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History and Philosophy of Quantum Mechanics II: The Hydrodynamical Interpretation

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Abstract:
Through a transformation similar to the one made by the Bohmian ontological approach, Madelung-Bohm-Takabayasi hydrodynamical interpretation of quantum mechanics transforms the Schrödinger equation into a set of hydrodynamical equations to express a causal and deterministic change of probability density over time. Then, the motion of probability density flow can be visualized in real space through its trajectory. This illustrative and metaphoric scheme provides intuitive understanding of quantum dynamical systems. In this computational scheme, the visual trajectories of the flow constitute a set of computational tools to solve the corresponding hydrodynamical equations of motion.

1. Hydrodynamical interpretation

There was also a line of independent development by Erwin Madelung (1926), geared toward understanding quantum phenomena. However, his approach to quantum mechanics based on stochastic classical fluid dynamics was not fully developed by Madelung himself and later on almost totally forgotten by most physicists. Nevertheless, right after Bohm's work on the ontological interpretation was published, a Japanese physicist Takehiko Takabayasi (1952) re-formulated the Bohmian ontological approach based on "quantum fluid" of motion to show that the work of Bohm could be extended to that of Madelung. Recently, quantum chemists and engineers working on quantum dynamical simulations finally recognize this series of developments as "Madelung-Bohm-Takabayasi hydrodynamical interpretation" of quantum mechanics (Wyatt 2005).

This interpretation transforms the Schrödinger equation into a form of hydrodynamical equations of fluid, very similar to the ones describing classical fluid motion. But, the "fluidal motion" in the hydrodynamical approach has nothing to do with the flow of any actual physical fluid. Mathematically it expresses a change of probability density over time. Nevertheless, since the flow can be described with a definite momentum in each position of motion, it is completely causal and thus deterministic. Thus, the motion of fluid can be visualized in real space through its trajectory. This again gives scientists an opportunity to gain a more intuitive understanding of the corresponding quantum systems.

The mathematical formulation of the hydrodynamical interpretation of quantum mechanics introduced originally by Madelung (1926), then later by Bohm and Takabayasi (Bohm 1952; Takabayashi 1952) looks deceivingly similar in a mathematical form with the ontological interpretation at first sight. Like Bohm, Madelung also started by introducing the wavefunction in polar form in the time-dependent Schrödinger equation, taking into account the definition of the velocity field v of equation (6), and

$$\rho = R^2 = \Psi^*\Psi , \qquad (15)$$

$$J = \rho v = R^2 \frac{\nabla S}{m}, \qquad (16)$$

where $\rho(r,t)$ is the probability density and $\mathbf{J}(r,t)$ is the quantum density current. By proceeding in this way, equation (3) and (4) transform to

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0 , \qquad (17)$$

$$\frac{\partial v}{\partial t} + (v \cdot \nabla) v = -\frac{1}{m}\nabla(Q+V) . \qquad (18)$$

These equations constitute the formal basis of the 'hydrodynamical interpretation' and are in direct correspondence with those of classical fluid mechanics if m is the mass of a piece of fluid with a closed surface, and ρ is the fluid density, and v is the velocity field of the flow (Landau and Lifshitz 1959).

