The Superposition Principle in Quantum Mechanics - did the rock enter the foundation surreptitiously?

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The superposition principle forms the very backbone of quantum theory. The resulting linear structure of quantum theory is structurally so rigid that tampering with it may have serious, seemingly unphysical, consequences. This principle has been successful at even the highest available accelerator energies. Is this aspect of quantum theory forever then? The present work is an attempt to understand the attitude of the founding fathers, particularly of Bohr and Dirac, towards this principle. The Heisenberg matrix mechanics on the one hand, and the Schrödinger wave mechanics on the other, are critically examined to shed light as to how this principle entered the very foundations of quantum theory.

I. INTRODUCTION

The superposition principle for quantum states can be said to be the very bedrock of quantum theory. To paraphrase Dirac, \textit{This principle forms the fundamental new idea of quantum mechanics and the basis for the departure from classical theory} (Dirac in the first edition of his book [1], \S 2, p.2). While commenting on the new laws required for the description of atomic phenomena, he emphasized that \textit{One of the most fundamental and most drastic of these is the Principle of superposition of states} (see \S 2 p.4 of [2]). Dirac went as far as to assert: \textit{’One could proceed to build up the theory of quantum mechanics on the basis of these ideas of superposition with the introduction of the minimum number of new assumptions necessary.’} (p.16 of \S 6 of [1]).

Immediately after the discovery of matrix mechanics and wave-mechanics [3], while Heisenberg’s uncertainty principle [4], Bohr’s complementarity principle [5], and Born’s probability rule [6] paved the way for a lasting physical interpretation of quantum theory, an equally important parallel development was the work of Dirac [1, 2, 7–9] who focussed on the nature of the quantum state. This eventually culminated in the formulation of the principle of superposition of states.

A. The Superposition Principle for Quantum States

Though it is customary to view the superposition principle within the mathematical framework of Hilbert Spaces, it is instructive to recall its purely operational meaning as elaborated by Dirac. He gives a very broad characterization of states as the embodiment of the collection of all possible measurement outcomes. Then superposition of states according to him is as follows: if A is a superposition of two or more states, say, B, C, ... every outcome of a measurement on A must also be a possible outcome of the same measurement on any of B, C, .. (p.15 \S 6 of [1]). Though this characterization of superposition may seem \\textit{ad hoc}, the customary, Hilbert Space based view is completely equivalent to it. but the Dirac characterization has the advantage of being purely operational and applicable even if there is no underlying Hilbert space structure.

Being about superposition of states, it is like no other superposition principle in either physics or mathematics. Examples of the latter are superposition of sound waves, of electromagnetic waves, of vectors etc... This was most emphatically stated by Dirac himself: \textit{’It is important to remember, however, that the superposition that occurs in quantum mechanics is of an essentially different nature from any occurring in the classical theory’} (The italics are Dirac’s). He further stated that \textit{The analogies are thus liable to be misleading}(p.11 \S 3 of [1], and p.14 \S 4 of [2]).

In the current formulation of quantum theory, this principle is given a precise mathematical meaning through the Hilbert Space formalism(actually one needs the density matrix formalism for a more satisfactory description, but that discussion is somewhat beyond the scope of this presentation). According to this, every physical state is representable by a family of vectors in a Hilbert space. A typical such vector is symbolically denoted by \textit{\psi}. Vectors belonging to a given family differ only in phase. This is the so called ray representation of states. If \textit{P1}, \textit{P2} are two distinct physical states meaning their rays are distinct, and if \textit{\psi} belongs to the ray of \textit{P1} and \textit{\psi} belongs to the ray of \textit{P2}, the principle of superposition of states states that the \textit{complex linear superpositions}

\[ \psi = \alpha \psi_1 + \beta \psi_2 \]

also represent quantum states of the system.
B. Illustration through an artistic example.

Imagine a rose atom which exists in only two colour states, say, $|\text{red}\rangle$ and $|\text{yellow}\rangle$. According to present day quantum mechanics, this means that if you observe colour, the outcome will be red if the system was in state $|\text{red}\rangle$, and yellow if the system was in $|\text{yellow}\rangle$. It should be emphasized that these rules of quantum measurements are themselves intimately tied to the superposition principle. Now, according to the principle of superposition of states, linear combinations of the type (and in fact infinitely more)

$$|\text{good}\rangle = \frac{1}{\sqrt{2}} \{ |\text{red}\rangle + |\text{yellow}\rangle \} \quad (2)$$

and

$$|\text{bad}\rangle = \frac{1}{\sqrt{2}} \{ |\text{red}\rangle - |\text{yellow}\rangle \} \quad (3)$$

also represent legitimate quantum states!

