreducible diagram $\Sigma^{(2a)}$ (fig. 7.14) really matter as building blocks.

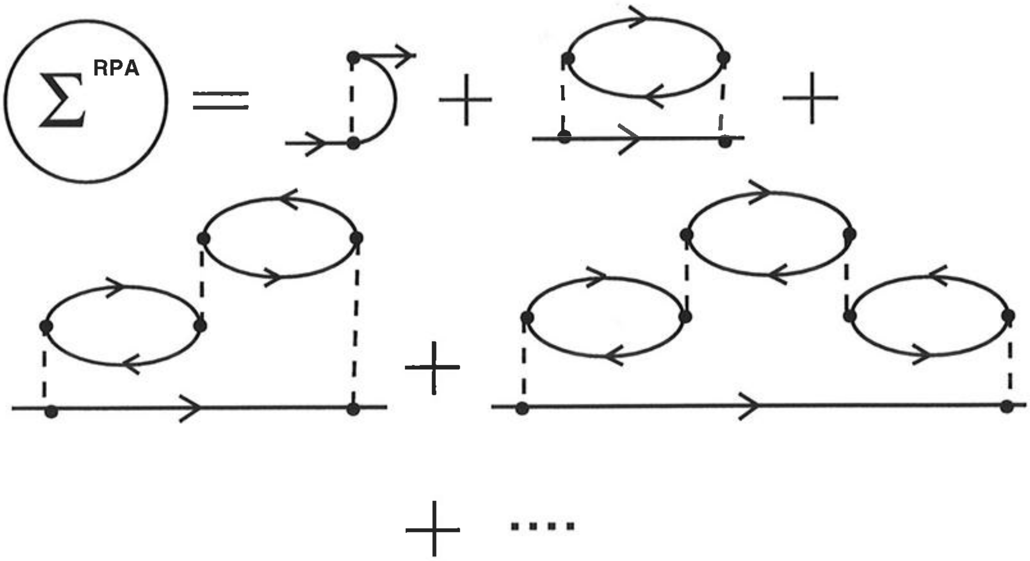

Figure 7.15

It starts out with the observation that the bubble appearing in the second order self-energy diagram fig. 7.14a also shows up as the basic building block of the RPA resummation fig. 7.11. Expanding the electron self-energy up to higher order, we will find among many other diagrams the ones shown in figure 7.15. For a good reason, I also included the diagram for the first order Hartree correction. Hence, this is like the RPA resummation, except that the bubble 'chains' are now connected to the external fermion line. Since we learned that bubbles have to be resummed to produce the correct physics, we expect that this resummation is also important for the electron self-energy. Using (7.73) and (7.108),

$$\frac{V_{\vec{q}}}{\varepsilon^{RPA}(\vec{q},\omega)} = V_{\vec{q}} + V_{\vec{q}}\chi^0(\vec{q},\omega)V_{\vec{q}} + V_{\vec{q}}\chi^0(\vec{q},\omega)V_{\vec{q}}\chi^0(\vec{q},\omega)V_{\vec{q}} + \cdots \tag{7.135}$$

The screened interaction V/ε becomes in RPA the diagram series as indicated in figure 7.16.

