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## An Overview on Quantum Trajectories I: Two Bohmian Interpretations

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### **Abstract:**

*The two interpretations of Bohmian quantum mechanics and their advantage over the standard interpretation are sketched. The Bohmian interpretations rearrange the original mathematical framework of quantum mechanics to expand its physical meaning so that visual intuition on underlying physical processes can be obtained. In particular, the 'quantum trajectory method' in the hydrodynamical formulation of Madelung-Bohm-Takabayasi quantum mechanics is an example of showing the cognitive importance of scientific illustrations and metaphors in computational quantum chemistry and electrical engineering. The method involves several numerical schemes of solving a set of hydrodynamical equations of motion for the probability density 'fluids,' based on the propagation of those probability density trajectories. On the other hand, the standard interpretation of quantum mechanics remains to be a probability-based minimalists' approach on a quantum process.*

**Keyword:** Bohmian quantum mechanics, hydrodynamical formulation, Madelung-Bohm-Takabayasi quantum mechanics, quantum trajectory method, probability density trajectories

### 1. Quantum Trajectory Method

The 'quantum trajectory method' in the hydrodynamical formulation of Madelung-Bohm-Takabayasi quantum mechanics is an example of showing the cognitive importance of scientific illustrations and metaphors, especially to its professional audiences, in this case, in computational quantum chemistry and electrical engineering. The method involves several numerical schemes of solving a set of hydrodynamical equations of motion for the probability density 'fluids,' based on the propagation of those probability density trajectories. 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. Thus, it invites many well-established computational approaches to the corresponding classical fluid motion.

When a set of the hydrodynamical equations for the probability density 'fluid' are solved, the trajectories are not only the goal of the computational scheme, but also, more importantly, "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 those fluid elements are first used to calculate the initial quantum potential and a related quantum force. Then, under the influence of both a classical force and a quantum force, which derives the propagation of the trajectories, a new set of trajectories is propagated along the motion of the initial fluid elements (Wyatt, 2005). The later set of positions for those trajectories is then used to calculate a new quantum potential which in turn drives the propagation of the fluid elements further. These procedures can then be re-iterated.

In this computational scheme, the trajectories and the wavefunctions--the solutions of the Schrödinger equation--are concurrently calculated along the motion of the probability density fluid. This quantum trajectory method thus has greater computational and cognitive advantages than the usual numerical method of integrating the Schrödinger equation directly since it visually illustrates how the fluid elements are being propagated in real space through time, based on the illustrative and metaphoric quantities, such as 'trajectories' and 'probability flows.'

However, it is notoriously difficult to numerically (not to mention analytically) solve the standard Schrödinger equation through a direct integration when more than four or five particles are actively involved. This quantum trajectory method thus provides a unique way of getting the solutions of the genuine quantum mechanical equations of motion for a multiple particle system (e.g. Garashchuck 2002, 2003a, 2003b, 2004). This visual computational scheme is feasible since the probability density flow and its trajectories are all well defined in every possible position of real space in any given time. So, the entire flow is completely causal and thus deterministic throughout its motion in real space. Therefore, this scheme strongly appeals to those who prioritize visual illustrations in theoretical understanding of quantum phenomena. However, whether

the numerical scheme falls to a category of realism or anti-realism is a rather unfruitful question in understanding this research program because the trajectories merely represent the flow of mathematical probability density.

Currently, some quantum chemists and electrical engineers are actively involved in applying the hydrodynamical interpretation of quantum mechanics. For example, continually miniaturized integrated circuits with more and more quantum effects are being developed as a major part of continuing engineering effort in nano-technology today. Within the hydrodynamical interpretation, some computational models have been developed to simulate key functions of the next generation integrated circuits incorporating genuine quantum mechanical effects. In these simulations, the hydrodynamical equations with an effective quantum correction from the quantum potential provide a research opportunity with classical efficiency on investigating the quantum transport behavior of the circuits (Wu, Tang, Nam, and Tsai, 2003).

There are also some hybrid numerical schemes of combining both the standard and the hydrodynamical quantum mechanics. For example, the Schrödinger equation is first solved numerically, and then the momentum of particles can be calculated (or rather 'assigned') at each position of space through the Bohmian 'guidance condition'.<sup>1</sup> This assignment of the particle momentum is initially introduced in the standard quantum mechanics only as a 'heuristic device' for classical understanding of the system. Nevertheless, this heuristic scheme allows researchers to visualize the trajectory of a particle within the standard quantum mechanics, and shows how constructively some key elements of classical metaphysics (such as realism and determinism) can be added to the standard quantum mechanics without provoking major interpretational issues (e.g. Heller 1975).

