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Revisiting Bohmian Quantum Mechanics with Quantum Trajectories

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Abstract:
The ontological interpretation of Bohmian quantum mechanics, through a particle's visual trajectory of motion, reconstitutes realism and determinism (and thus causality) in a quantum system. There also exists a similar but distinctive class of interpretation under Bohmian quantum mechanics, called the hydrodynamical interpretation. Here, the trajectories of the probability fluid flow play a significant computational role. The flow of the probability density visually helps chemists and engineers to solve the corresponding quantum hydrodynamical equations of motion. This particular computational scheme for the numerical solutions is called 'the quantum trajectory method.' The success of the quantum trajectory method demonstrates the power of visual illustrations and metaphors in representing and analyzing quantum systems.

Keywords: *History and philosophy of science, Bohmian quantum mechanics, ontological interpretation of quantum mechanics, history and philosophy of quantum mechanics*

1. Introduction

Some of the main ideas behind quantum mechanics are indeterminism, the correspondence principle, the statistical interpretation of the wave function, and the complementarity of quantum phenomena. In particular, the familiar physical properties of particles' having a definite position, velocity or energy etc. are all denied in quantum mechanics. These intrinsic features of quantum systems emphasize that causality and determinism have no place in quantum mechanics. So, quantum mechanical processes are not thought to be composed of causally-connected visual sequences in space and time, which means that quantum particles do not follow any definite trajectories in their dynamical motions. Thus, quantum mechanics as we know it prohibits a comprehensible (that is, understandable in terms of our 'customary intuition') account on the quantum world through direct visualization of fundamental phenomena. Consequently, our 'customary intuition' and the 'benefit of direct visualize ability' from classical mechanics are fully replaced by its mathematical formulation. In other words, in understanding the quantum world, our intuitive and perceptual metaphors and illustrations are not considered to be 'illuminative' or 'functional,' and sometimes even taken to be 'trash' at least by Werner Heisenberg.

2. Different Interpretations of Quantum Mechanics

Ever since the birth of this Copenhagen interpretation, philosophers and physicists have tried to introduce different interpretations of quantum mechanics, not by questioning the general validity of its mathematical formalism, but rather by rearranging some of the mathematical formalisms so that new physical insights into it can be achieved. For example, Hugh Everett (1957)'s relative-state formulation was an attempt to explain why observers get determinate measurement records, which further led to the many-worlds interpretation (e.g. Barrett 1999). On the other hand, The GRWP theory (Ghirardi, Rimini and Weber 1985, 1986) was a mathematical attempt to introduce an additional 'noise' term to the Schrödinger equation. These new interpretations were all designed to tackle the measurement problem in one way or another.

When it comes to their usefulness in application, however, their achievements cannot possibly be compared with the successful empirical outcomes the standard quantum mechanics has shown. Nonetheless, for example, the many-world interpretation seems to work very well with the physical situations caused by the environmental decoherence. According to this interpretation, the environmental interactions in a surrounding neighbor of a laboratory setting can effectively erase a quantum superposition, realizing a particular measurement outcome out of all possible ones. The existence of many coexisting worlds with ours thus provides an effective 'intuition pump' for understanding the interaction processes with the environment in modern condensed matter physics. This many-world concept could generate further experimental developments in the future. On the other hand, according to the GRWP theory, there is a cosmic background of 'noise' from which the basic equation of quantum mechanics should be modified. This could also lead to a different calculational outcome in a given problem in the future.

3. Visualization on Quantum World

However, all of these interpretations do not necessarily increase the 'benefit of direct visualizability' based on our 'customary intuition,' any more than the standard quantum mechanics. This 'direct' visualization is critical for stimulating further usefulness in its application, which then, as claimed in this work, works as an 'intuition pump' for the quantum computability and some possible generation of new experimental outcomes. In fact, a desire for visualizable models or causal explanations is as an essential part of any scientific endeavors, and the world often becomes comprehensible in terms of our inherent patterns of thought through visualizing fundamental phenomena, according to Cushing. In other words, the mathematical formulation itself cannot possibly replace the perceptual metaphors and intuitive illustrations about the world, that is, they cannot be simply abandoned as something 'trash.'

The reason is rather obvious. The cognitive importance of illustrations and metaphors occupy a central place in the course of developing scientists' research as in Heller's and Feynman's research. They convey cognitive information for which verbal and mathematical descriptions have a limited capability of conveying a cognitive meaning. These forms of representation then perform diverse and unique cognitive (and social) functions to provide better understandings of the theories and there is no predetermined single function for a given representative form. They include [1] mathematical notations or formalisms, [2] illustrations, graphic models, and visual images, and [3] a whole body of metaphors and verbal analogies (Cat, 2001). Especially, when representative forms are consistently coupled together, they give rise to a series of powerful constructive intuitions and further research motivations for the model, eventually motivating some experiments. This is due to the fact that those illustrative and metaphoric quantities could call to mind more concrete and clear conceptions of further experimental (and theoretical) developments (Cat, 2001).