This immediately leads to the problematic question “What will be the outcome of a colour measurement on these new states?” If the measurement scheme follows the standard lore, the outcome can only be red or yellow, it can not be any mixture of these colours. The answer is that on a single copy the outcome for both the new states will be randomly red or yellow. Further, if the outcome is yellow, the state after measurement is $|\text{yellow}\rangle$ etc. That on an ensemble, the probability of each outcome is 50%. This is a generalization of the famous Born probability rule given originally in the context of collisions, an essential pillar of quantum theory. It should now be clear why no other superposition principle has the same depth as the principle of superposition of states.

C. Superposition principle and Heisenberg uncertainty

It is easy to invert the previous combinations, to get

$$|\text{red}\rangle = \frac{1}{\sqrt{2}} \{ |\text{good}\rangle + |\text{bad}\rangle \} \quad (4)$$

and

$$|\text{yellow}\rangle = \frac{1}{\sqrt{2}} \{ |\text{good}\rangle - |\text{bad}\rangle \} \quad (5)$$

It turns out that the states $|\text{good}\rangle, |\text{bad}\rangle$ have definite values of some other attribute which we could call smell! Suppose we start with $|\text{good}\rangle$ and make a colour measurement. The outcome will be red or yellow with equal probability. If it is red, the state after the measurement is $|\text{red}\rangle$, and likewise for the outcome yellow. Let us say that the outcome is red. Now imagine a smell measurement on the system. Because the state after the last measurement i.e $|\text{red}\rangle$ is an equal superposition of the good and bad smell states, the outcome will be one of these randomly and with equal probability. Therefore, even though we started with a state whose smell was certain i.e good, an intervening colour measurement has completely destroyed this certainty! Instead, the smell information has become totally unpredictable! This is the inherent indeterminacy of quantum theory. This is also a demonstration that the pair of observables colour, smell are mutually incompatible. Existence of incompatible observables is the essential content of the Heisenberg Uncertainty Relations.

D. Superposition principle and complimentarity

The superposition principle incorporates complimentarity in a natural way. To see this, note that a given state $|\psi\rangle$ can be equivalently expressed, in the context of the so called wave and particle aspects as

$$|\psi\rangle = \sum_i \alpha_i |W_i\rangle = \sum_i \beta_i |P_i\rangle \quad (6)$$

where $P_i, W_i$ are just a symbolic shorthand for the particle and wave aspects. Bohr’s great vision lay in the recognition of the role of measurements in quantum theory. We immediately see the superposition principle as an embodiment of this i.e the same $|\psi\rangle$ above reveals either the $P_i$ or the $W_i$, depending on the measurement scheme whose outcomes are one or the other. Bohr,
in his Como lecture [5], recognized another face of complementarity whereby states are superpositions of what may be called classically incompatible states. For example, in the rose atom case, the two colors are classically distinct and mutually exclusive. The states |good⟩, |bad⟩ are indeed such superpositions of classically incompatible states.

In summary, we see the superposition principle as the glue, in a precisely stated manner, of the three milestones that underlie the physical interpretation of quantum theory, namely, the uncertainty principle, complementarity principle and the probability interpretation. It should be emphasized that this is so only in conjunction with suitable rules for quantum measurements. Such rules are anyway essential for a consistent interpretation of the superposition principle itself.

II. WHY THE ROCK?

In addition to its central role elaborated above, it turns out that the principle is rather rigid. All efforts to modify it have resulted both in serious mathematical as well as conceptual difficulties. From the mathematical side the chief difficulty is in finding a smooth deformation of the Hilbert Space structure. From the conceptual side, difficulties include apparently unphysical effects like superluminal signal propagation etc. [10–12]. Even the probability interpretation may itself become very fragile as a result of such modifications. It is therefore apt to call the principle a Rock!

It should however be noted that many of these attempts at modifying quantum mechanics still maintain some essential features of the present theory while modifying some other features. These failures may only be an indication that if at all, the whole structure may have to be overhauled. Nevertheless, from the perspectives of a satisfactory scientific method too, it is important to find such modifications. It is only when one has such a broader framework that tests of quantum theory become complete. It is also important to have the conceptual space to handle any future empirical developments.