Although the foundations of this hydrodynamical formulation of quantum mechanics were established by de Broglie, Madelung, Bohm, and Takabayasi etc., it is distinct from the de Broglie-Bohm interpretation of quantum mechanics. "The purpose of which [de Broglie-Bohm interpretation] is not to solve the time-dependent Schrödinger Equation (TDSE) per se, but to provide insight. Frequently, interpretative terms such as "pilot wave", "ontological status of the wavefunction", and "hidden variable" are associated with this approach" (Wyatt 2005, p.2). It seems that this distinction between the de Broglie-Bohm and the Madelung-Bohm-Takabayasi approaches has not yet been fully noticed even by some philosophers of physics working on the foundation of quantum mechanics. Just knowing of the equations of motion for 'quantum trajectories' is not good enough to distinguish the subtle but profound difference between two approaches. Even Cushing (1994) wrote, "although Madelung claimed that this model gave an intuitively clear picture of quantum phenomena, it is not wholly evident, at least to a modern reader, just *what* this ideal fluid was" (Cushing 1994, p.125). Most philosophers of physics (with Bohm himself included) seem to have been primarily interested in the ontological implications and the difficulties associated with the quantum potential term in the de Broglie-Bohm interpretation. Thus, they did not pay much attention to its subtle differences from the hydrodynamical formulation. It was, in fact, due to quantum computational chemists that the hydrodynamical formulation with more profound implications in numerical applications became quite distinct from the original de Broglie-Bohm interpretation. Those chemists are particularly interested in a mesoscale (i.e. molecular level) system with multiple particles involved. The standard time dependent Schrödinger equation and also the Bohmian ontological equations are both notoriously difficult to solve in a direct numerical integration for the multiple particle system like that.

Why have most philosophers and physicists not paid much attention to the subtle differences between the ontological and the hydrodynamical interpretation? It seems that the quantum potential alone causes so numerous difficulties in accepting de Broglie-Bohm's quantum mechanics as a 'workable' physical theory to many physicists that many have been reluctant to accept de Broglie-Bohm's interpretation in the first place, not to mention the hydrodynamical version of it which seems to offer no real distinction from the original ontological interpretation anyway. People already had to understand various (unphysical) features in the de Broglie-Bohm formulation, appreciating a subtle difference between the two sister interpretations was a less important issue. Further topics on the hydrodynamical interpretation will be discussed in 2.5 in contrast with the ontological interpretation. Before that, in the following section, difficulties under these Bohmian interpretations are discussed first.

Conclusion: Through a transformation similar to the one made by the Bohmian ontological approach, the work of Madelung on stochastic fluid dynamics can be re-formulated to be consistent with the quantum fluid of motion. This Madelung-Bohm-Takabayasi hydrodynamical interpretation of quantum mechanics transforms the Schrödinger equation into a set of hydrodynamical equations to express a causal and deterministic change of probability density over time. Then, the motion of probability density flow can be visualized in real space through its trajectory. This illustrative and metaphoric scheme provides intuitive understanding of quantum dynamical systems.

2. Difficulties in Bohm's Theory

The two interpretations of Bohmian quantum mechanics have been shown to be logically consistent and numerically identical with all aspects of the non-relativistic standard quantum mechanics (e.g. Cushing 1994; Wyatt 2005). However, a majority of contemporary physicists have never paid much attention to these alternative interpretations of quantum mechanics. According to Cushing (1994), the ontological interpretation of Bohmian quantum mechanics was nearly destined to be unrecognized because it was only published well after the standard quantum mechanics was firmly established and widely practiced by a generation of working physicists in the area. Also, according to Wyatt (2005), the numerical advantage based on the hydrodynamical interpretation was fully incorporated in quantum dynamical simulations only in 1999 with huge time gaps between major developments. Thus, most physicists and philosophers do not recognize the success of this particular computational approach primarily by quantum chemists and electrical engineers. This may be a rather understandable situation. Communities formed by physicists and philosophers on one hand and by chemists and engineers on the other hand are generally quite independent. They rarely communicate directly with each other and exercise distinctive sets of strategies and values in pursuing their research.

Various other studies in history of physics also point out that the recognition of Bohmian quantum mechanics was delayed due to the social, political, and physical isolation David Bohm encountered during much of his professional life (e.g. Olwell 1999; Friere 2005). On top of this, foundational research on quantum mechanics has not received much attention by working physicists. Even for those whose interested are in the foundational issues of quantum mechanics, Bohmian quantum mechanics seems to have a profound conceptual problem. That is, the quantum potential term in the Bohmian equations of motion seems to have no physical reality whatsoever. It sometimes diverges even in a region with no wavefunction present, while instantly affecting every corner of the Universe. Consequently, Bohmian quantum mechanics has had to remain in the area of a philosophical interpretation rather than of an applicable physical theory.

