On Quantum Mechanics

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1 Introduction

Quantum mechanics is about hundred years old. After the invention of classical mechanics by Newton, it is the greatest discovery in physics with the largest impact on our view on the nature of matter. Everbody will agree that quantum mechanics contains counterintuitive notions and libraries are filled with books on the proper interpretation. So why trying to add something to seemingly endless and often grotesque discussions (e.g. superpositions of dead and alive cats) on the proper perspective on quantum mechanics?

This note is purely didactic and concerns the question of how to introduce most adequately new students to the strange world of quantum mechanics. The advice that I want to give is: abandon the historic route elaborating on the analogy with waves (particle-wave duality) and rather stress the analogy with stochastic processes governed by the Master Equation and with Brownian motion in particular. Historically, stochastic processes were seen as less fundamental and driven by an underlying chaotic mechanics. With the advent of quantum mechanics the situation is reversed: stochastic evolution is the basic principle and mechanics derives from it. I will show that the Schrödinger Equation is a sort of square root out of the Master Equation. So I start with a short discussion of the Master Equation.

2 The Master Equation

A stochastic process is governed by transition rates $W(Y|Y')$ of state Y' to Y. The probability $P(Y,t)$ on state Y obeys the Master Equation (ME)

$$\frac{\partial P(Y,t)}{\partial t} = \sum_{Y'} [W(Y|Y')P(Y',t) - W(Y'|Y)P(Y,t)] = \sum_{Y'} H_{Y,Y'} P(Y',t), \qquad (1)$$

The first term gives the gain to state Y and the second term the loss from state Y. The equation is deterministic i.e. the probability at any later time t is determined by the probability at an earlier time (e.g. $t = 0$). Somewhat more precise: $P(Y,t)$ gives the conditional probability to find the system in state Y at time t given the probability distribution $P(Y,0)$ at time $t = 0$. In this discrete formulation the time evolution results from a matrix operation on the distribution. The matrix $H_{Y,Y'}$ is called *stochastic* since the sum over the columns vanishes, as (1) shows. This property guarantees the conservation of probability

$$\sum_Y P(Y,t) = \sum_Y P(Y,0), \qquad (2)$$

implying that one of the eigenvalues of $H_{Y,Y'}$ is zero; the others must have a negative real part, otherwise the probability distribution blows up.

A specific example of the ME is the Brownian particle. The state of the particle is the position $\mathbf{r}$. When the transition probabilities are confined to small steps, the ME can be written in the form of a Fokker-Planck equation. Introduce the step

$$\mathbf{s} = \mathbf{r} - \mathbf{r}' \tag{3}$$

and write the transition probability as

$$W(\mathbf{r}|\mathbf{r}') = W(\mathbf{r}';\mathbf{s}). \tag{4}$$

Using this notation the ME gets the form

$$\frac{\partial P(\mathbf{r},t)}{\partial t} = \int d\mathbf{s}\, W(\mathbf{r}-\mathbf{s};\mathbf{s})P(\mathbf{r}-\mathbf{s},t) - P(\mathbf{r},t)\int d\mathbf{s}\, W(\mathbf{r};-\mathbf{s}). \tag{5}$$

The assumption is that W and the probability P depend smoothly on the first argument $\mathbf{r}$. Then we may expand the first term in the Master Equation with respect to $\mathbf{r}$, will keeping the second argument in its full glory

$$W(\mathbf{r}-\mathbf{s};\mathbf{s})P(\mathbf{r}-\mathbf{s},t) = W(\mathbf{r};\mathbf{s})P(\mathbf{r},t) - [\mathbf{s}\cdot\nabla]W(\mathbf{r};\mathbf{s})P(\mathbf{r},t) + \cdots \tag{6}$$