A. How did the rock enter the foundation?

Because of the central nature of the superposition principle, as well as its extreme allergy to any change, it is important to understand its genesis. One needs to get a historical as well as a conceptual perspective on it. History of an idea is as important as the idea itself. In particular, it is of value to know the attitude of the founding fathers towards such a deep and central principle. Such an exercise is not just of historic value, it may prove critical should a need arise in the future to modify this principle. With that spirit, I have tried to uncover the development of this concept during various stages of the creation of quantum theory. I have mainly used Bohr’s Como lecture [5], the first two editions of the book by Dirac [1, 2], the early papers of Dirac [7–9], the original papers on the discovery of quantum theory [3], including the Bohr triology [14], the two papers by Born on the probability interpretation [6], Heisenberg’s uncertainty paper [4], as well a paper by Schrödinger [13] that played an important role in Bohr’s analysis of the uncertainty relations. Thanks to Bacciagaluppi and Valentini [15] the proceedings of the famous Solvay meeting in 1927 was available in english. Initially I went carefully through this very valuable source but did not find much explicit reference to the broader nuances of the superposition principle there.

B. Early Views

Before undertaking this exercise, it is worthwhile to look at some early attitudes towards the superposition principle. As articulated by Bohr on many occasions, and as explicitly elaborated in his Como lecture [5], the superposition principle was viewed essentially in a wave theory perspective. This was manifest when Bohr sought to correct Heisenberg’s initially flawed thinking on the uncertainty principle. Bohr, following Schrödinger [13], had sought to view states with sharply localized position as a superposition of plane waves, the latter corresponding to states of definite momentum. But I had earlier said that the principle of superposition of states is unlike any other superposition principle, including the one in wave mechanics. The subtlety here is that the superposition of waves of different wavelengths should really be understood as a superposition of states and the probability interpretation invoked to understand the outcomes of measurements. This latter element is not present in the classical wave superposition. Thus it is really the superposition principle for states which is at the heart of Bohr’s explanation of the uncertainty principle on the basis of complementarity. In the discussions at the Solvay meeting of 1927 too (following the report of Bragg on X-ray scattering) [15], superposition principle was essentially seen as the manifestation of wave behaviour.

C. States in quantum theory

It is clear that in understanding the genesis of this principle, it is first necessary to understand the genesis of the notion of a quantum state. It is often implicitly understood that the superposition principle follows simply on the basis that the Schrödinger equation is linear. This is not quite so. All that the linearity of the Schrödinger equation provides is a superposition principle
for wavefunctions. This does not, however, immediately translate into a superposition principle for states. This is because in the early stages it was not obvious that every wavefunction should be associated with a physical state. Bohr, in his Como lecture, does provide an interesting example of how superposition of the wavefunctions of two stationary states also represents a bona fide physical state. It should also be stressed that at the time Schrödinger proposed his wave equation, Solitons (originally discovered by Scott Russell in 1834) were well known, and there was no fundamental justification for a linear wave equation. In fact we shall see that even in Heisenberg’s matrix mechanics, the nature of quantum states was obscure in the beginning. We shall return to these points soon.

D. The Bohr Atom: the seed of the banyan tree

The idea of a quantum state can rightly be considered to have been born with the Bohr model for atoms. The central concept there was that of the stationary states. The states of the Bohr atom were truly schizophrenic - one part, the stationary states, looking boldly into the future, surviving all the epoch-making developments of quantum theory. The other, the orbits, looking embarrassingly into a classical past! Taking the legitimate point of view that the stationary states are quantum states, a number of fundamental questions would arise regarding the nature of the quantum states. The most important of these would be “Do the stationary states represent ALL the quantum states?” The Bohr theory had no ready answers to this important question.

However, even at that stage, Bohr’s correspondence principle would have something very relevant to say. The ‘number’ of classical states of a Keplerian system are far more than the ‘number’ of stationary states of the Bohr atom. This means there ought to be many more quantum states than the stationary states. The question is, What are these additional states? It is clear that there was nothing even remotely like the superposition principle in the Bohr model. Even the remarkable extensions by the Bohr-sommerfeld model did not change this situation. However, an interesting clue in that direction was revealed by the analysis of the Stark effect within the Bohr-Sommerfeld theory. Starting with zero electric field in certain stationary states, turning on the electric field and eventually turning off the field would not return the atom to the starting state. The eventual resolution of this was to be found in the superposition principle applied to the degenerate states of the atom in zero field.

E. States in Heisenberg Matrix Mechanics

The next revolutionary development was Heisenberg’s Matrix Mechanics. While this retained Bohr’s stationary states, it completely did away with the classical trajectories. Instead, it associated the classical observables like position and momentum with matrices whose rows and columns were labelled by the stationary states. Thus, as far as the question of the totality of quantum states was concerned, the Heisenberg matrix mechanics had gone no further than Bohr’s atomic model. As mentioned before, Bohr, in the Como lecture had discussed how superposing the wavefunctions of two stationary states of an atom led to a description of the physical circumstance of radiating charges. Though a pointer in the right direction, this was insufficient to arrive at the principle of superposition of states in its entirety.