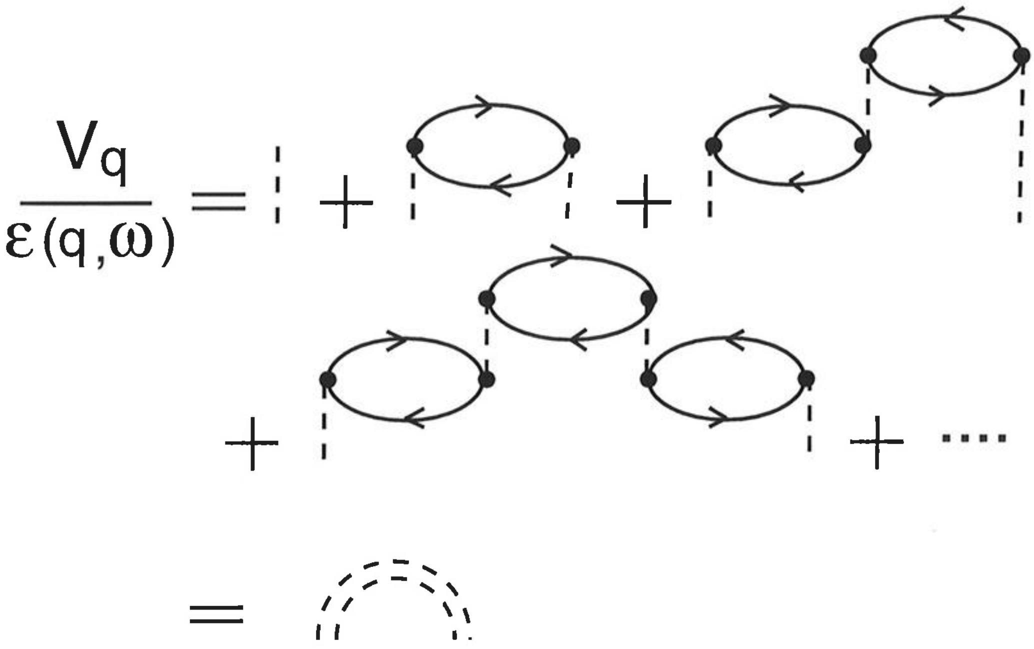

Figure 7.16

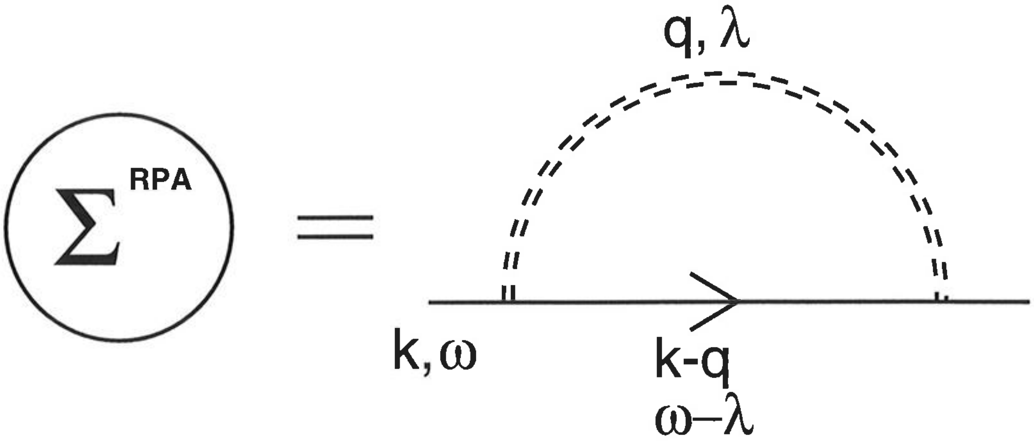

Figure 7.17

Because of the frequency dependence of ε^{RPA}, the screened interaction (double dashed line, figure 7.16) is now time dependent and it is no longer necessary to draw it straight upwards. Alternatively, one can look at the screened interaction as being a boson like excitation. Comparing figure 7.15 and figure 7.16 we see directly that the RPA-level self-energy can be represented by the simple diagram shown in figure 7.17. In algebraic form,

$$\Sigma_{RPA}(\vec{k},\omega) = \sum_{\vec{q}} \int d\lambda \frac{V_q}{\varepsilon_{RPA}(\vec{q},\lambda)} G^0(\vec{k}-\vec{q},\omega-\lambda) \tag{7.136}$$

and this is the typical form of a lowest order electron self-energy related to the exchange of a boson. For instance, the lowest order electron self-energy coming from the interactions with phonons is given by glueing together to elementary diagrams of the type figure 4.4. This yields figure 7.18, with the doubly dashed line replaced by the wiggly phonon line. This corresponds with a convolution type integral as in (7.136), with $\frac{1}{\varepsilon^{RPA}(\vec{q},\omega)}$ replaced by the $\vec{q}$ and ω dependent phonon Greens function.

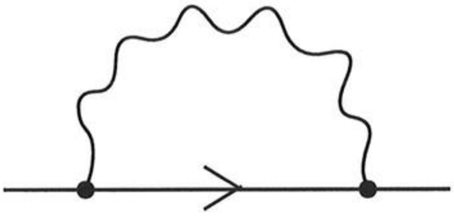

Figure 7.18

What is the physical meaning of figure 7.17/(7.136)? It *proves* that the electron only knows about the *screened* Coulomb interaction! Recalling the discussion in the previous section, the effective low energy theory which can be extracted by analyzing (7.110), (7.73) and (7.136) for low energies is characterized by much smaller interactions than the theory in terms of the bare electrons. This gives a first glimpse on the renormalization principle which makes it possible for the Fermi-liquid to exist: the coupling strength itself is a function of energy. Starting with a rather strongly interacting system at high energies, the interaction strength decreases with decreasing energy, to vanish alltogether in the infrared where the effective system becomes 'free' (non-interacting).

There is more to be dressed up. Up to now we have used the bare fermion lines to calculate the bubble. However, the bare fermions donot exist, and we better dress up these bubble fermions with self-energy diagrams as well: figure 7.19. Hence, it is easy to improve the RPA by using the full electron Greens functions instead of the bare fermion propagators in the calculation of χ^0. Finally, we should also dress up the remaining internal fermion line in the self-energy diagram, figure 7.20: the electron itself is also scattered into a dressed state after the exchange with a (dressed) RPA charge fluctuation.

This series of resummations defines the GW approximation. It corresponds with the following system of equations,

$$G_{GW}(\vec{k},\omega) = \frac{1}{\omega - \varepsilon_{\vec{k}} - \Sigma_{GW}(\vec{k},\omega)}$$

