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History and Philosophy of Quantum Mechanics VI: Application in the Semiclassical Domain

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Abstract:
Based on the hydrodynamical interpretation of Bohmian quantum mechanics, computational models have been developed to simulate the key functions of MOSFET integrated circuits. Those numerical simulations originally evolved from a classical electron transport theory. Thus, with the classical efficiency intact, those simulations use the hydrodynamical equations of motion with an effective quantum correction from the quantum potential. The Bohmian computational approaches allow some hybrid numerical schemes in which the Schrödinger equation is first solved numerically, and then the particles' momentum can be assigned through the Bohmian guidance condition. This gives researchers a rare opportunity to visualize the trajectory of a particle under the standard quantum mechanics.

1. Introduction

With ever decreasing physical circuit dimensions involved, developing high integrated circuits still forms a major continuing engineering effort in a current day nano-technology. In a dynamical simulation of such circuits, researchers now have to incorporate more aspects of quantum effects previously ignored. Based on the hydrodynamical interpretation, some computational models have been developed to simulate the key dynamical functions of the high integrated circuits (e.g. Wu, Tang, Nam, and Tsai, 2003).

2. Application: Electron Transfer Theory

There are many examples of the use of the hyrodynamical formulation in research activities, especially in the fields of physical chemistry and electrical engineering. Based on the quantum trajectory method, quantum transport systems have already been simulated in the semi-classical domain (e.g. Garashchuck and Rassolov 2002, 2003a, 2003b, and 2004).[1] These semi-classical transport simulations constitute the major part of the now-well-recognized 'hydrodynamical interpretation of quantum mechanics' (Sanz, Borondo, and Miret-Artés 2002).[2]

As a more concrete example of the quantum trajectory method in the semi-classical electron transfer theory, some recent developments in simulating a MOSFET semi-conducting device can be discussed (for example, Wu, Tang, Nam, and Tsai 2003). Developing an electron transport theory in the semi-classical domain while preserving genuine full quantum effects is challenging because transport theory itself has evolved with time-dependent classical dynamical properties such as electron momentum, trajectories and collisions. While taking full advantage of the genuine quantum mechanical correction in the semi-classical region, it is possible to mobilize a classical, ontological and deterministic program in electron transport research under the Bohmian hydrodynamical version of quantum mechanics. The Bohmian pictures, as emphasized, provide an effective middle path of developing a dynamical theory of motion between classical and quantum mechanical domains.

[1] The titles of these papers are very illuminating. They are as follows.
(2002) "Semiclassical Dynamics Based on Quantum Trajectories."
(2003a) "Semiclassical Dynamics with quantum Trajectories: Formulation Comparison with the Semiclassical Initial Value Representation Propagator."
(2003b) "Quantum Dynamics with Bohmian Trajectories: Energy Conservation Approximation to the quantum Potential."
(2004) "Modified quantum Trajectory Dynamics Using a Mixed Wavefunction Representation."

[2] For further applications of the quantum trajectory method outside the semi-classical transport system, Sanz, Borondo, and Miret-Artés (2002) cite other quantum phenomena such as superconductivity and Bose-Einstein condensation, through the presence of vortices. Some developments of the quantum theory of magnetic monopoles, which generalizes the concept of quantum vortex, can also be included in the applications (Bialynicki-Birula and Bialynicka-Birula 1971). The concept was also applied to the well-known Aharonov-Bohm effect (Aharonov and Bohm 1959).

On the classical physics side, the limitation of the classical transport theory in the semi-classical domain is obvious. With the scaling down (i.e. miniaturization) of semi-conducting devices, it becomes increasingly important to consider various types of quantum effects, such as short channel effects (SCE), gate leakage currents, statistical dopant fluctuation, carrier confinement, and tunneling, etc. While it is temping to add some proper, but simple, quantum mechanical corrections based on the classical theory, finding such a simple and proper quantum correction is not easy because of conceptual inconsistencies between classical and quantum physics-tunneling itself being a primary example. Part of the inconsistency, of course, arises from the fact that the standard quantum mechanics does not have many of crucial classical concepts.

The problem of missing classical concepts in the standard quantum mechanics simply disappears in both de Broglie-Bohm ontological and Madelung-Bohm-Takabayasi hydrodynamical interpretations of quantum mechanics, since a particle's momentum and its trajectory at a given position are always well defined.[3] It is thus possible to develop a dynamical transport theory with genuine quantum corrections in the mesoscale based on these Bohmian models, since a single term called the quantum potential is responsible for all the quantum features. The 'wild' features in the quantum potential term become manageable at the mesoscale region because they are relatively small in magnitude and thus expandable in a mathematical series. After taking only a few of the dominating terms in the series expansion of the quantum potential, the Bohmian ontological quantum mechanics gives an effective, quantum-mechanically-corrected, electron transport theory in the mesoscale domain. The sum of the neglected terms in the series expansion can be taken as the calculation error involved in approximating the quantum potential.