Objections on de Broglie-Bohm's ontological interpretation are typically associated with the classical pictures on quantum phenomena and the various unphysical features of the quantum potential. The objections go as follows. First, the Bohmian ontological picture involving particle ontology and its trajectory together with the 'hidden' position variables forces physicists to accept a heavier metaphysical commitment toward the quantum mechanical world. In accordance with the Copenhagen version of quantum mechanics, many physicists deny the claim that quantum particles can have a definite position, velocity and energy in their dynamical motion. They are happy with an essential, minimal set of working rules for computing the likely outcomes of measurement. Anything more constitutes unnecessary metaphysics to them. To those physicists, gaining an intuitive or cognitive advantage from various forms of representation as in the Bohmian picture may not be a great concern. In a terminology of 'satisficing' decision making, they simply have some higher priority, among their selection options, for mathematical simplicity, elegance or purity of their models.

Second, as discussed previously, the quantum potential Bohm introduces has so many notorious unphysical properties involving non-local, unbound, singular, non-linear, and time dependent features that it is hard for physicists to take it as something real and physical, governing all fundamental features of quantum mechanics. This may be the most reasonable and understandable objection to the Bohmian approach. The term of quantum potential single-handedly causes so many features usually not acceptable in physics as a workable component of a theory. To those physicists, on top of the burdensome metaphysics already imposed by the Bohmian quantum mechanics, the unphysical nature of quantum potential seemed to demand too big a task for them to appreciate the approach and its subtle application.

Third, there may be some historically–contingent biases against the Bohmian interpretation being generally accepted as a physical theory. Cushing concludes that the Copenhagen interpretation became widely accepted not because it is a better explanation of subatomic phenomena than Bohm's, but because Bohm's idea came in 1952, after a generation of physicists had accepted the Copenhagen interpretation of quantum mechanics (Cushing 1994, 2000). Olwell also present several reasons why the Bohmian *ontological* interpretation has been marginalized in the general physics community (Olwell 1999). His reasons include: [1] massive military patronage of science which emphasized extending the current calculational methods rather than the addressing foundational issues,[1] [2] McCarthyism in American science in the 1950s and Bohm's well-publicized security problems, [3] Bohm's exile and loss of American citizenship in Brazil, which led to his physical isolation, and [4] Bohm's prior political or philosophical commitments against empiricism. However, Oliver Friere argues against the role of McCarthyism as an influential factor in the battle between the Copenhagen and its opponents (Friere 2005). According to Friere, McCarthyism did not prevent American physicists from discussing Bohm's interpretation. Friere also points out that Hugh Everett's relative-state interpretation, which was renamed the many-worlds-interpretation, was also poorly received although he was working for the Pentagon in the 1950s. Therefore, Friere claims that the broader cultural context of physics, in which the Copenhagen interpretation was already dominant and where foundational issues held low status, explains better than any particular personal biases against David Bohm why Bohm's interpretation has failed to gather support. We could also introduce a Kuhnian theme here. Within the Copenhagen interpretation, the pressing problems (i.e. anomalies) of the standard framework such as the measurement problem had not emerged convincingly and explicitly yet. The projection postulation was thought to be good enough to handle the fundamental issues in measurement for a long time. Therefore, the supporters of the Copenhagen felt that there was little demand for an alternative interpretation. However, eventually, the fact that the Bohmian interpretation (and GRW theory also) did solve away of the pressing problem of measurement gave some physicists a clear second thought on pursuing an alternative form of quantum mechanics. Whatever the reasons, however, there is little doubt that the two Bohmian interpretations have been neglected from the beginning, delaying recognition that they are empirically equivalent to every aspect of the standard non-relativistic quantum mechanics. Due to the delay, the numerical advantages from the hydrodynamical interpretation were only demonstrated in the late 1990s in the actual computational schemes in quantum chemistry.