Inserting this expansion in the ME (5), the first term in the expansion cancels the second term in the ME. Thus the ME transforms into the Fokker-Planck equation

$$\frac{\partial P(\mathbf{r},t)}{\partial t} = -\nabla\cdot\mathbf{a}_1(\mathbf{r})P(\mathbf{r},t) + \frac{1}{2}\nabla\nabla\cdot\mathbf{a}_2(\mathbf{r})P(\mathbf{r},t). \tag{7}$$

where the $\mathbf{a}_i(\mathbf{r})$ are the jump moments

$$\mathbf{a}_i(\mathbf{r}) = \int d\mathbf{s}\,\mathbf{s}^i\, W(\mathbf{r};\mathbf{s}). \tag{8}$$

If the jumps are isotropically distributed, $\mathbf{a}_1 = 0$ and if they are independent of the position one has

$$\mathbf{a}_2(\mathbf{r}) = 2D\,\mathbf{I} \tag{9}$$

and the Fokker-Planck equation gets the form

$$\frac{\partial P(\mathbf{r})}{\partial t} = D\Delta P(\mathbf{r},t). \tag{10}$$

D is the diffusion coeffient of the Brownian particle. There are good mathematical reasons to terminate the expansion (6) after the second term, but that is not important for the discussion here. We repeat that $P(\mathbf{r},t)$ is that the probability to find the Brownian particle at position $\mathbf{r}$ at time t given the distribution $P(\mathbf{r},0)$. If it was found to be at $t = 0$ at the origin $P(\mathbf{r},t)$ would be a δ function at the origin, which would spread out as a Gaussian. If at t it was found to be at position $\mathbf{r}'$, the distribution $P(\mathbf{r},t)$ would start again as a δ function around position $\mathbf{r}'$. No one would see the probability distribution as some physical property of the Brownian particle.

By fourier decomposition one sees that all the eigenvalues of the diffusion operator are negative except one. All the wave components with finite wave vectors decay, the one with wave vector zero is invariant.

To phrase the physics of the Brownian particle in a formulation akin to the quantum mechanical: the brownian particle is in a state, which can be found by measurement of the position. By measuring the position again at a later time one finds a new state with a probability given by the solution of the ME with the original state as starting point. So the ME gives the transition probabilities from state to state. One can only measure displacements of the Brownian particle, it has no velocity. Although the evolution of the ME is deterministic the dynamics is not deterministic within the frame work of the stochastic process.[1]

3 The Schrödinger Equation

The Schrödinger Equation (SE) has the form

$$i\hbar \frac{\partial \Psi(Y,t)}{\partial t} = \mathcal{H}\, \Psi(Y,t), \tag{11}$$

where Ψ is the wavefunction (state) of the system. This is also a deterministic equation, since the initial value of the wavefunction $\Psi(Y,0)$ determines the behavior at later times. The operator $\mathcal{H}$ is hermitian and this yields the conservation law

$$\int dY |\Psi(Y,t)|^2 = \int dY |\Psi(Y,0)|^2, \tag{12}$$

which is interpreted as conservation of probability. Usually the variable Y gives the spatial state of the system and the operator $\mathcal{H}$ is a differential operator. For a free particle it is given by the kinetic energy operator

$$\mathcal{H} = -\frac{\hbar^2}{2m}\Delta \tag{13}$$

and Eq. (11) becomes

$$\frac{\partial \Psi(\mathbf{r},t)}{\partial t} = \frac{i\hbar}{2m}\Delta\Psi(\mathbf{r},t). \tag{14}$$

The mathematical analogy between Eq. (10) and Eq. (14) is striking. Our viewpoint is that the SE is a sort of square root out of the ME and we want to show that this analogy is didactically very instructive. Square roots are not innocent though. To mention a few profound differences: the wave function is complex and the time evolution is unitary and not decaying. So while a plane wave decays in the ME, it evolves via a phase factor in the SE.