4. Bohmian Quantum Theory

In this respect, the Bohmian ontological quantum theory of motion combines the accurate quantum mechanical predictions with 'functional' visual illustrations and metaphors on the quantum processes. These visual illustrations and metaphors are not cosmetic or ornamental embellishments of the mathematical formulation. Rather, they are utterly indispensable; they provide more effective computability through a visual insight, thus working as an 'intuition pump' on the quantum dynamical processes. That was possible because, under this Bohmian formalism, each particle always has a definite momentum and a position throughout its entire deterministic motion, allowing us to see what happens in the dynamical process, while the standard quantum mechanics just calculate the final outcomes (i.e. the expectation values) of the dynamical processes. Currently, the 'quantum trajectory method' in Madelung-Bohm-Takabayasi hydrodynamical formulation seems to pave a way for new and important experimental (and computational) works in chemistry and engineering. These (often simulated) experimental works motivated by Bohmian mechanics establish a claim that successful computability could potentially lead to a prolific generation of empirical outcomes.

According to Jordi Cat (2001, p.410), the history of the 19th century electromagnetism also demonstrates that the cognitive importance of scientific illustrations and metaphors should not be dismissed as merely an ornamental or an educational tool. They can occupy a rather central place in research developments, in technical writings and addresses to professional and general audiences. As already claimed, the 'quantum trajectory method' can also be an example of showing this cognitive importance of scientific illustrations in computational quantum chemistry. The method involves a set of the hydrodynamical equations of motion for the probability density 'fluids' with those (probability density) trajectories. The trajectories are 'guiding lights' for the entire hydrodynamic scheme, providing a visual direction of the propagation of the fluid itself. In this method, the actual (and current) locations of the trajectories are used to calculate a new quantum potential which in turn derives the propagation of the trajectories sometimelater (Wyatt, 2005). Although the trajectory itself may not be taken literal or empirical, it is nonetheless a powerful computational tool because the time dependent 'flow' of the probability density can be described in almost the same way as in the flow of classical fluid. This quantum trajectory method thus has greater computational/cognitive advantages since it visually illustrates how the fluid elements are being propagated, based on the illustrative and metaphoric quantities, such as 'trajectories' and 'probability flows.' So, 'metaphors remind us what a certain quantity may be more clearly conceived as, by pointing to a property of the illustrative model' (Cat, 2001, p.425). Therefore, it strongly appeals to some computational chemists and electrical engineers, who have a high priority for such visual illustrations.

However, among philosophers of physics, this hydrodynamical method has not yet been recognized either as an independent interpretation, or as an effective computational scheme with many successful applications. This may be due to the philosophers' stereo-typical attitude toward those subject matters in chemistry and engineering, which are to them considered to be more 'practical' (or 'dirty') than 'conceptual' (or 'clean'). Consequently, to many of the philosophers, the subtle (and distinct) difference between the hydrodynamical formulation and de Broglie-Bohm ontological interpretation has not yet been appreciated.

Although the quantum trajectory is not to be taken literally and empirically, it is still *a powerful imaginary computational tool*. Unlike many of the philosophers, to those computational quantum chemists and engineers, their concerns are not the issues of realism and ontology for the trajectories, however. As Jordi Cat (2001) would argues from his study on Maxwell, the dichotomy between realism and instrumentalism seems inadequate for making sense of the chemists and engineers' position. Their pattern of commitment to metaphorical and literal understanding of theoretical terms such as the 'trajectories', the 'probability density fluid', and the 'quantum potential' is rather irregular and diverse both over time and within each separate discussion. This diversity leaves the realism/instrumentalism dichotomy with little use for insight.

5. Applications

To the chemists and engineers, in conclusion, the Bohmian trajectory model is an effective and pragmatic middle path to accommodate both quantum and classical physics, at the same time, giving a visual and intuitive advantage which, they have cherished so much. Specifically, for example, an electron transport theory based on the Bohmian quantum mechanical BTE (Boltzman Transport Equation), with particle ontology and a visual trajectory, extends classical causal intuition into the semi-classical domain, while successfully taking care of all genuine quantum effects. This is possible because a single term called the quantum potential introduces all quantum effects in Bohmian quantum mechanics. Through a series expansion or a Gaussian fitting of the quantum potential, it can also provide an effective error estimate for the simulation. Scientists may then use a single particle equation of motion in Bohmian quantum mechanics with the quantum potential corresponding to the single particle and a mean field approximation for the rest of the particles involved.

