

An expository medley on the probabilistic aspects and insights of the Schrödinger systems

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Abstract

Calculus, as a starting point to everyone's study of mathematics, was developed along with classical mechanics. Though not rigorously formulated, the intuition for differential form and infinitesimal motion makes calculus not hard to understand. And hence it does not require great effort to grasp the principles of classical mechanics. However, the situation becomes quite different when it comes to the quantum world. Given a particle system, what of interest is always the physical quantity of this system, such as energy, position, momentum, entropy, etc. But it is no longer straightforward.

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1 Introduction

In this essay, we discuss the mathematical formalism of quantum mechanics and its internal connection to probability theory. Very heuristically, physicists try to explain the uncertainty phenomena which they observed in experiments with mathematical tools known to them. Surprisingly, people find the widely-accepted classical formalism of mechanics could not explain the structure of a particle systems at a microscopic level. Hence the quantum mechanics was introduced after unremitting efforts at the first half of 20th century. The philosophy of quantum mechanics changes our understanding of the structure of atoms and their mutual interactions at a fundamental level. With the exception of gravity, which is described by another beautiful branch of physics, general relativity,

all microscopic interactions so far can be described within the framework of quantum mechanics and its further theory, quantum fields.

Quantum mechanics has become the basis of modern physics. But the investigation of its physical and philosophical purpose has been accompanied with incessant debate; and there has been no unanimously accepted perspective. The quantum formalism is very hard to comprehend, partly due to its distant formalism to Newtonian and Lagrangian physics, and partly due to its adoption of abstract mathematics.

Calculus, as a starting point to everyone's study of mathematics, was developed along with classical mechanics. Though not rigorously formulated, the intuition for differential form and infinitesimal motion makes calculus not hard to understand. And hence it does not require great effort to grasp the principles of classical mechanics. However, the situation becomes quite different when it comes to the quantum world. Given a particle system, what of interest is always the physical quantity of this system, such as energy, position, momentum, entropy, etc. But it is no longer straightforward to *compute* these quantities of interest from the given particle system. Instead of simply calculating position and momentum like in the Newtonian physics, such operation of computing itself has non-trivial meaning: The action to compute certain physical quantities from a particle system is now regarded as an operator acting on a Hilbert space. This Hilbert is intuitively the space of the total information of the given particle system. For example, the information of all the relevant physical quantities of this given system is stored in some fixed Hilbert space

$$\mathbb{H} \equiv \text{span}(e_1, \dots, e_J),$$

so does the information of the system's time evolution. On the other hand, any observation to this space \mathbb{H} of information becomes an operator X , which we call *observable*, on this Hilbert space \mathbb{H} . Remark that all realizable observables correspond to a Hermitian operator, i.e.

$$X^\dagger = X$$

After proposing the information Hilbert space \mathbb{H} , the total information of any given particle system is equivalent to the particle system itself, because an object is essentially the collection of its total information. Hence from now

on, we will use $|\psi\rangle$ to denote the vector of the information with respect to the given particle system, and $|\psi\rangle$ can also indicate the particle system itself without any confusion. Some physicists call this $|\psi\rangle$ the wave vector, because its time evolution satisfies the well known Schrödinger equation which is a complex wave equation in the language of partial differential equations. Notice that time evolution is also a very special type of operator acting on the information vector $|\psi\rangle$, which is a unitary operator on \mathbb{H} and can be written as

$$\mathcal{U}(t) = e^{-i\mathcal{H}t/\hbar}$$

where \mathcal{H} is the Hamiltonian, or the energy observable, of the system and \hbar is the Planck constant. And its Schrödinger equation can be written as

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} \mathcal{U}(t - t_0) |\psi(t_0)\rangle = \mathcal{H} |\psi(t)\rangle.$$

From the above equation, one can see the partial derivative with respect to time t , so the Schrödinger equation is really the equation of motion for the given particle system $|\psi\rangle$. One can also inspect the complex identity $i \in \mathbb{C}$ from the above equation. Indeed, the state vector $|\psi\rangle$ is a \mathbb{C} -vector. Many people confuse about such complex parameter, since in real world there is no complex number. However, such formalism does not hurt the faithfulness of quantum mechanics. The complex numbers only appear as the *amplitude* of a state vector $|\psi\rangle$ rather than the realization of its observables.