However, the same term 'trajectory' means two ontologically distinct things in the two sister interpretations of Bohmian quantum mechanics. A trajectory in de Broglie-Bohm ontological interpretation rather means a causal dynamical propagation of a realistic particle (i.e. a corpuscular trajectory) in usual space-temporal locations, whereas a trajectory in Madelung-Bohm-Takabayashi hydrodynamical formulation means a mathematical progression of the probability density flow (i.e. a quantum trajectory), which does not imply a physical motion of any ontological objects. In this respect, the quantum trajectory within the hydrodynamical formulation does not intend to mean any real physical flow in an ontological sense, as some philosophers would put it. It is rather an imaginary computational tool that lacks empirical status. Here, however, to those computational quantum chemists, their concerns are not focused on the realism or the ontology of the trajectories. Unlike many philosophers, the trajectory method primarily serves the function of illustrations and metaphors, similar to the way Jordi Cat (2001) argues for the visual and intuitive role of ether in his study on Maxwellian electromagnetism. The chemists' pattern of commitment to metaphorical and literal understanding of the theoretical terms such as 'trajectories', 'probability density flows', and the 'quantum potential' is rather irregular and diverse both over time and within each separate discussion. As Cat argues in his discussion of ether, this diversity is, however, "compatible with a pluralism about what counts as understanding, or conversely, what counts as explanation. Hence it leaves the realism/instrumentalism dichotomy with little use for insight" (Cat, 2001, p.437).

Nevertheless, Cat also emphasizes that, "illustrative models attached to metaphors can have an indirect heuristic value: they can suggest experiments and introduce additional structure in the theoretical representation of phenomena and enhance its deductive structure and, thereby, its computational and predictive power" (p.432). In his view, metaphoric devices can not only increase the computational power of an illustrative model, but also suggest experimental tests of the model itself. So, a heuristic tool can make a big difference in empirical aspects. Thus, according to Cat, a cognitive approach based on pictorial representations, rather than a mathematical approach based on formal equations, had played an essential role in Maxwell's development of the 19th century electro-magnetic theory, giving rise to a series of experimental activities to test the electromagnetic theory itself.

Since illustrations and metaphors can suggest actual experiments, Bohmian quantum mechanics could also lead to some deeper cognitive understanding of quantum processes through some intuitive, pictorial and visual representations on them. The quantum trajectory methods in this respect could thus potentially yield novel results, even a possible kind of 'crucial' experiment in the future.

## 2. Hydro Dynamical and Ontological Interpretations

Now, it seems necessary to show what exactly it is meant by the hydrodynamical interpretation in relation to its sister interpretation, the ontological interpretation and also to the standard quantum mechanics. First of all, the standard quantum mechanics, formulated in its present mathematical form in the early 1930s, has been one of the most successful physical theories in history of science. However, ever since its formulation, it has been a constant source of debate for its possible interpretations among physicists and philosophers of physics. One reason for the debate is that the standard quantum mechanics, or "the Copenhagen Interpretation," provides only bare mathematical descriptions. Some underlying micro-physical processes possibly involved in the descriptions are almost never provided. This formal approach primarily based on mathematical equations virtually eliminated all forms of realism, causality and related determinism from classical mechanics, all of which were believed to be part of 'unnecessary metaphysics' for the foundations of quantum mechanics. So, the earlier founding fathers of quantum mechanics replaced 'metaphysics' with the mathematical recipe for calculating probable "expectation values" of the corresponding physical quantities. This may have been due to the form of empiricism shared by

<sup>1</sup> It was de Broglie who first introduced the guidance condition in quantum mechanics.

those founding fathers (Cushing 1994). Therefore, in the standard quantum mechanics, a cognitive approach based on visual illustrations and intuitive metaphors is usually considered only educational and ornamental, rather than genuine. That is, they are not genuine representations on any underlying quantum processes. Due to this, some philosophers and physicists seriously doubt whether quantum mechanics in its present form is a legitimate physical theory for describing the quantum world.