As Eq. (12) shows Ψ is not a probability but the "square root" of a probability. Also position and velocity become on equal footing. If one is sharp the other is undetermined and in general the product of their uncertanties is given by $\hbar$. Both the ME and the SE have, as linear equations, the superposition principle. One can add wavefunctions in the SE and probabilities in the ME.[2]

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[1] One should not invoke the fact that there is, in the case of the Brownian particle, an underlying deterministic theory in a more detailed description.

[2] This is in fact the basis of the ME, as it is derived with the aid of the Kolmogorov theorem, which states that the transition probabilities from Y' at $t = 0$ to Y at t is the sum of all paths from Y to Y'' at some intermediate time t' (with $0 < t' < t$) and from Y'' at t' to Y at t.

The analogy with stochastic processes is even stronger for many particles. Probabilities for more than one particle are naturally defined in the product space of the particles. The probability on a pair of particles is a function in a six-dimensional space. So the wavefunction of two particles is a function in a six-dimensional space. This makes the analogy with waves even more obscure. For two well-separated particles a new twist of quantum mechanics comes into play. Due to superposition, the probability distribution does not have to be the product of the probabilities on the particles, what one would expect for independent systems. So funny correlations (entanglement) between the particles may arise, which can not occur in the classical ME.

4 Stochastic evolution by path-integrals

An instructive way to appreciate the similarities and differences between the SE and the ME, is to look to the solution of the equations as a weighted sum (integral) over paths. In the ME a path of the system is generated in two steps. From a starting state Y one remains in that state for a time Δt drawn from a probability distribution, related to the diagonal elements of the matrix H. After this Δt one makes a transition to a state Y' based on the transition rate $W(Y'|Y)$. The solution is realized by generating "all" paths and adding the contributions of each path. This procedure resembles the experimental way of finding out probabilities. One can either repeat the experiment in the same circumstances or observe the system for a long time.

The solution of the SE may be generated by the Feynman path integral formalism. All paths going from an allowed initial state to an allowed final state contribute. Curiously enough, the classical path gives the largest contribution. The fundamental difference is that in the ME the weight of a path is essentially positive, while it is not in quantummechanics. The difference between the ME and the SE is that in the former the probabilities are added and in the latter the wavefunctions. So the phases in the wavefunctions, which do not enter in the probabilities, are important in doing the path integral. In the two-slit experiments there are positions on the screen where the two paths destructively interfere.

Of course path integrals are not the only way to obtain the solution of the equation. In some cases an analytic solution is possible. Then path-integrals are a clumsy way to reach the same result.

5 Differences between the equations

To illustrate the differences, we take one of famous experiments in quantum mechanics: the two-slit experiment. An electron is fired at a barrier with two open slits. After passing through the slits, the electron is detected at a screen. According to the ME the probability to arrive at a point at the screen is the sum of the probabilities to pass via one of the slits. Since probabilities are essentially positive all points on the screen have a positive probability for detecting the electron.

However, the screen displays an interference pattern, since in quantum mechanics one must add the wave function and not the absolute squares. The interference pattern is reminiscent of coherent light passing through the two slits. No wonder that the analogy with waves is invoked and that the SE is seen as a *wave equation*. An unfortunate misnomer, suggesting that Ψ is a wave of a field, as Schrödinger originally thought. The analogy is misleading, since one can also detect the passing of the electron through the slits. The outcome is that the electron is always detected as passing through one of the slits, never through both at the same time. Detection of the electron at one of the slits destroys the interference pattern. A wave, on the contrary, interferes with itself, since it is half present at both slits. The result for the electron is not strange if one realizes that quantum evolution is a stochastic process. So if the electron is found at one slit one must continue with that new initial value for the wavefunction.