Soon after Heisenberg’s paper on matrix mechanics, Dirac made an astute, and fundamental, observation. He noted that labelling the matrices only by the stationary states was unnecessarily restrictive. He proposed that it was sufficient to have the observables obey the same algebraic properties of matrices and that the labelling could be arbitrary. This observation is what really opened up the space of physical states eventually, though not immediately. This was also the proposal of Born and Jordan, and Born, Heisenberg and Jordan. But it is also this proposal that put quantum theory into the linear straitjacket! The arbitrariness in the labelling of the matrices meant that vectors used for labelling can be transformed among each other (hence the name transformation theory). In the original Heisenberg formulation, these vectors corresponded to the stationary states. Hence they represented quantum states. Now the question is whether every vector into which the stationary state vectors are transformed also represented quantum states? This is analogous to the question raised previously as to whether every superposition of Schrödinger wavefunctions represents physical states.

What led to a clarification of this question, and eventually to the superposition principle, was a critical observation by Dirac. His position was based on the centrality of the eigenvalues of the Hamiltonian(energy) in matrix mechanics, namely, that the eigenvalues of the energy matrix in the stationary states were to be interpreted as the value of energy in the corresponding stationary state. What gave support to this rather mathematical conjecture was the empirical success in identifying the eigenvalues with the terms of the spectra of atoms. Another important property of the Hamiltonian matrix, noted in Heisenberg’s matrix mechanics paper, was that it was Hermitian.

Dirac’s crucial clarification is to be understood in two parts. In the first part, Dirac dealt with the so called constants of motion. In the version of matrix mechanics elaborated by Dirac, these were constant matrices. Extrapolating the hermiticity requirement to these constant matrices also, Dirac made the suggestion that their eigenvalues in the stationary states are to be interpreted as the values of these constants of integration in the corresponding stationary states. This was consistent because the matrix mechanics required these matrices to commute with the Hamiltonian matrix (see eqn.(11) of §2 of [9]). Unlike the empirical support for the eigenvalue idea for the Hamiltonian, the eigenvalue idea for observables did not have such an immediate empirical support. The
second part consists of the reasonable extension that just as stationary states were states with definite values of energy, there ought to be quantum states with definite values for a set of compatible observables, even in the general case when these are not constants of motion.

III. BACK TO THE SUPERPOSITION PRINCIPLE..

It was then natural to consider the so called eigenstates of any observable, say, position(or momentum), as also physical states. The principle of superposition of states then follows as a consequence of the transformation theory, which had only remained as a mathematical property till then. One thus ends up with many more physical states than the stationary states. The irony is that now one ends up with far too many states than the totality of classical physical states!

A. Dirac and the superposition principle

Dirac, more than anyone else, dwelt at length on the meaning of the superposition principle in quantum theory, and commented both extensively and emphatically on it. This is evident from his masterly exposition of the principle in the first and second editions of his classic book on quantum mechanics \[1,2\]. In them, he explicitly showed the deep connection between the superposition principle and the foundational aspects of quantum theory like indeterminacy, compatibility of observables etc. He saw in it the fountainhead for a systematic and logical exposition of quantum theory, though he admitted that that may not be the most convenient road to take. He even sought to determine the dynamical laws governing quantum mechanics through their consistency with the superposition principle.

B. More of the principle..

The ramifications of this principle in later developments of quantum theory have been astounding. With the development of areas like high energy physics, superposition principle plays a central role in systems with spin, isospin and other exotic quantum properties. There are no descriptions for them with anything remotely resembling waves in three-dimensional space and superposition understood in a wave theory context are irrelevant for them. Nevertheless, the principle of superposition of states has given completely successful description of them. Entanglement, a key ingredient in the fast developing areas of Quantum Information and Quantum Computing, is a direct consequence of the superposition of states. Early sources of the conceptual challenges to quantum theory like the EPR paradox, and the Schrödinger-cat paradox are all based on entanglement.

IV. SURREPTITIOUS OR NOT?

Despite its centrality in quantum theory, the development of the principle of superposition of states appears to have been driven more by reactions to various local issues. Every stage of this development, like the basis independence prompted by the transformation theory, the legitimacy of including eigenvalues and eigenfunctions of generic observables etc. though very reasonable, do not seem inevitable. The entire development can be said to be more of an evolution rather than a revolution! This is in stark contrast to other great principles like the ones in special relativity, general relativity etc. In short, its entry into the very foundations can be considered somewhat surreptitious. Should future experiments belie the expectations of this principle, one may need the great intuitive powers of Bohr, Heisenberg, Schrödinger and Born, as well the meticulous systematics of Dirac and the critical creativity of Einstein to get past the crisis!

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