Ever since the beginning of quantum mechanics, some physicists, such as Einstein, have contested the probability-based minimalism of the Copenhagen interpretation. Among those, David Bohm, in particular, took a clear position against it. He published his own alternative form of quantum mechanics under the title of 'hidden variable theory' (Bohm 1952), which was later renamed the 'causal interpretation' and then eventually the 'ontological interpretation.' The ideas behind the ontological Bohmian interpretation are similar with ones developed independently by Louis de Broglie who verbally presented his ideas at the 1927 Solvay Conference, although de Broglie himself was eventually persuaded to move on to other issues in the standard quantum mechanics; thus the ontological interpretation is also referred to as the de Broglie-Bohm theory. Nevertheless, there are differences between de Broglie's ontological approach and Bohm's, especially on their ontological formalisms. The Bohmian ontological approach begins by transforming the basic equation of motion in the standard quantum mechanics, the Schrödinger equation, into a set of equations very similar to Newton's second law of motion. Since the second law embraces classical dynamical features such as realism and causality, Bohm's ontological interpretation also reconstitutes classical ontology and determinism into the corresponding quantum system. On the other hand, de Broglie's approach is defined by two equations; the Schrödinger equation and the guidance condition, through which de Broglie directly defines a velocity of particles. This velocity field defined by the condition then gives rise to a whole set of classical dynamical features such as particle trajectories. In a sense, Bohm reformulated the Schrödinger equation to arrive at the Newtonian form of second law, while de Broglie was not interested in arriving at the Newtonian form and instead contradicted Newtonian mechanics by taking the guidance condition as an axiom. However, they virtually invoked the same (classical) metaphysics in quantum mechanics. Throughout this work, de Broglie-Bohm ontological interpretation simply means the particular ontological approach historically established by Bohm.

Let's contrast the (Bohmian) ontological interpretation of quantum mechanics with the standard Copenhagen one using, for example, the Young's double slit experiment. The linear Schrödinger equation in the standard quantum mechanics naturally suggests a linear combination (superposition) of various quantum states as a general solution. The interference patterns in the double slit experiment is usually said to be an outcome of a superposition and then an interference of two different waves coming from the two slits. In the standard interpretation of quantum mechanics, there is no particle actually going through any one of the slits. It is the waves that interfere with each other in forming the pattern. The moment we have the information about which slit the particle went through, the pattern disappears. Therefore, the nature of quantum system in the standard quantum mechanics is either a particle or a wave, not both at a given situation. In the ontological interpretation of quantum mechanics, however, a Bohmian particle consists of both a particle and a wave at the same time. The Bohmian particle actually goes through one of the slits following a definite trajectory of motion. In this case, an ensemble of trajectories can be found for the two-slit experiment under Bohmian ontological quantum mechanics (i.e. Stanford Encyclopedia of Philosophy on Bohmian Mechanics by Sheldon Goldstein <http://plato.stanford.edu/entries/qm-bohm/>). It is also guided by a wave (i.e. the pilot wave) through the quantum potential. For an ensemble of particles, all the points in the screen made by the particles collectively form an interference pattern on the screen, although each one of them is totally deterministic.

### 3. Visualizing Trajectories

Thus, for a Bohmian particle, its particle behavior can be described by 'the second law of motion,' and its wave behavior by the Schrödinger equation. The wave, also known as 'the pilot-wave', guides a particle's motion throughout its dynamical trajectory, generating all kinds of quantum effects such as 'wholeness' or 'non-locality.' In this respect, one of the most appealing features of the ontological interpretation is that, by visualizing particles' trajectories over time, the intuitive and cognitive representations of their dynamical motions can have legitimate physical meanings for the corresponding quantum phenomena. For example, 80 Bohmian trajectories can be visualized ([http://bohm-c705.uibk.ac.at/visu\\_daten/frei/picturesandmovies/free2traj.gif](http://bohm-c705.uibk.ac.at/visu_daten/frei/picturesandmovies/free2traj.gif)). This visualization shows what happens in freely evolving trajectories when 80 different Bohmian particles moving with the same speed in 1-D opposite directions meet at the center. Also, the hydrogen atom can be visualized with an orbiting electron for a state of quantum number  $n=10$ ,  $l=8$ ,  $m=3$  ([http://bohm-c705.uibk.ac.at/visu\\_daten/dreid/picturesandmovies/Hstate10k3.gif](http://bohm-c705.uibk.ac.at/visu_daten/dreid/picturesandmovies/Hstate10k3.gif)). Here, an electron circles about the z-axis with constant angular velocity. These pictures are from the Bohmian mechanics research group webpage at the University of Innsbruck.