Conclusion: The reasons why Bohmian quantum mechanics have never been paid much attention by the majority of contemporary physicists go as follows. First, the ontological interpretation was only published well after the standard quantum mechanics was firmly established. Second, the workable numerical schemes within the hydrodynamical interpretation were fully incorporated in quantum dynamical simulations only in 1999. Third, Bohm's social, political, and physical isolation and the low status of the foundational issue all contribute to the further delay on the recognition of his theory. Fourth, to physicists, the quantum potential has no physical reality whatsoever.

3. Ontological Formulation vs. Hydrodynamical Formulation

The ontological and the hydrodynamical interpretations seem to be similar at first sight. However, they are two separate and thus independent formulations of quantum mechanics. The ontological interpretation, by re-introducing causality and realism in quantum systems, is mainly concerned with the ontology of sub-atomic particles and subsequently their deterministic dynamics. On the other hand, the hydrodynamical interpretation is about visually describing the flow of probability density over time in a computational scheme. Since probability density is only a mathematical entity, this approach does not constitute a claim of realism. Rather, with the available visual trajectories, the fluidal flow offers a set of computational tools for solving the corresponding hydrodynamical equations of motion. In other words, the ontological interpretation has something to do with realistic metaphysics while the hydrodynamical interpretation with computational devices.

When it comes to Madelung's work in the hydrodynamical formulation of quantum mechanics, it receives even less attention than de Broglie-Bohm's ontological interpretation by philosophers and physicists. There have been long time gaps between major developments on the hydrodynamical side, further delaying its recognition even by chemists and engineers who have eventually become the interpretation's active supporters. Even if some philosophers happened to notice Madelung's work before, they were usually more interested in the ontological or physical meanings of those 'fluids' in the hydrodynamical formulation, than in their potential applicability in a numerical scheme. It is, in fact, de Broglie-Bohm interpretation itself that finally gave some computational chemists a deeper look into the hydrodynamical formulation in numerical applications. Some of them then realized that there were interesting possibilities in the numerical application of the trajectory approach, regardless of the ontological status of the trajectories themselves.

At this point, we should also keep in mind that not all things Bohmian are Bohm's. Madelung's and Takabayasi's pioneering works are primary examples on this. However, it seems to me that philosophers working in Bohm's ontological quantum mechanics have in a sense recreated some of their own history to give a rather conspicuous image for Bohm in the development of the ontological interpretation of quantum mechanics. They seem to appeal to Bohm's ingenious authority to 'bolster' their own claims. In doing so, again, it seems to me that the subtle but quite distinct differences between de Broglie-Bohm interpretation and

[1] It may seem ironic that the current users of the hydrodynamical approach are engineers and applied scientists who are interested in computational methods in quantum mechanics. However, the applicable numerical schemes within the hydrodynamical framework were not fully developed until the late 1990s. All the calculational methods mentioned here were ones used in theoretical high energy particle physics research.