The fact that the electron sometimes behaves as a particle (when hitting the screen) and sometimes as a wave (when passing through slits) is seen as particle-wave duality, which is lifted by Bohr to an even deeper (and correspondingly less understandable) *Complementarity Principle*. One has invented for the detection of the electron the term *collapse of the wavefunction*. This was confusing: do measurements collapse the wavefunction? Does the wavefunction stop to obey the Schrödinger during the measurement? Following Bohr the answer is no, because the electron interacts with the measuring device and this causes the wave function to collapse. There is a whole industry persuing the unholy route of studying the evolution of the electron in interaction with the measurement device. It is of course interesting to show that, in a weak measurement, the density matrix of the measuring device gradually becomes diagonal, such that it behaves classically. Then the idea is that classical distributions may be "collapsed", but one forgets that it implies a simultaneous collapse of the electron component.

A further analysis would require to include the interaction of the eyes of the observer with the measurement device etc. Ultimately one has to acknowledge the stochastic nature of quantummechanics. No calculation, with all the interaction of the environment included, can tell through which of the two slits the electron passes. Including of the measurement device is also unnecessary, since in a good measurement the transition probabilities are determined by the quantum system (electron) and not by the measurement device. It is the beauty of quantum mechanics that one can show, within the theory, that no hidden parameters exist from which the transitions could be derived.

No one is surprised that a measurement leads to a reduction of the probability distribution. If one detects a Brownian particle, somewhere away from the origin where it started, everyone will continue with that knowledge on the probability distribution. One could call that a "collapse of the probability distribution", but there is nothing physical in this "collapse". In the same way the outcome of the measurement has changed the initial condition in the SE for the probabilities in further experiments.

6 Psychology of the Schrödinger Equation

The stochastic character of quantum evolution is obvious and unavoidable. Anyone has to agree that the outcome of a two slit-experiment is intrinsically unpredictable (no hidden variables). Still the SE is given some status as the exact mechanics of the wave function. Nico van Kampen summarizes his opinion aptly in his fourth theorem (with a slight modification):

Theorem IV: *Whoever endows the wave function with more meaning than is needed for computing transition probabilities, is responsible for the consequences.*

The psychology of the status of the SE is understandable. Quantum mechanics was developped to replace the classical determinisitic mechanics and in fact the quantum equations are mostly constructed from the classical equations by replacing variables, as position and momentum, in a well defined way, by operators. Later on there appeared operators without a classical analog such as spin, (which Dirac derived by studying the square root out of the Klein-Gordon equation!). As the hamiltonian is the basic ingredient in the evolution of the wavefunction, all the experience with hamiltonians, such as conservation laws, can be exploited in the SE.

Stochastic processes were, so far, known to be approximate. One knew the underlying mechanistic motion of the Brownian particle. Moreover the ME cannot be fundamental, since it is not time reversal invariant, while a fundamental theory has to have this property. In fact in quantum mechanics the situation is opposite: the SE is time reversal invariant and von Neumann showed that there cannot be an underlying deterministic mechanics.

There is an intimate connection between quantum and classical mechanics following from the construction of the quantummechanical hamiltonian operator. One can calculate under what conditions the quantum theory starts to coincide with classical mechanics. The cross-over from quantum to classical behavior is controlled by $\hbar$ in combination with other appropriate variables to dimensionless combinations. Sufficiently far beyond the cross-over value, the predicitions of quantum mechanics are, for all practical purposes, the same as that of classical mechanics.

The unitary evolution of the wave function of a quantum system is denoted as *conservation of information*. This becomes a big point in astrophysics: can quantum information escape from a black hole? As soon as the word information is used, the discussion becomes a bit vague. The sort of information carried by the wavefunction is nothing else than a means to calculate probabilities.

Let me use again the two-slit experiment as illustration. One would think that by measuring the passage at the slit, information is gained on the electron. One the other hand information on the electron is destroyed since its wave function “collapses”. I presume that the proponents of the “conservation of information” will argue that the combined system of electron and measuring device evolves unitarily, so total information is conserved. But by unitary evolution the combined system remains forever in a superposition of possible outcomes, while in reality only one happens. So the sort of information carried by the unitary wavefunction of the combination is at odds with the reality.