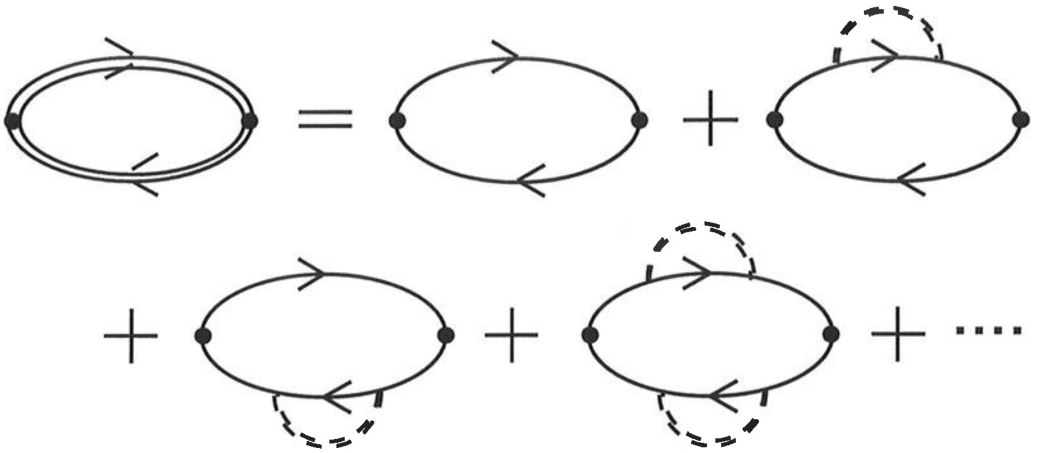

Figure 7.19

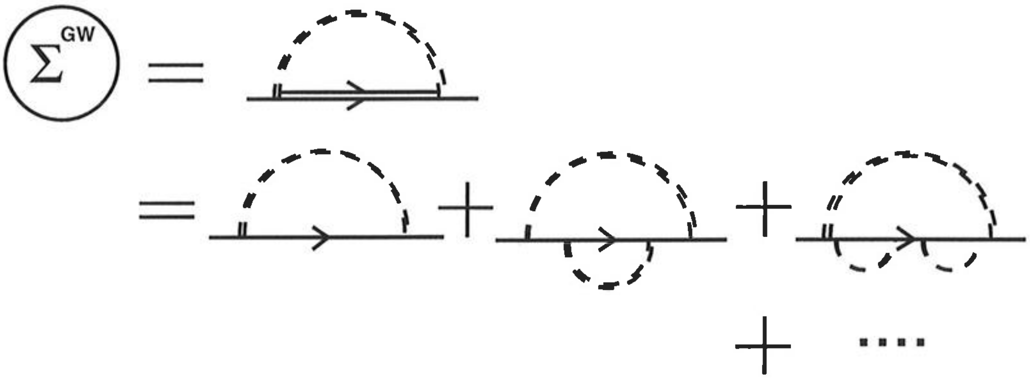

Figure 7.20

$$
\begin{aligned}
\Sigma_{GW}(\vec{k},\omega) &= \sum_{\vec{q}} \int d\lambda \frac{V_q}{\varepsilon_{GW}(\vec{q},\lambda)} G_{GW}(\vec{k}-\vec{q},\omega-\lambda) \\
\varepsilon_{GW}(\vec{q},\lambda) &= 1 - V_{\vec{q}}\chi^0_{GW}(\vec{q},\omega) \qquad (7.137)
\end{aligned}
$$

where the imaginary part of χ^0_{GW} relates to the density of states of fully dressed particle-hole excitations, which can be calculated from G_{GW}. It is called GW, because the self-energy has the form $\Sigma \sim GW$, where W is the screened interaction and G the dressed Greens function. This system of non-linear equations can be solved numerically and it turns out to yield a rather accurate description for the jellium. In addition it can be generalized to apply to inhomogeneous electron systems as well. (7.137) takes now a matrix form, because the equations become non-diagonal in $\vec{k}$ space: in analogy to the scattering of independent electrons against a periodic potential, points in $\vec{k}$ space displaced by reciprocal lattice vectors $\vec{K}$ start to communicate with each other. For the simplest realistic electron systems, this problem can be approximately solved, and it turns out to yield a near to *exact* description of the electronic structure of for instance silicon[13]. These results give the best rational available for the succes of the local density approximation (LDA), commonly used in band structure calculation to treat the interaction effects. LDA has a far simpler

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[13] See, e.g., M. S. Hybertsen and S. G. Louie, Phys. Rev. B34, 5390 (1986).

structure than GW: it is a simple mean-field theory with an adjusted relationship between the vacuum expectation values (charge densities) and mean-field potentials. It turns out, that this LDA 'exchange-correlation' potential can be understood as the static $\omega \rightarrow 0$ and local $(\Sigma(\vec{k}, \vec{k}') \rightarrow \delta(\vec{k} - \vec{k}')\Sigma(\vec{k}))$ limit of the GW self-energy, which suffices when the system is not too inhomogeneous[14].