Madelung-Bohm-Takabayasi interpretation have gone unnoticed by philosophers of physics. Subsequently, any developments of the trajectory method in computational quantum chemistry might have been seen just as the usual Bohmian ontological approach.
Another reason why Madelung-Bohm-Takabayasi approach has been less attractive, even compared with de Broglie-Bohm interpretation, could be due to the fact that the earlier researchers in this field tried to avoid the numerical solution of these hydrodynamic equations. Coupled systems of nonlinear differential equations containing possible singularities are notoriously difficult to solve. Issues of computational stability and accuracy, especially in calculating spatial derivatives (see below), still play a significant role in constructing computational algorithms for systems of this type. Consequently, the usefulness of the quantum trajectory method as a computational tool within the hydrodynamical formulation for solving the time-dependent Schrödinger equation was not fully appreciated, or at least demonstrated, until 1999 in computational quantum chemistry (Wyatt 2005). While some concerned philosophers were primarily still preoccupied with possible physical meanings of those fluid trajectories, quantum chemists were rather interested in workable numerical applications of the fluid trajectories. This again indicates "lingering prejudice against the use of trajectories in quantum mechanics" (Wyatt 2005, p.200), even among philosophers of quantum mechanics.
To be more specific, according to Robert Wyatt (2005, p.3), almost nothing happened in the hydrodynamical interpretation for 25 years between 1927 and 1952. After a couple of papers by Bohm in 1952, the first *numerical* implementation of Madelung-Bohm-Takabayasi approach in computational chemistry was developed during the period from the late 1960s through the 1970s by Weiner *et al*. (Weiner and Parton, 1969). "Surprisingly, the first few of these papers made no mention of the much earlier work by Bohm [in 1950s]" (Wyatt 2005, p.3). Stimulated by these studies, Wyatt continues, a number of attempts were made to use the same computational methods, but the algorithms were too immature and simple to permit any promising results. According to Mike Towler who recently developed a graduate course on de Broglie-Bohm pilot-wave theory in 2009 as a member of Theory of Condensed Matter Group at the Cavendish Laboratory of Cambridge University, the main trouble in those early numerical attempts is to accurately calculate the spatial derivatives appearing in functions such as ∇S (also Q) and $\nabla \cdot v$.[2] Those spatial derivatives make equations of motion difficult to integrate even numerically, but at the same, they need to be known very precisely since they bring all nonlocal effects into the dynamics. Evaluation of accurate derivatives still remains to be one of the most challenging and important problem in (any) numerical analysis. (This problem is even more serious in the case of the Schrödinger equation than in the case of the hydrodynamical equations because the Schrödinger equation involves second derivatives whereas the hydrodynamical equations are only concerned with first derivative.) Because of the difficulty in accurately calculating the spatial derivatives, there were a series of long gaps between the earlier works' successes and failures mentioned by Wyatt. Then, in 1999, two groups, working independently, published studies involving ensembles of quantum trajectories. They finally developed some good approximate techniques for calculating the spatial derivatives in their specific applications. The first of these (Lopreore and Wyatt, 1999) introduced a computational approach called the 'quantum trajectory method' (QTM). The other study (Sales-Mayor, Askar, and Rabitz, 1999) developed what was called the 'quantum fluid dynamics' (QFD). Although different computational methods were employed, both methods solve the quantum hydrodynamical equation of motion by evolving ensembles of quantum trajectories.
Computational quantum chemists do not worry about the physical meaning of the fluid to begin with. To them, those fluids only characterize statistical events at each point in space and time, in spite of the fact that the time evolution of these events can be better understood when compared with the motion of ordinary fluids. Moreover, whereas the classical concept of a fluid can be applied to describe the statistical behavior of a macroscopic ensemble of particles, in quantum mechanics it is applied even to a single particle (Bialynicki-Birula, Cieplak and Kaminski 1992, Ch. 9).
Based on this similarity between the quantum fluid and the classical ensemble of particles, they were able to come up with an effective numerical scheme to understand a quantum system through the quantum trajectory method. Whether the trajectories are physically real or not is not the kind of question those quantum chemists are worried about. In this analogy, equation (17) of section 2.3

$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0 , \qquad (17)$$

can be interpreted as the continuity equation for the quantum flow, which in terms of the standard quantum mechanics translates into the equation of probability density conservation. Then, equation (18) of 2.3

$$\frac{\partial v}{\partial t} + (v \cdot \nabla) v = -\frac{1}{m} \nabla (Q + V) . \qquad (18)$$