The essentials of quantum mechanics lies in its probabilistic perspective to particle systems. The axiom of localization is a prerequisite to classical mechanics: all particles are simultaneously localized to a point in the phase space, which is usually \mathbb{R}^{6N} where N denotes the particle number and 6 denotes the sum of position and momentum coordinates. On the other hand, quantum mechanics assumes that all particles do not delocalized to points in the phase space simultaneously; they spread out the whole space \mathbb{R}^3 with a particular probability distribution. And any physical observation, which corresponds to a Hermitian operator on \mathcal{H} , can be seen as a multivariate random variable: its realization depends on whatever events that occur.

Now that the formalism of quantum mechanics forces us to step into one of the richest realm of pure and applied mathematics, *probability theory*, it is good timing that we begin some discussion on this part of mathematical theory and

try to give an overview. The evolution of theoretical probability was based more on intuition and its interactions to other sciences than some axiomatic principles during its early but polished development. In the year 1933, the great mathematician A. N. Kolmogorov provided an rigorously written axiomatic foundation for probability theory, which now becomes the most universally accepted model. But of course, there have been many different approaches to the theory of probability. Nonetheless, we will follow the path of A. N. Kolmogorov, whose framework has been tested by time and practice. The basic intuition in probability is the idea of randomness. There are realizable experiments whose results are not predictable and can only be estimated after performing them and then observing the statistics of the outcomes. The easiest and most familiar example is the tossing of a biased coin and the throwing of a biased die with N faces. In the first experiment, the result can either be a head with probability p or a tail with probability $1 - p$. In the second example a score of any integer k from 1 through N can be attained with probability p_k such that

$$\sum_{k=1}^N p_k = 1.$$

Indeed, these two realizable experiments are examples with a finite number of discrete alternate outcomes. It is then natural to conceive experiments whose outcomes are countably infinite or even continuous.

Abstractly, one could rephrase as follows. There is the *unobserved* ground probability space Ω containing all possible outcomes. Certain nice subsets of Ω are called events, and each one of them corresponds to a collection of possible outcomes. If the outcome ω is contained in one of the nice subsets $A \subseteq \Omega$, then the event A is said to have occurred. The readers would then naturally expect that probabilities should be associated to a *probability function* $f(\omega)$ which indicates the probability of the outcome $\omega \in \Omega$. In the case of the aforementioned biased coin toss, we could write $\Omega = \{H, T\}$ and

$$f(H) = p \quad \text{and} \quad f(T) = 1 - p.$$

Or in the case of a die where $\Omega = \{1, 2, \dots, N\}$ and

$$f(k) = p_k \quad \text{for all } k = 1, \dots, N.$$

Since probability is naturally conceived to be normalized, certainty then corresponds to probability 1. One then expects

$$\sum_{\omega \in \Omega} f(\omega) = 1.$$

It would then be problematic when Ω is uncountable, say, a continuous interval $[0, 1] \subseteq \mathbb{R}$. There is no reasonable method to sum an uncountable set of real numbers. The above remark then implies that it might not be possible to start with assigning probabilities to discrete outcomes before building any meaningful theory. An alternative narrative is to begin with the idea that probabilities are already defined for some nice events. In this situation, the probability $\mathbb{P}(A)$ is defined for a class \mathcal{B} of nice events in Ω . To avoid any nuisance, it is reasonable to require that the class \mathcal{B} of nice events should satisfy some properties. First, the whole unobserved ground space Ω and the empty set \emptyset are in \mathcal{B} . Second, for any two events A and B in class \mathcal{B} , their intersection $A \cap B$ and their union $A \cup B$ are in class \mathcal{B} . Third, the complement $\Omega \setminus A$ for any arbitrary $A \in \mathcal{B}$ is contained in \mathcal{B} . Another condition that is somehow more technical but necessary from a mathematical point-view, is that of a countable additivity. The class \mathcal{B} , in addition to satisfying the above three conditions, has to be closed under countable union and countable intersection. Such a class \mathcal{B} is called a σ -field. And the so-called *nice* event A is simply an arbitrary subset of Ω contained in the class \mathcal{B} . And this is the most essential fundamentals to a fantastic realm of mathematics, *probability theory*.