However, almost all physicists are still reluctant to accept the ontological interpretation as an alternative form of quantum mechanics. One of their primary objections is to the newly introduced term called the 'quantum potential' in the mathematical transformation by Bohm.<sup>2</sup> The term sometimes diverges; in other words, its value goes to infinity even in a region where no wavefunction exists, and at the same time, it instantly affects every corner of the Universe. Even more problematically, it does not seem to originate from any known physical source whatsoever, giving physicists (but not to the

<sup>2</sup> However, the quantum potential term can be avoided in the ontological interpretation through the guidance condition as an axiom as suggested by de Broglie.

chemists and engineers who have developed effective computational schemes out of this quantum potential term) a strong suspicion that it is only a spurious mathematical entity, not a physical one. Consequently, the Bohmian ontological quantum mechanics has primarily remained a possible interpretation, rather than an applicable dynamical theory of physics.

Then, here comes the sister interpretation, the hydrodynamical interpretation. This began as an attempt to understand quantum phenomena based on stochastic classical fluid dynamics first by Erwin Madelung in 1926. Unfortunately, however, the approach was not fully developed by Madelung himself, and was almost totally forgotten by other physicists at least in the western hemisphere. However, right after Bohm's work on the ontological interpretation, Japanese physicist Takehiko Takabayasi (1952) reformulated Bohm's ontological work into a set of dynamical equations for 'quantum fluidal motion' to show a possible link from Madelung's stochastic quantum fluid dynamics. Once again, however, the work of the Japanese was not noticed by most physicists. Finally, only recently, some quantum chemists and electrical engineers working on quantum dynamical simulations rediscovered these developments. They now call them Madelung-Bohm-Takabayasi hydrodynamical interpretation of quantum mechanics (Wyatt 2005).

The hydrodynamical interpretation transforms the Schrödinger equation into a set of equations reminiscent of those in classical fluid mechanics. However, the fluidal motion in the hydrodynamical approach has nothing to do with the physical flow of any actual entities. Mathematically, the hydrodynamical equations only describe the flow of quantum probability density over time. Nevertheless, since the flow can be described with a definite momentum in each actual position of the fluid, its motion becomes totally deterministic and perfectly traceable. Thus, the motion can be visualized by its trajectory throughout its entire motion in real space over time. This trajectory method gives scientists an excellent research opportunity for some visual, intuitive and cognitive representations for the corresponding quantum processes. However, the same quantum potential appears again in the hydrodynamical interpretation, and most physicists and philosophers are still unaware of its successful applications in quantum chemistry and engineering, not to mention its separate existence from the ontological one.

The two interpretations of Bohmian quantum mechanics are logically consistent and numerically identical with all aspects of non-relativistic standard quantum mechanics (e.g. Cushing 1994; Wyatt 2005). However, contemporary physicists have never paid much attention to them. One primary reason is that the 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. These time gaps indicate that solving the corresponding equations of motion even under the hydrodynamical approach often becomes a major numerical task even nowadays, and there is still a lingering prejudice against the use of trajectories in quantum mechanical calculations, according to Wyatt. Various other studies in history of physics also show that Bohmian quantum mechanics had not given a proper consideration and its recognition has been seriously delayed due to some social, political, and cultural obstacles Bohm himself had to endure throughout his research career (e.g. Olwell 1999; Friere 2005). Furthermore, physics research in US, especially during the Cold War, had been driven by its military applications. So, the majority of working physicists had no compelling reason to contemplate on the foundational issues of quantum mechanics. To them, alternative interpretations of quantum mechanics were simply not included as one of their usual research topics.

Although similar looking sets of equations at first sight, the ontological and the hydrodynamical interpretations nonetheless are two distinctive and thus independent formulations of quantum mechanics, according to some quantum chemists and electrical engineers. The former, through causality and realism for quantum systems, is mainly concerned with establishing the ontology and determinism for sub-atomic particles in their dynamical motions. On the other hand, the latter is designed to visually describe the flow of probability density over time in a computational scheme. Since the probability density is only a mathematical entity, this approach has nothing to do with any realistic ontology of quantum system, but has something to do with a set of computational tools to solve the fluidal equations of motion through visual trajectories. In other words, the former is related with ontological metaphysics while the latter with computational methodology.

The real virtue and advantage of the hydrodynamical interpretation lies in its application primarily in the mesoscale domain. Between the classical and the quantum domain, there exists an intermediate region called the mesoscale domain. In recent years, in the name of nano-science and -technology, some major research activities have been conducted particularly in this region. Here, while classical mechanics with its well-defined parameters and concepts can be effectively employed, some quantum effects can also play a key major role in the overall dynamical behaviors. In condensed matter physics, for example, the so-called semi-classical method has long been a standard approach in which the quantum mechanical variables are simply combined with the classical ones within a framework of easy-to-handle classical models (e.g. Ashcroft and Mermin, 1976, Chapter 2 and 12).