Suppose that we did a two slit experiment with *classical* particles, in which not only the arrival distribution at the screen is observed, but also through which slit the particle has passed. Then one has two options to calculate the distribution at the screen: use the information of detection at the slits or ignore it. Both lead to the same result. Using it, one can calculate two sub-distributions related each to a passage at one of the slits. The sub-distributions contain more information. Their sum yields, by Kolmogorov's theorem, the same as calculated without the knowledge of passing.

The situation in quantum mechanics is different. Measuring both passing through the slit and arrival at the screen, gives no interference pattern. So, if the passing through the slits is measured but ignored (may be someone else has measured them), one draws the wrong conclusion about the probability distribution at the screen. This is the clue why eaves dropping shows up in transmission of quantum information and not in classical information. It prompts me to formulate the following theorem:

Theorem IVa: *Anyone ignoring information provided by measurements, draws wrong conclusions.*

It is remarkable that even Einstein, one of the founding fathers of Brownian motion theory, had such a trouble accepting the stochastic nature of quantum mechanics. Originally he set up a stochastic interpretation, but later got convinced that "God does not play dice", on which Bohr replied: "How do you know what God does?"

7 Measurements of Quantum Systems

In a discussion on Quantum Mechanics one cannot omit the role of the measurement. The reason is that Bohr, in his famous discussion with Einstein, placed such a large role on the disturbative character of the measurements due to the uncertainty principle. In the quantum world everything fluctuates, so one may ask what the measurement of a property means.

Before discussing this question it is good to note that there are few measurements that probe the wavefunction in a fundamental way as e.g. in the two-slit experiment. The most striking success of quantummechanics is the prediction of properties of matter: the values of spectral lines, the possible elements in the periodic table, the covalent bonds, magnetism and superconductivity, the existence of bosons and fermions and their profound implications. All these properties do not require an interpretation of the wavefunction or a theory of the measurement.

In my opinion there is nothing special about a quantum measurement. Measuring is the art of amplification, in particular for small systems. (Or of minuscule effects, such as measuring gravity waves, although this has nothing to do with quantum physics.) To detect a property of a particle is to amplify maximally the effect of the particle on the measuring device, with the minimal change of the measured property. So the game is to transfer an effect of the particle to the macroscopic world. The trace of an elementary particle in a bubble chamber is a nice example.

Thus the problem of quantum measurement seems to boil down to the question: is there a fundamental difference between the micro and macro world? Quantummechanics tells that there is no fundamental difference, but a cross-over from the micro regime to the macro regime. In the quantum theory one can indicate where the cross-over to classical behaviour occurs. For instance a particle with mass behaves quantum-mechanically, if the mass is of the order of the electron, but classically when it is of the order of the mass of the moon. Sufficiently far beyond the cross-over regime, quantum fluctuations play no role anymore.

It is the cross-over to classical physics that allows for sensible measurements in quantum mechanics. A valuable measurement leaves an imprint in the macroscopic world where values do not fluctuate and are permanent.

The distinction between the quantum mechanical and the classical world, looks controversial but it is a matter on which side of the cross-over one is. So it is in my view a tautology: the classical world is the domain where quantum fluctuations do not matter and values remain "forever" (or are completely determined, such as the position of the moon).

8 Conclusion

By accepting that the quantum evolution is fundamentally a stochastic process, one avoids difficulties appearing in the interpretation of quantum mechanics as the "mechanics of the wavefunction". The mathematical description of a stochastic process is just as well defined as the solution of classical deterministic equations of motion. On the other hand, one should stress, the difference in the rules of calculating transition probabilities in quantum and classical stochastic processes. The fact that superposition holds for the wavefunction and not for the probability distribution, is the origin of the fundamental differences between quantum and classical stochastic processes and all counterintuitive results, as for instance the Bell inequalities, can be traced to this difference.

In order to introduce students to the amazing world of quantum processes, it is wiser to make them familiar with stochastic processes, than to bother them with such vague notions as particle-wave duality or with useless superpositions of micro- and macro objects.

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