This effective potential (i.e. a mean field approximation) approach has also been routinely conducted in other numerical scheme such as Density Functional Theory (DFT), in which the 'local-density approximation' (LDA) is commonly used to model the effective potential of electrons. The computational costs of DFT are relatively low compared to the standard (semi-classical) quantum mechanical calculations from the complicated many-electron wavefunction. Now, the success of DFT as an important experimental (and computational) work in chemistry also successfully argues for a case that effective numerical computability could lead to a prolific generation of empirical outcomes. This point, as claimed before, can also be shared with the hydrodynamical interpretation of Bohmian quantum mechanics. However, although DFT offers an improved computational scheme, it does not necessarily offer better and more direct visualization than the standard (semi-classical) approach. Bohmian quantum mechanics with quantum trajectories, therefore, not only becomes an effective computational scheme but also provides functional illustrations and metaphors on quantum dynamical processes.

In the meantime, a wider variety of investigations on the foundations of quantum mechanics are on their way. They could potentially give rise to an opportunity to witness Leggett's 'Stage 3' type experiments of testing/refuting the standard quantum mechanics in the near future. Among them, the Bohmian hydrodynamical simulations with quantum trajectory can also be included. According to Cat (2001), this is possible because the illustrative and metaphoric quantities such as 'trajectories' and 'fluids' can 'call to mind some more concrete and clear conceptions of further developments.' Those illustrative models with trajectories can thus introduce additional structure in the theoretical representation of (current and future) phenomena, and potentially suggest some possible future experiments. Some of such future experiments might become crucial enough to avoid the Duhem-Quine type complication. This 'crucial' experiment can serve as more or less clear-cut experimental evidence, favoring one side rather than the other in a scientific dispute, and afterward, 'satisficed' scientists could form a widespread satisfactory consensus in choosing one model rather than the other. This whole decision-making process called a 'satisficing strategy', thus, can end a scientific dispute.

6. General Overviews

Although they have been with us around for a long time, the Bohmian interpretations still have not yet achieved the status of an applicable model for most in the physics community. Even within a philosophical circle, the interpretations have long been considered marginally possible 'interpretations' with excessively heavy baggage in metaphysical commitments such as ontology and determinism, not to mention the non-local (and thus physically unacceptable) features inside. However, they finally give rise to, for example, an authentic quantum electron transport theory of motion to, among others, the classically-minded applied scientists who probably have less of a commitment to traditional quantum mechanics. The communities those scientists are involved are in quantum chemistry and electrical engineering. They were not the usual audience of quantum mechanics and nowadays they simply choose to use a non-Copenhagen type interpretation (in this case, the Bohmian hydrodynamical quantum mechanics in particular) to their advantage. Thus, the metaphysical issues physicists had a trouble with are not the main concern of the scientists.

One primary reason why contemporary physicisthas never paid much attention to Bohmian quantum mechanics is that the Bohmian ontological interpretation was published well after the standard quantum mechanics was widely practiced by a generation of working physicists (Cushing 1994). Also, according to Wyatt (2005), the numerical advantage based on the hydrodynamical interpretation in quantum dynamical simulations was fully realized and incorporated only in 1999 with some huge time gaps between major research developments since the time of Madelung. Even in philosophy of science, as seen already, the hydrodynamical quantum mechanics has not given a proper attention. Nonetheless, with the advantages of a visual and illustrative trajectory, the Bohmian quantum theory of motion effectively bridges quantum and classical physics, especially, in the mesoscale domain. Without having an abrupt shift in actions and beliefs from the classical to the quantum world, scientists and engineers may be able to enjoy human cognitive capacities extended into the quantum mechanical domain.

7. Conclusions

Finally, a list of summaries can be made as follows:

- The ontological interpretation of Bohmian quantum mechanics, through a particle's visual trajectory of motion, reconstitutes realism and determinism (and thus causality) in a quantum system.
- There also exists a similar but distinctive class of interpretation under Bohmian quantum mechanics, called the hydrodynamical interpretation. Here, the trajectories of the probability fluid flow play a significant computational role. The flow of the probability density visually helps chemists and engineers to solve the corresponding

quantum hydrodynamical equations of motion. This particular computational scheme for the numerical solutions is called 'the quantum trajectory method.'

- The success of the quantum trajectory method demonstrates the power of visual illustrations and metaphors in representing and analyzing quantum systems.
- The power of such pictorial and diagrammatic representations is clearly noticeable throughout history of science, for example, in the 19th century development of electromagnetism by Maxwell.
- The Bohmian visual scheme may help develop in the future some potentially 'crucial' experimental tests on the standard quantum mechanics itself.
- As Leggett (2007) claims, the on-going experiments routinely conducted on the SQUIDs could set a preliminary stage for potentially testing the limit on the validity of the standard quantum mechanics and, at the same time, various other interpretations of quantum mechanics. In this possible situation, the SQUID technology may help avoid the situation of continuing debate on the foundational issues in quantum mechanics.

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