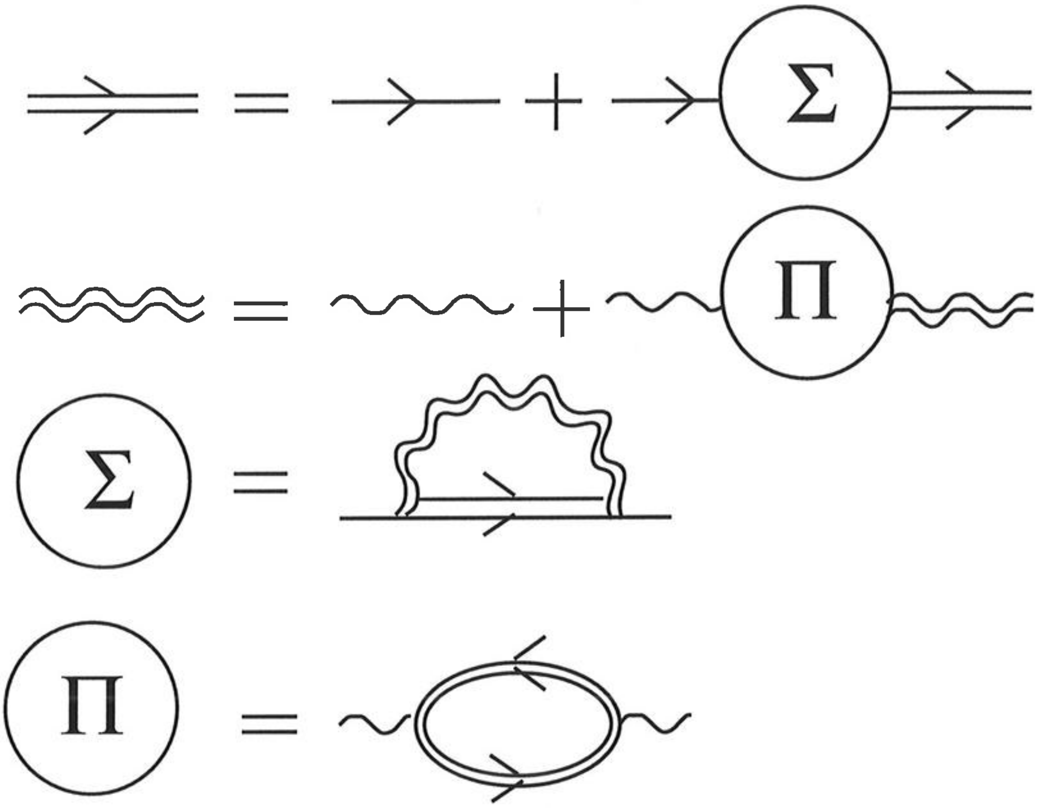

Figure 7.21

Despite the GW resummations, there are still infinities of diagrams which are neglected. It can be rigorously shown that all the neglected processes act to renormalize the interaction points ('vertices') where the Greens function lines connect. These are called vertex corrections and are usually much harder to calculate and to resum. GW is best characterized as the theory of interacting fermions under the 'complete neglect of vertex corrections'. In the case of GW, this is an uncontrollable approximation and it is a matter of trial and error to find out if it makes any sense. This is different in the context of electron-phonon coupling in metals, where it can be proven (Migdal's theorem) that the vertex corrections start to contribute for the first time in the order ω_E / E_F. Because the ratio of the phonon frequency and the Fermi energy is a very small number, one can neglect the vertex corrections safely, also in the context of the quantitative theory. In diagrams, the structure of the very successful Migdal theory for the electron-phonon coupling is indicated in figure 7.21. Notice that the phonon-self energy (Π) is the dressed version of the second order diagram, describing the

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[14] Quite often, LDA is sold by referral to the (in itself significant) density functional theorems by Hohenberg, Kohn and Sham. I find these rationalizations to belong to the domain of scientific myth.

decay of a phonon in an electron-hole pair. This theory is straightforwardly extended to include a superconducting condensate as well, and this is the 'strong coupling' or 'Eliashberg' theory for superconducivity, which is very accurate even when the electron-phonon coupling becomes large.

Despite their quantitative accuracy, the above 'pragmatic' theories do not show any light on the question of principle: does the Fermi-liquid exist? At the end, an infinity of diagrams has been neglected and only one of those has to be singular in order to render the Fermi-liquid condensate unstable. The structure of the perturbation theory around the Fermi-liquid can be further analyzed, and it turns out that one can actually *prove* that the Fermi liquid *can* exist when the dimensionality of the system $d \geq 2$. More specifically, it can be shown that the Fermi liquid is internally consistent: the perturbation theory around the Fermi liquid is well behaved in all orders. Notice that this does not imply that the Fermi-liquid *has* to exist: the proof amounts to saying that the fully renormalized Fermi-liquid corresponds with a minimum of energy and this is not necessarily the global minimum. The full argument is far too complicated to be presented here, and needs the full machinery of field-theory style perturbation theory: I refer the reader to the specialized books[15]. A central piece in this proof is the stability criterium itself: what question should we ask in order to find out whether or not the Fermi-liquid survives?

The self-energy is the central quantity. In the context of crystals we started out, assuming that the Taylor expansion (4.15) exists, which was trivially the case in the classical limit, but not necessarily so in the quantum system (the one dimensional 'crystal', section 4.6). In the present context, the existence of the Fermi-liquid as a stable state depends on the analytic character of the self-energy. We have to demand that the imaginary part of Σ'' can be written as a power series in ω which starts with a quadratic contribution,

$$\Sigma''(\vec{k}, \omega) = \sum_{n=2}^{\infty} a_n(\vec{k}) \omega^n \tag{7.138}$$

In the Fermi-liquid Σ'' has to vanish at the Fermi-energy, because otherwise the discontinuity would be smoothed out, because of the fuzziness of the quasiparticles. This means that the fermion states at E_F and k_F live for an infinite time, which can only be the case when these fermions are non-interacting. In addition, we assume that Σ'' is a non-singular function of $\vec{k}$. When Σ'' is of the form (7.138) it follows from the Kramers-Kronig relation that all derivatives of Σ' exist. This implies that the real part of the self energy can be written as a Taylor expansion around $\omega = 0$ and $\vec{k} = \vec{k}_F$,

$$\begin{aligned} \Sigma'(\vec{k}, \omega) &= \Sigma'(k_F, 0) + \left(\frac{\delta \Sigma'(k_f, \omega)}{\delta \omega} \right)_{\omega=0} \omega + \left(\frac{\delta \Sigma'(k, 0)}{\delta k} \right)_{k=k_F} (k - k_F) \\ &\quad + \left(\frac{\delta^2 \Sigma'(k_f, \omega)}{\delta \omega^2} \right)_{\omega=0} \omega^2 + \cdots \end{aligned} \tag{7.139}$$

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[15] Especially 'AGD' has a reputation to loose in this regard.