represents the quantum Euler equation, analogous to the classical one for an ideal classical fluid of incompressible and non-viscous flow.
Using these equations, "the Schrödinger equation for both stationary and non-stationary states may be solved exactly by propagating quantum trajectories, at least in principle. The probability amplitude and the phase of the wavefunction are transported along these trajectories and observables may be computed directly in terms of this information" (Wyatt 2005, p.1). Thus, rather than guiding quantum trajectories with a pre-computed wavefunction as in the pilot wave of de Broglie-Bohm interpretation of quantum mechanics, "the trajectories and the hydrodynamical fields are computed with concurrently, on the fly" (Wyatt 2005, p.2). Thus, this approach becomes the *computational tool* for solving the quantum hydrodynamic equations of motion. Wyatt (Wyatt 2005, p.4) then summarizes the reasons why we solve the hydrodynamic equations with quantum

[2] The course material is available on Web from www.tcm.phy.cam.ac.uk/~mtd26/pilot_waves.html

trajectories in the first place; he lists a number of advantages of solving the hydrodynamical equations with the quantum trajectories;

- Exact quantum-dynamical equations of motion are solved.
- The trajectories follow the evolving probability density.
- A relatively small number of moving grid points (fluid elements) may be needed.
- *x(t)* describes where the 'particle' has been, and *dx/dt* tells where it is going next.
- The equations of motion bring in elementary dynamical concepts, such as forces.
- The trajectories can be used for informative analysis, such as phase space plots.
- New insights may arise, because the trajectories show how the process takes place.
- New computational approaches can be developed (e.g., for density matrix evolution for mixed states and for mixed quantum-classical dynamics).
- The computational effort scales linearly with the number of trajectories.
- [The trajectory method] can possibly avoid the traditional exponential scaling of computational effort with respect to the number of degrees of freedom.
- There are no large basis sets or large fixed grids.
- There is no need for absorbing potentials at the edges of the grids.

The most appealing feature of the trajectory scheme in the hyrodynamical formulation described above is to solve the exact quantum dynamical equations of motion. Thus, this numerical scheme is equivalent to that of conventional quantum mechanics. In addition, these trajectories may provide a very economical way of solving the TDSE (Time Dependent Schrödinger Equation). This alleged economical advantage is surprising to many physicists because the hydrodynamic equations include a set of non-linear coupled equations, instead of the single linear Schrödinger equation in the standard quantum mechanics. Usually, non-linear coupled equations require a much greater burden in any feasible numerical schemes. However, the 'simple' linearity of the Schrödinger equation is somewhat misleading since it fails to provide us any practical (easy and stable) numerical schemes for a system with more then a couple of particles involved. The linearity is an advantage only for a system with a deceptively small number (one, two or three) of particles involved. This may explain why chemists and electrical engineers were originally interested in the hydrodynamical approach. Their research focuses on dynamical mesoscale systems with multiple particles, which must actively interact with each other under realistic circumstances. Finding an exact solution of the Schrödinger equation describing those multiple particles is almost impossible. This is not simply due to the number of particles involved. Even for a system of a few particles, physics in its usual analytical mode requires a symmetric boundary condition in order to get a solution of (any) differential equations. However, the real-world circumstances in electrical engineering often demand a complicated and ugly boundary condition, which rules out the usual symmetric approaches of physics in the first place. Physicists thus are not simply trained to handle a situation like that in a standard method of physics.

Consequently, the hydrodynamical formulation has much better advantage in a numerical scheme for a realistic N particle system. In addition, "we may gain new insights into the dynamics. Unlike conventional computational methods, quantum trajectories provide detailed information about how the process takes place. These insights may lead to improved algorithms for treating systems of increasing complexity and dimensionality" (Wyatt 2005, p.4). This numerical advantage will be discussed with a greater detail in the next chapter in the applications of the trajectory method.

4. Conclusion

The ontological interpretation is designed to re-introduce particle ontology and dynamical determinism in quantum systems. On the other hand, the hydrodynamical interpretation is concerned with visually describing the flow of probability density over time. In this computational scheme, the visual trajectories of the flow constitute a set of computational tools to solve the corresponding hydrodynamical equations of motion.

5. References

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