In realistic situations, hardly do we need explicitly specify the ground space Ω and hence the phrase, *unobserved*. Indeed, probability theory provides the necessary tools to describe *randomness* in a rigorous fashion. However, the mathematical language of probability theory cannot, and will not, tell what is a genuine randomness: anything satisfying the axioms proposed by A. N. Kolmogorov can be rephrased into a stochastic system, either an algebraic lattice or a topological space. That said, they are but self-contained logic. The satisfactory explanation to *randomness* should be sought from physics. The principles of quantum mechanics support the realization of a random atomic fluctuation. They endorse the idea that a probabilistic distribution like a wave spreading over the spacetime is the nature of particles. Indeed such distributions admit a time evolution, and our observations on them are simply realizations of a certain probability event.

There has been intense debating around the mathematical interpretation of the quantum observations. Some physicists argue that [4] the particular observed value to a certain physical quantity is due to the *collapse* of the wave, or information, vector $|\psi\rangle$ of the particle system. However, after taking a careful look, one could comfortably reconcile with the idea that the wave $|\psi\rangle$ is actually equivalent to the probability distribution to the information encoded by the particle system. And then we could use the theory proposed by A. N. Kolmogorov to rigorously investigate the spreading and collapsing of the quantum waves. Indeed, without a rigorous formalism, contradictions often arise due to the lack of a precise language. And via introducing the theory of probability invented partially by A. N. Kolmogorov, certain confusions in quantum mechanics could be clarified without debate, which will ultimately lead us to a deeper understanding of theoretical physics and the laws that govern our world.

On the other hand, [9] quantum mechanics is still far from complete even with the help from probability theory. Indeed, quantum physics has fixed the issue of particle localization from classical physics. The quantum particle waves $|\psi\rangle$ spread in the space \mathbb{R}^3 in the sense of a probability distribution, and hence its localization is generally impossible. This is remarkable progress. But there are still other serious issues to be discussed. For example, the red shift of the galaxy and stars. Such issues relate to the dilation and compression of space-time, when the observers are no longer static at their coordinates. To put it less formal, there is no notion of a consistency and invariance of time in the universe. At different spacetime coordinates, time runs at different *speed*. And the mathematical notion of a *light cone* prevents a closed spacetime curve, and hence prevents a genuine time travel. Such issues are not discussed in quantum physics, and cannot be worked out with probability theory. Actually, the discussion of such issues has led to the development of a totally different branch of physics: General Relativity. And this realm relies on Riemannian Geometry, whose [3] object, smooth [5] manifold, suits the topic of spacetime. Nonetheless, the realm [8] of General Relativity is also flawed: it does not encode the probabilistic description of a particle system [7]. Indeed, in General Relativity we still live with classical particles, which is not completely compatible with the quantum world.

However, the community of physicists and mathematicians have not been idle. They made incessant effort to combine Quantum Mechanics and General Relativity. Some of their models and results are included in the topics of Quan-

tum Field Theory and Quantum Statistical Physics. But both branches reaches mathematical contradictions and the problems could not be solved easily.

Still, the realm of probability theory has shed light on some of their progress to combine quantum mechanics with other advanced branches of physics. One sub-realm of probability theory [6] is called *Random Geometry*. Those mathematicians in favor of this realm study the stochastic evolution of planar random processes and investigate their conformal invariance properties. Of all these random objects, Brownian motion is one of the most studied processes: it has strong Markovian property and Hölder regularity to its sample paths. Indeed, people from random geometry are currently using discrete lattice models, such as harmonic crystal, and continuous planar processes, such as Schramm–Loewner evolution, to investigate the new frontier of Liouville Quantum Gravity. This realm is very promising, even though it only explains the stochastic and relativistic evolution to the 2+1D spacetime. Hopefully in the future, the probabilistic approach to Liouville Quantum Gravity will eventually help us to understand [2] our genuine four-dimensional spacetime.

Indeed, ever since the first half of the last century, probability theory has become essentially important in the rigorous formalism of quantum mechanics. And without probability theory, the notion of wave collapsing would not be properly defined, not to mention its future discussion. Even though there are still open problems in mathematical quantum mechanics, despite that many mathematicians regard such open problems not so important, these mathematical issues are still essential to the further development of a more precise, or even [1] rigorous, language of theoretical physics and its frontier.

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