(7.139) is the actual stability criterion for the Fermi-liquid: only when Σ' can be written as this Taylor series, the Fermi-liquid exists, as we will see in a moment. Notice that Σ' is finite on the Fermi-surface, in contrast to Σ'' (because of the Kramers-Kronig relation, $\Sigma'(k_F, 0) \sim -\int d\omega' \Sigma''(k_F, \omega')/\omega' \neq 0$ and $\Sigma'(k_F, 0)$ redefines the thermodynamic potential). Notice also that the first derivative of Σ' to ω is always negative,

$$\left(\frac{\delta\Sigma'(k,\omega)}{\delta\omega}\right)_{\omega=0} = -\frac{1}{\pi}P\int d\omega' \frac{1}{\omega'}\frac{\delta\Sigma''(k,\omega')}{\delta\omega'} < 0 \tag{7.140}$$

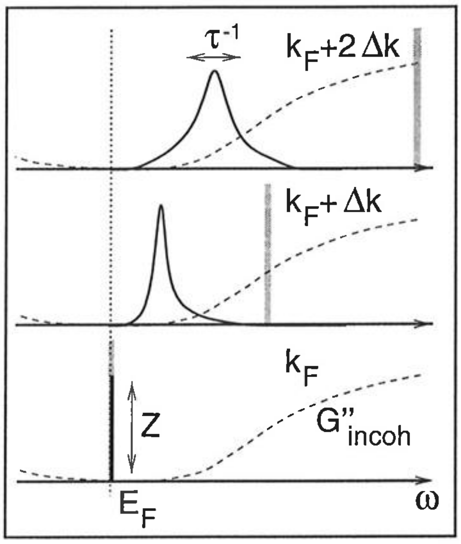

Figure 7.22: *the consequences for the (unoccupied part) of the single particle spectral function, implied by the analytic structure (7.138,7.139) of the self-energy.*

Assuming that the self-energy can be written as (7.138,7.139), interesting statements can be made, regarding the nature of the one particle spectral function: this is the elegant core of the argument. G_1 is divided in a part describing the $\omega \to 0$ limit of $A_1 = ImG_1$ (the quasiparticle part) and the remainder which does not contribute when the energy is sufficiently low ($ImG_{incoh} = 0$ when $\omega \to 0$, the "incoherent" part).

$$\begin{aligned} G_1(k,\omega) &= \frac{1}{\omega - \varepsilon_k - \Sigma(\vec{k},\omega)} && (7.141)\\ &= \frac{1}{\omega - \varepsilon_k - \left(\frac{\delta\Sigma'}{\delta\omega}\right)_{\omega=0}\omega - \left(\frac{\delta\Sigma'}{\delta k}\right)_{k=k_F}(k-k_F) - ia_2(k)\omega^2} \\ &\quad + G_{incoh}(k,\omega) && (7.142) \end{aligned}$$

This can also be written as ($\varepsilon_k \to \frac{k_F}{m}(k - k_F)$ when $k \to k_F$),

$$G_1(k,\omega) = \frac{Z_k}{\omega - \frac{k_F}{m_k^*}(k-k_F) - i\tau_k^{-1}(\omega)} + G_{incoh}(k,\omega) \tag{7.143}$$

with

$$Z_k = \frac{1}{1-\left(\frac{\delta\Sigma'}{\delta\omega}\right)_{\omega=0}} \tag{7.144}$$

$$m_k^* = \frac{1}{Z_k}\frac{1}{\frac{1}{k_F}\left(\frac{\delta\Sigma'}{\delta k}\right)_{k=k_F}+\frac{1}{m}} \tag{7.145}$$

$$\tau_k^{-1}(\omega) = \frac{a_2(k)}{Z_k}\omega^2 \tag{7.146}$$

Because the k dependence is in many cases quite weak, it is often neglected alltogether,

$$G_1(k,\omega)) = \frac{Z}{\omega-\frac{k_F}{m^*}(k-k_F)-i\tau^{-1}(\omega)}+G_{incoh}(k,\omega) \tag{7.147}$$

$$Z = \frac{1}{1-\left(\frac{\delta\Sigma'}{\delta\omega}\right)_{\omega=0}} \tag{7.148}$$

$$\frac{m^*}{m} = \frac{1}{Z} \tag{7.149}$$

$$\tau^{-1}(\omega) = \frac{a_2}{Z}\omega^2 \tag{7.150}$$

This is a very important result. It links the analytical structure of the self-energy to the following physical consequences: *When the imaginary part of the self-energy can be written as the power series (7.138), it follows that the low energy regime of the fermionic excitation spectrum is completely defined in terms of fermions with a mass m^* which do not interact, and which are in other regards identical to the bare electronic degrees of freedom.* This can be inferred directly from the one particle spectral function A_1, figure 7.22. Momenta close to k_F are considered and the grey lines indicate where the poles would be located when the electrons would be truely non-interacting. The full spectral function is characterized by the incoherent part (dashed lines) and the quasiparticle part dominating the low energy regime (full lines), corresponding with a resonance. The quasiparticle has the following properties:

(i) For every non-interacting electron state there is exactly one quasiparticle state (see figure 7.22). This means that there are precisely as many quasiparticles as there would be bare fermions when the bare particles would not have interacted. There is a one-to-one correspondence between the interacting- and non interacting systems. This has (among others) the consequence that the volume in $\vec{k}$ space enclosed by the Fermi-surface is the same in the interacting- and non-interacting systems (Luttinger's theorem).

(ii) The quasiparticle peak is not a sharp state away from k_F. At any finite energy it has a width (or inverse lifetime) which increases asymptotically as $1/\tau_k \sim \Sigma''(E_k,k) \sim E_k^2$, where E_k is the quasiparticle energy. At the Fermi-energy, the lifetime becomes infinite and the quasiparticles become truely independent, sharply defined excitations.

(iii) Because $\delta\Sigma'/\delta\omega < 0$ (7.140), $Z < 1$ (7.148). The overall weight of the quasiparticle resonance is Z and this is always a fraction of the weight of the free state. Z is called the 'quasiparticle pole strength' and it expresses the overlap between the quasiparticle and the non-interacting electron. Notice that the remainder of the weight in A_1 disappears in the incoherent continuum at higher energies. Z actually corresponds precisely with the overlap A^2 between the single determinant state and the fully renormalized vacuum as defined by (7.32): only the quasiparticles are present at E_F and they are therefore responsible for the discontinuity. Hence, as long as Z is finite, the classical state dictates the properties and the system is a Fermi-liquid. *The stability of the Fermi liquid is therefore controlled by the analytical structure of the one particle self-energy.*

(iv) Although there is a one-to-one correspondence between the non-interacting electrons and the quasiparticles, the quasiparticle energy is different from the kinetic energy of the free electron. The dispersions can always be linearized close to E_F and because of the correspondence principle, the energy differences can be completely absorbed in a redefinition of the mass, (7.147): the quasiparticle mass m^* is always *larger* than the bare electron mass. The highlight, (7.149): *the mass enhancement is inversely proportional to the pole strength, and the mass of the quasiparticle is a direct measure of the magnitude of the Fermi liquid order parameter.* Hence, in a heavy fermion system, the quasiparticle mass is enhanced by three orders of magnitude, and this implies that the weight of the classical state in the true ground state is only 1/1000 - a reason to find heavy fermion systems interesting.

It remains to be demonstrated that the imaginary part of the self-energy has the analytic structure (7.138). In fact, this can be checked directly by experiment. The simplest way is to consider the DC resistivity. According to semiclassical transport theory, the resistivity is directly proportional to the inverse of the transport life-time $\rho \sim 1/\tau_{tr}$ and, taking some care, the transport life-time can be associated with the single particle life time, such that $\rho \sim \Sigma''(\omega = 0, T)$. At finite temperatures and zero energy, one can simply exchange ω and T in the expressions for Σ'', and one expects $\rho \sim T^2$: this is the universal behaviour of the DC resistivity at low temperatures in normal metals. When this is not observed, as for instance in high T_c superconductors ($\rho \sim T$ from 10 to 1000 K), it is considered as evidence for the system being a non-Fermi liquid.

The existence proof for the Fermi-liquid actually amounts to the demonstration that the full perturbation expansion (including all diagrams) produces the series expansion (7.138) for the imaginary part of the self-energy. The actual proof is quite complicated[16], but the physical essence is not hard to understand: because of the Pauli exclusion principle, severe kinematic constraints (energy- and momentum conservation) are present for the production of real excitations, needed as a decay channel for the quasiparticle. Moreover, these constraints become more severe when one considers diagrams of increasing complexity. As a consequence, the asymptotic behaviour

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[16] see J. M. Luttinger, Phys. Rev. 121, 942 (1961).

of Σ'' (counting the real excitations) is completely dominated by the lowest order diagrams. The most dangerous contribution is actually coming from the familiar bubble diagram, figure 7.23.

