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History and Philosophy of Quantum Mechanics V: Numerical schemes

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Abstract:
In the hydrodynamical interpretation, the time dependent "flow" of the probability density can be described in almost the same way as for the flow of classical fluid. On the contrary, however, this kind of visual computational approach on solving the equations is not possible under the standard quantum mechanics. The Schrödinger equation does not easily allow some effective computational schemes, especially for a system with more than a couple particles involved.

1. Introduction
In the hydrodynamical interpretation, the time dependent "flow" of the probability density in the quantum fluid equations of motion can be described in almost the same way as for the flow of a classical fluid. The interpretation provides many classical computational approaches to solving the quantum fluid equations. Here, chemists and engineers first estimate the initial value for the quantum potential to propagate the entire trajectory of the fluid. This trajectory thus gives them a visual advantage in solving the fluid equations. This cognitive scheme is feasible since the entire flow is completely causal and deterministic throughout its motion in real space. On the contrary, however, in the standard quantum mechanics, the Schrödinger equation does not easily allow effective computational schemes, not to mention any cognitive approaches, when there are more than three or four particles are involved (e.g. Garashchuck and Rassolov 2002, 2003a, 2003b, 2004).

2. Hydrodynamical Solutions
There are a variety of applications of the hydrodynamical interpretation. First, it should be also noted that a significant feature of Bohm's work both in the hydrodynamical formulation and in the ontological interpretation is that the quantum potential was identified as the localized origin of all quantum effects, including non-locality. This quantum potential leads to an additional force, the 'quantum force,' acting to guide the trajectory, in addition to the classical force. "As a result, in the hydrodynamic formulation, the trajectories lose their independence and are organized (correlated) by the quantum potential" (Wyatt 2005, p.9). "Through the quantum potential, each fluid element is influenced by the motions of the other elements, and the ensuing correlation brings all quantum effects into the dynamics" (p.11).
In practice, however, in the hydrodynamical formulation, scientists have a complication just to get the trajectory method started. Since the quantum force derives the ensemble of trajectories, scientists need to know the quantum potential at the beginning to propagate the initial trajectory within the hydrodynamical formulation. The quantum potential is defined in terms of the curvature (the second partial derivative) of the amplitude R of a wave function. Thus, in order to run the hydrodynamic scheme, they need to have a complete knowledge of the wave function, which is the goal of solving the hydrodynamical equations in the first place.
Quantum chemists try to avoid this complication by estimating the quantum potential from an independent fitting function rather than calculating it from a complete knowledge of a wave function in a 3N configuration space. This can be called 'semi-empirical thinking' (not to be confused with a semi-classical method). Several methods have been developed to estimate the initial value of the quantum potential. Their basic idea is to use the standard statistical meaning of probability and wave function in quantum mechanics. The fundamental statistical postulation of quantum mechanics says that the probability of having a position measurement in the element of space d^3x around the point **x** is given by

$$P(x,t)d^3x = \left|\Psi(x,t)\right|^2 d^3x \,.$$

This $P(x,t)$ becomes a probability of finding a particle (or 'fluid element' and its trajectory in the hydrodynamical formulation) in the given region. Also, this P is the same as the probability density ρ from the hydrodynamical formulation. What scientists have to do then is to estimate this probability of finding fluid elements at the beginning. Specifically, a parameterized function representing 'most likely' probable (initial) positions of the fluid elements can be used to find the (initial) probability density P or ρ. (For example, in the simplest case, the fluid elements are uniformly distributed throughout a given volume of space, then P is unity inside the space and zero outside.) This is always possible because both each fluid element and its later trajectory have well defined (and visually traceable) position in real space under the hydrodynamical formulation. Then, since the probability density P

or ρ is also defined as a square of the amplitude (the real part) of a wave function, $P = \rho = R^2$, scientists can calculate the amplitude R accordingly. Note that this is also the equation (15) of 3.3. as follows,

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

Based on this R, they can finally determine the quantum potential from the curvature (the second partial derivative) of the amplitude R, using the following definition of quantum potential.

$$Q = -\frac{(h/2\pi)^2}{2m} \frac{\nabla^2 R}{R} .$$

Then, depending on a method of finding parameters for the parameterized fitting function, there is either an 'expectation-maximization' (Maddox and Bittner, 2003), or a 'least square fitting' method (Garashchuk and Rassolov, 2002).