For a large N system, as in the beginning of this chapter, the quantum potential is not so easily expandable in this sense. Scientists may then have to use a single particle equation of motion with the quantum potential corresponding to the single particle and a mean field approximation for the rest of the particles involved.[4] Alternatively, they can estimate the quantum potential term by trying a Gaussian functional fit to the quantum potential using the actual positional distribution of probability fluid elements, as seen earlier in the hydrodynamical formulation.

In particular, in the simulations by Wu, Tang, Nam, and Tsai (2003), electron transport in MOSFET devices was modeled for each electron based on a hydrodynamical (and ontological) picture of the underlying electron motions. This *single* particle Bohmian calculation was done very effectively with a minimum amount of computing time. Then, instead of repeating the Bohmian calculation over and over again for a whole bunch of other electrons, they performed a statistical Monte Carlo simulation of each electron's dynamical transport properties for an ensemble of electrons with the help of classical Boltzmann Transport Equation (BTE). At this stage, using the Bohmian calculation for a single particle as a template, they simulated various statistical deviations of each electron's dynamical properties under different initial conditions. Since the Bohmian scheme is applicable to both quantum and classical physics, this classical Monte Carlo simulation does not inherit any conceptual inconsistency from a usual semiclassical method. They call this scheme 'an effective conduction-band edge (ECBE) method' based on Madelung-Bohm-Takabayasi hyrodynamical formulation of a single-particle. Their dynamical simulations of the quantum mechanical BTE with particle ontology and visual trajectory extend classical ontology and causality directly into the mesoscale domain, with successful incorporation of many genuine quantum effects.

3. More Numerical Schemes

Regarding some more computational developments on Bohmian quantum mechanics, there are various "hybrid numerical schemes." For example, first, the Schrödinger equation from the standard quantum mechanics can be solved numerically, but later on the particles' momentum can be assigned for each given position of space through the Bohmian "guidance condition" introduced only as a "heuristic device." This thus gives researchers an opportunity to visualize the trajectory of a particle under the standard quantum mechanics. Although the hybrid scheme directly follows the standard framework, it nonetheless shows how constructively we could add or rather assign some key elements of classical metaphysics (such as realism and determinism) to a quantum system to develop some wider discussions without provoking any major interpretational issues (e.g. Heller 1975).

Wyatt (2005, p.94) summarizes the main computational features of the quantum trajectory methods as follows.

- Trajectories follow the main features of the [probability] density.
- [The methods] evolve an ensemble of N correlated trajectories.
- [The methods] integrate coupled equations of motion for density and action.
- Trajectory dynamics [is] correlated through the quantum potential.
- The quantum potential introduces all quantum effects.
- [The methods] can synthesize wavefunction along each evolving trajectory.
- [The methods require] no large basis sets or space fixed grids.
- [The methods require] no absorbing potentials at edges of region to absorb amplitude.

[3] Of course, it is the flows of probability density, not particles, that are always well defined at a given position and time in the hydrodynamical interpretation.

[4] In this way, the many-body problem of interacting electrons in a static external potential can be routinely handled by an effective potential or a mean field approximation. In Density Functional Theory (DFT), in particular, the so-called "local-density approximation" (LDA) is also commonly used to approximate the effective potential of the Coulomb interactions among electrons. Thus, in this DFT, the computational costs become low compared to the standard (semi-classical) quantum mechanical calculations such as Hartree-Fock theory, which is based on the complicated many-electron wavefunction. However, DFT does not necessarily offer better visualization on the quantum dynamical processes than the standard (semi-classical) approach.

- [In the methods] only the "classical" potential is needed, not the [classical] force.
- [The methods] could compute classical potential *V(r)* on the fly (a quantum Molecular Dynamics algorithm)
- [In the methods] computational effort scales as N, the number of fluid elements.
- [In the methods] computer code can be parallelized [for each trajectory of the flow].

As mentioned previously, however, de Broglie-Bohm ontological interpretation was not especially concerned with these numerical schemes; rather, the focus was on 'corpuscle propagation' using information gleaned from a pre-computed wavefunction. The ontological interpretation simply takes the wavefunction as a given solution of a quantum system in a form of 'a pilot wave.' In fact, it may be more practical just to get a solution directly from the linear Schrödinger equation; there is a group of (rather traditional) methods in which the wavefunction is obtained directly from the time-dependent Schrödinger equation by a suitable 'time propagation' scheme. Then, once Ψ (r,t) is known, quantum trajectories are then calculated by means of the guidance condition as a final step.