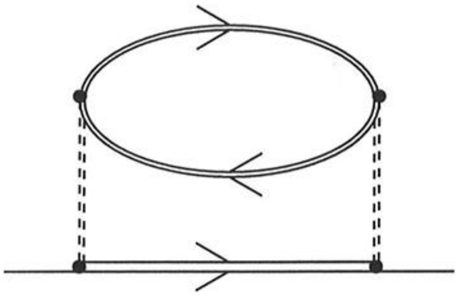

Figure 7.23

Because only quasiparticles exist as real excitations in the $\omega \rightarrow 0$ limit, the lines in the diagram now refer to the fully dressed quasiparticles, interacting via screened interactions. The calculation of the imaginary part is not different from the calculation of the phonon life-time, considered in section 4.4, except that we now have to count fermions. The effective interaction is short ranged and we can neglect its momentum dependence alltogether. According to the golden rule, we have to determine the probability that the test quasiparticle with momentum $\vec{k}_1 > k_F$ and energy $E_1 = k_F(k_1 - k_F)/m^*$ decays in a quasiparticle with momentum $\vec{k}_4 > k_F$ and energy E_4, thereby exciting a quasihole ($\vec{k}_2 < k_F, E_2$) - quasiparticle ($\vec{k}_3 > k_F, E_3$) excitation (figure 7.25). We infer directly that the test particle ('1') cannot decay when it is on the Fermi-surface, and its lifetime becomes infinite. We learned, however, that this is a necessary but insufficient condition for the existence of the Fermi-liquid. We also have to know how Σ'' approaches zero. We have only to account for the kinematics,

$$\begin{aligned} \vec{k}_1 + \vec{k}_2 &= \vec{k}_3 + \vec{k}_4 && (7.151) \\ E_1 + E_2 &= E_3 + E_4 && (7.152) \end{aligned}$$

Initially we have the test quasiparticle at E_1 and the quasihole-to-be at E_2, while the final state consists of two quasiparticles outside the Fermi sea, at E_3 and E_4. Momentum conservation (7.151) implies, that the center of mass momentum of the initial pair of quasiparticles has to be the same as that of the final pair of quasiparticles. This implies that the two final state quasiparticles ('2' and '4') have to lie on a sphere in $\vec{k}$ space centered around the center of mass momentum of the initial state pair (figure 7.24b).

In addition, it is immediately clear that particle 2 has to be within a shell $\sim E_1 - E_F = \omega$ from the fermi-energy in order for the conservation laws to be satisfied (figure 7.24a). The density of states can be taken to be constant (N_0) and the number of states for particle 2 is therefore $\sim N_0\omega$. The final state pair '3' and '4' can still be freely choosen except that the momentum of '3' is fixed when a momentum for '4' is choosen, and vice versa (figure 7.24b). In addition, both must lie within a shell ω

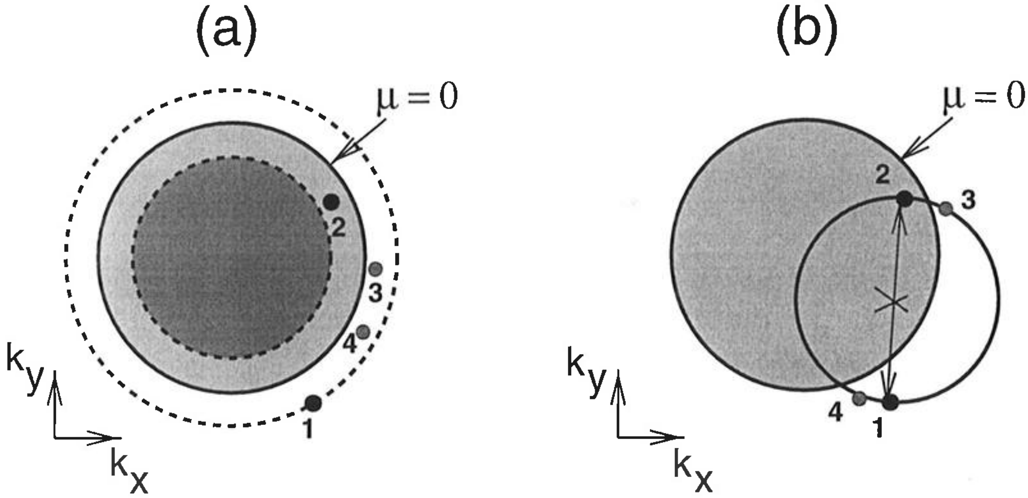

Figure 7.24: *consequences of energy- (a) and momentum conservation (b) for the lowest order decay process of the quasiparticle (figure 7.23)*

from E_F (figure 7.24a), and the total number of final states is therefore $\sim N_0\omega$ as well. Because '3' together with '4' can be choosen independently from '2', we find

$$\Sigma_2''(k,\omega) \sim a\omega^2 \tag{7.153}$$

Hence, the most 'dangerous' decay process contributes precisely the lowest allowed power to the expansion for Σ''.

The above excercise in kinematics is valid in three dimensions. This does not change in two dimensions, but it works really different in one dimension. We already anticipate difficulties because of the divergencies expected in the zero sound channel. Also in the fermionic channel the perturbation theory gets out of hand. One finds that the leading (bubble) order contribution to $\Sigma''(k,\omega) \sim \omega$. This implies that the full self-energy behaves as $\Sigma(k,\omega) \sim \omega\ln(i\omega)$ such that $\Sigma'(k,\omega) \sim \omega\ln|\omega|$. It follows directly that $\delta\Sigma'/\delta\omega \sim ln\omega$ and the first derivative of Σ' at $\omega = 0$ *diverges logarithmically.* Therefore, the effective mass diverges as wel, while the pole strength goes to zero. As the other classical states, the Fermi-liquid cannot exist in one dimension, and to find this out one can as well look at the fermions.