In the first method, a 'most likely' probability density carried by the fluid elements and their trajectories is obtained by summing contributions from the 'joint probability' of randomly chosen fluid elements that are located at position r. The joint probability is a Gaussian functional form parameterized by a weight, a mean position vector, and a vector of variances. An iterative procedure called expectation-maximization can be used to find the parameters that best approximate the input data. This fitted density is then used to compute an approximate quantum force that derives the ensemble of trajectories.

In the second method, the parameters of the Gaussian functions are determined by minimization of the least-square error functional. However, the total energy is not strictly conserved in this least-square fitting method. An alternative way of approximating the quantum potential is to fit to the log derivative of the probability density (Garashchuk and Rassolov, 2003b).

In this quantum trajectory method, first of all, an initial wave packet is discretized in terms of N fluid elements, small chunks of the probability density flow. The initial quantum potential is then calculated for these N fluid elements of probability as described above. The hardest part of the problem is now over. Once the initial quantum potential is calculated (or rather, estimated) to get the initial trajectories going, the time evolutions of those trajectories can be solved from the hydrodynamical equations. This requires integrating corresponding two coupled equations of motion (for real and imaginary parts of a wave function, respectively), and the procedure is pretty straightforward since scientists know how to get the solutions in many types of classical fluids. Specifically, equation, (17) and (18) from 3.3 must be solved together with the guidance condition of equation (6) as follows.[1]

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

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

$$v = \dot{r} = \frac{\nabla S}{m} \qquad (6)$$

While solving these equations, the only difference from classical fluid mechanics is, as we already expect, "the total force guiding each quantum trajectory includes the classical force […] plus the quantum force […] [which] depends on the *shape of the density surrounding each trajectory* and brings in all quantum effects" (Wyatt 2005, p.2).

According to this set of equations, the calculated quantum potential starts to propagate (or drive) quantum trajectories out of the initial fluid elements; the hydrodynamical equations of motion with the quantum potential describing the probability fluid are then integrated from the first time step to the next, at the same time, generating a new ensemble of N quantum trajectories through the guidance condition. Then, along each quantum trajectory of probability fluid, the amplitude and action of a wave function are computed and integrated 'on the fly.' From these, the wave function is readily constructed for an ensemble of quantum trajectories, giving us a complete solution of the system. At the same, based on the new positional configuration of the trajectory, a new quantum potential is up-dated along with the progression of the fluid elements for each integration time step. These N fluid elements are now correlated with and influenced by one another through the quantum potential.

In solving equations (17) and (18) directly, a wide variety of specialized computational methods are already available, based on different computational strategies. However, three kinds of numerical schemes are standard: [1] the spatial or Eulerian scheme (Sales-Mayor, Askar and Rabitz 1999), [2] the material or Lagrangian scheme (Weiner and Partom 1969; Weiner and Askar 1971), and [3] the arbitrary Lagrangian-Eulerian (ALE) scheme. In the Eulerian scheme, the equations are solved in a fixed spatial grid or basis set and then the streamlines are obtained. Alternatively, if the Lagrangian description is considered, equations are set up in a reference frame moving with the fluid that distorts as trajectories progress. This method implies the evaluation of third-order spatial derivatives, which is a very difficult computational task, except for low-dimensional problems (Lopreore and Wyatt 1999; Wyatt 1999; Lopreore and Wyatt 2000). The ALE scheme allows for 'adaptive grid point motion' and is more useful than the standard Eulerian or Lagrangian scheme.

However, "the Lagrangian and ALE pictures, in which trajectories are used to solve QHEM (the quantum hydrodynamic equations of motion), provide a very different computational approach from those used in the conventional formulations of quantum dynamics. […] The full power and elegance of the hydrodynamic formulation are exposed only by evolving quantum trajectories in the dynamical pictures [of the Lagrangian and ALE pictures]" (Wyatt 2005, p.3). Thus, "the hydrodynamic

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[1] It is even possible to directly get some analytic solutions, although it is not part of our discussions here. (See Holland (1993) for many types of the analytic solutions.)

formulation […] is considerably more than "just an interpretation"; it presents nontraditional computational techniques for solving quantum dynamical problems in addition to utilizing the descriptive terminology of fluid mechanics" (Wyatt 2005, p.2).

As Wyatt claims here, the hydrodynamical scheme is more than just an interpretation and provides many computational approaches to solving the quantum fluid equations. Here, the trajectories of the fluid give chemists and engineers a visual and intuitive advantage on solving the fluid equations. This cognitive scheme is feasible since the entire flow is completely causal and deterministic throughout its motion in real space.

3. References

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