However, developing a logically consistent and, at the same time, successfully working semi-classical model remains to be one of the most challenging areas of contemporary condensed matter physics. It is a bit ironic that semi-classical approaches seem to be even more complicated than full quantum mechanical ones. Thus, it is not surprising that not only physicists but also engineers and chemists all participate in the area, actively forming an interdisciplinary research group. One of the fundamental difficulties in this area of research is the fact that the standard quantum mechanics does not seem to overlap with classical mechanics. The physical variables from two theories are often said to be 'incommensurable', and the so-called 'quantum leap' apparently exists in the mesoscale region between the classical and the quantum domain.

However, in all two Bohmian interpretations, all classical variables can be continuously applicable to the mesoscale and then to the quantum domain with no apparent discontinuity anywhere in between. This is achievable by adjusting the contribution from the quantum potential term through some series expansions of it. In particular, under the Bohmian schemes, developing a separate semi-classical model based on a hybridization of both quantum and classical mechanics is simply a redundant effort. Within the Bohmian schemes, the conceptual incommensurability between classical and quantum variables does not exist.

One of the difficulties in the standard quantum mechanics is that the exact source of the quantum mechanical effects in the Schrödinger equation cannot be isolated within the equation itself. Rather, the entire equation as a whole is said to be the source of all the quantum effects. In Bohmian quantum mechanics, however, all the effects originate from the single source, the quantum potential. Depending on its contribution, Bohmian quantum mechanics becomes either classical mechanics or the standard quantum mechanics. In this respect, taming the quantum potential makes Bohmian mechanics applicable to all possible physical domains of scales, by adjusting its contribution to the dynamical equations of motion. For example, in the mesoscale region, the quantum potential cannot be ignored, but its contribution is relatively small. Thus, it can be expanded in a rapidly converging series before its first few terms are summed up to make an effective correction for all the quantum effects in the intermediate region. Afterwards, the sum of the discarded remaining terms constitutes a numerical error involved in this approximation scheme. Consequently, its series expansion gives chemists and engineers a powerful numerical scheme in applying their dynamical models in the mesoscale region.

Another difficulty in the standard quantum mechanics that is relevant in today's condensed matter physics arises in determining how much time a particle spends during tunneling. Calculating tunneling time is conceptually challenging, or nearly impossible, to formulate properly within the standard framework, but it can be meaningfully formulated under the Bohmian ontological interpretation. Tunneling occurs when a particle appears on the other side of a potential barrier even though it has less energy than the barrier. Within the standard quantum mechanics, physicists simply state that such a particle has some intrinsic probabilities of either reflecting back by or tunneling through the barrier. The reason why calculating tunneling time is challenging in the standard frame is mainly due to the fact that time is not an observable physical quantity and it is only a mathematical parameter with no corresponding Hermitian operator. Thus, calculating the expectation value of time is fundamentally impossible within the standard quantum mechanics. All the attempts in the standard quantum mechanics for tunneling time have so far deep conceptual problems, serious enough to reject all (Hauge and Stövneng, 1989).

However, under the ontological interpretation, tunneling is nothing but a dynamical motion of a particle over the barrier with some additional boost from the quantum potential. Whether it tunnels through or reflects back by the barrier depends on its initial position. Since the initial positions are unknown as 'hidden variables' within the ontological interpretation, probability comes in only for an ensemble of particles while each particle still has a definite trajectory of motion with its well-defined momentum throughout. Thus, for each small segment of the trajectory, actual flight-time can be calculated, and then for the entire path, the flight-time can be added, giving rise to the tunneling time calculation (e.g. Dewdney 1992; Leavens 1990a, 1990b). This is all possible because the visual particle trajectory is readily available in the ontological interpretation with clear cognitive advantage on understanding the tunneling process itself.

So far, the two interpretations of Bohmian quantum mechanics and their advantage over the standard interpretation have been sketched. The Bohmian interpretations rearrange the original mathematical framework of quantum mechanics to expand its physical meaning so that visual intuition on underlying physical processes can be obtained. On the other hand, the standard interpretation of quantum mechanics remains to be a probability-based minimalists' approach on a quantum process.

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