In this rather standard and direct computational approach within de Broglie-Bohm ontological interpretation, the corpuscle trajectories themselves are not used to solve the equations of motion as in the hydrodynamical formulation. Nonetheless, these trajectories are still "a means of understanding and exploring quantum behavior, that is, as a heuristic tool" (Bowman, 2002). Consequently, the (corpuscle) trajectories also play a significant role in de Broglie-Bohm formulation although actual calculations of the trajectories are rather done by a direct integration of the Schrödinger equation.

This direct computational scheme from the Schrödinger equation is more practically available for simple systems (i.e. one particle system as in the tunneling time calculation) where the time evolution of the wavefunction from the Schrödinger equation can be easily obtained (Dewdney and Malik 1993; Parmenter and Valentine 1995) by using the so-called 'spectral methods', in which Ψ (r,0) is projected onto the eigenstates of the corresponding Hamiltonians. For problems with more complicated potentials, the evolution of Ψ (r,t) is obtained by more sophisticated methods within a direct computational scheme, such as 'wave packet propagation' or the 'discretization' methods. The former scheme can be that of Heller (1975), in which the wavefunction is given in terms of Gaussian functions, whose evolution in time is calculated by a direct numerical integration.[5] The latter scheme is, on the other hand, based on a grid method, a discretization of the system both in space and time (Feit, Fleck and Steiger 1982; Kosloff and Kosloff 1983; Tal-Ezer and Kosloff 1984). This scheme includes the modern fast Fourier transform (FFT) methods (Press, Flannery, Teukolsky and Vetterling 1986, Ch. 12), Feynman path integrals (Philippidis, Dewdney and Hiley 1979) and Monte Carlo techniques (Oriols, Martín and Suñé 1996) to compute Bohmian trajectories.

Finally, a hybrid method of mixing the hydrodynamical scheme with classical dynamics, where some coordinates are considered classical while the others are described in terms of the hydrodynamical trajectories, has also been attempted (Gindensperger, Meier and Beswick 2000; Gindensperger, Meier and Beswick 2002; Gindensperger, Meier, Beswick and Heitz 2002). This method employs a quantum mechanical description of light particles such as electrons and protons, and classical trajectory evolution for heavier particles such as atomic nuclei. "There are consistent and accurate ways of handling this problem that make use of quantum trajectories for the quantum subsystem" (Wyatt 2005, p.27). This hybrid scheme shows the quantum trajectory scheme in the hydrodynamical formulation can be used to embrace both classical and quantum mechanical variables in a hybrid fashion with no abrupt 'quantum leap', or incommensurability inside. The hybrid scheme within the hydrodynamical formulation thus provides better conceptual justifications and faster and more stable numerical solutions in computational quantum chemistry than a usual semi-classical method in physics.

4. Summary

In this series of papers III - VI, a semi-classical method within the standard quantum mechanics is discussed as a common approach in which quantum mechanical variables are simply forced to work with classical variables in a frame of classical mechanics. However, this standard semiclassical approach seems to have some fundamental conceptual difficulties due to the incommensurability of the physical variables from classical and quantum mechanics. Furthermore, these standard hybrid models lack internal flexibility of adjusting their domains of application. Within Bohmian quantum mechanics, however, by adjusting the contribution of the quantum potential, it can be applicable to all the possible scales of physical domains. Thus, it is directly applicable to mesoscale domain and does not require any separate semiclassical approaches as in the standard quantum mechanics. Nevertheless, the Bohmian computational approaches also allow some other (Bohmian type) hybrid numerical schemes, too. In one form of the Bohmian hybrid scheme, the Schrödinger equation is first solved numerically, and then the particles' momentum can be later assigned through the Bohmian guidance condition. This gives researchers an opportunity to visualize the trajectory of a particle under the standard quantum mechanics. In a second form of the hybrid scheme, the hydrodynamical scheme is directly mixed with classical dynamics, where some coordinates are considered classical while the others are described in terms of hydrodynamical trajectories. These hybrid schemes show practical versatility and applicability of the Bohmian interpretations in various dynamical situations.

Furthermore, under the Bohmian ontological interpretation, tunneling is nothing but a simple dynamical motion of a particle that actually goes over the barrier with some additional boost from the quantum potential. Since a particle's visual trajectory is readily available, a particle's actual flight-time can be calculated for the entire path. On the other hand, 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. However, in order to run the hydrodynamical scheme, scientists need to have a complete knowledge of the

[5] Heller's art works previously also correspond to this direct numerical scheme of the Schrödinger equation combined with the guidance condition of the ontological interpretation.

wavefunction, 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 wavefunction in a 3N configuration space. This can be called 'semi-empirical thinking' (not to be confused with the semiclassical method). Several methods have been developed to estimate the initial value of the quantum potential. Based on this hydrodynamical interpretation, computational models have been developed to simulate the key functions of MOSFET integrated circuits. With the classical efficiency intact, these simulations have an effective quantum correction from the quantum potential.

5. References

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