I already hinted at the state which is realized instead: the Luttinger liquid. Interestingly, in this state it is not possible to identify fermions as fundamental excitations, although the collective modes still exist in the sense of the floating solid (section 4.6). The physical picture is that the electron decays into a charge- and a spin mode which propagate with different velocities. Hence, they can never find back each other to recombine into the fermion, and in this way the fermion gets 'lost' in the sea of fluctuating charge- and spin modes. Intellects in a one dimensional universe would not worry about fermions!

7.5 Excercises

7.1 Consider the nearest-neighbor tight binding model in $d = 1$ and assume that the system is half filled. Sketch $A_{k\sigma}(\omega)$ for $k = 0, \pi/4, \pi/2, 3\pi/4$ and π.

7.2 Derive (7.16) from (7.9), (7.14) and (7.15).

7.3 Derive (7.17) and (7.19) from (7.10-7.16).

7.4 (7.22) is equivalent to the so-called Kramers-Kronig relations connecting the real and imaginary part of response functions. Consider the analytic continuation of the susceptibility $\chi(z)$, with $z = \omega' + iImz$.

a. Argue that χ is analytic in the upper half-plane. What is the relationship with causality?

b. Assume that χ/z vanishes when $|z| \to \infty$. Show that

$$\oint \frac{\chi(q,z)}{\omega - z} dz = P \int_{-\infty}^{\infty} \frac{\chi(q,\omega')}{\omega - \omega'} d\omega' + i\pi\chi(q,\omega) = 0 \tag{7.154}$$

using the integration contour fig. 7.25.

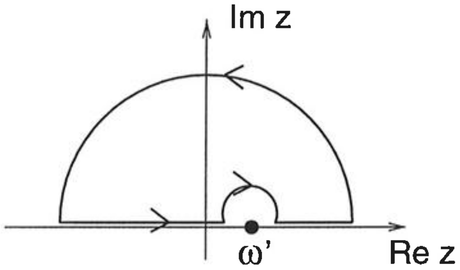

Figure 7.25

c. Show that the Kramers-Kronig relations follow from the result (b.),

$$\begin{aligned} \chi'(q,\omega) &= -\frac{1}{\pi} P \int \frac{\chi''(q,\omega')}{\omega - \omega'} d\omega' \\ \chi''(q,\omega) &= \frac{1}{\pi} P \int \frac{\chi'(q,\omega')}{\omega - \omega'} d\omega' \end{aligned}$$

7.5 The density operator in reals space is given by,

$$\rho(\vec{r}) = \sum_i \delta(\vec{r} - \vec{r}_i) \tag{7.155}$$

Derive the jellium quantities (7.34-7.35).

7.6 Derive (7.41) directly from the definition of χ, (7.19).

7.7 The Lindhard function χ_0. It is not too hard to obtain the imaginary part.

a. Show that the imaginary part of (7.40) can be written as,

$$\chi_0''(\vec{q}.\omega) = 2\pi \int_0^{p_F} \frac{d^3p}{(2\pi)^3} \left[\delta(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}} + \omega) - \delta(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}} - \omega)\right] \tag{7.156}$$

b. Show that this simplifies to,

$$\chi_0''(\vec{q},\omega) = \frac{1}{2\pi} \int_0^{k_F} p^2 dp \int_{-1}^{1} d\nu \left[\delta(\varepsilon_q + \frac{pq}{m}\nu - \omega) - \delta(\varepsilon_q + \frac{pq}{m}\nu + \omega)\right] \tag{7.157}$$

c. Integrate first over ν and show that the remaining integral yields (7.50,7.51).

7.8 How do the upper- and lower bounds of the particle-hole continuum of figure 7.3 behave precisely as function of q/k_F and ω/E_F?

7.9 Derive (7.57) from (7.52) and (7.56).

7.10 Derive (7.60) from (7.57).

7.11 Derive (7.68-7.69) (use (7.52) for χ_0').

7.12 The Anderson impurity model is an important model in the context of heavy fermion physics. It represents a tight-binding like, correlated impurity state 'd', hybridizing via V_k with band states (recall excercise 5.11),

$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \varepsilon_d \sum_{\sigma} n_{d\sigma} + \sum_{k\sigma} V_k (c^\dagger_{k\sigma} d_\sigma + h.c.) + U n_{d\uparrow} n_{d\downarrow} \tag{7.158}$$

When $U = 0$ (no interactions), this model is easily solved using Greens functions, illustrating the idea of self-energy.

a. Use the Dyson equation to derive the impurity Greens function,

$$G_{dd} = \langle d|\hat{G}(z)|d\rangle = \frac{1}{z - \varepsilon_d - \Sigma_{dd}(z)} \tag{7.159}$$

with the *self-energy* (compare with Clogston-Wolff !!),

$$\Sigma(z) = \sum_k \frac{V_k^2}{z - \varepsilon_k} \tag{7.160}$$

b. Assume $V_k = V$, while the density of states of the band electrons has the 'box' form (7.100-7.101). Sketch and discuss the impurity spectral function $A_{dd}(\omega) = Im G_{dd}(\omega - i\eta)$ for the following cases:
(i) $\varepsilon_d = 0$ and $V^2\rho = W/10$.
(ii) $\varepsilon_d = 0$ and $V^2\rho = W$.
(iii) $\varepsilon_d = 3W/4$ and $V^2\rho = W/10$.
(iv) $\varepsilon_d = 3W/4$ and $V^2\rho = W$.