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History and Philosophy of Quantum Mechanics IV: Tunneling Time Calculation

Yeuncheol Jeong
Department of History, Sejong University, Seoul, South Korea

Abstract:
Within Bohmian quantum mechanics, all the quantum effects originate from a single source of term called the quantum potential. Thus, by adjusting its contribution in the dynamical equations of motion, Bohmian mechanics can be applicable to all the possible scales of physical domains. Within the standard quantum mechanics, however, no dynamical process is given for tunneling. Thus, calculating expectation values of time from some other related physical processes is the only way to calculate the tunneling time. However, all the standard approaches suggested so far have deep conceptual problems that are serious enough to reject them all. However, under the 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 in the ontological formulation. On the other hand, the trajectories and the solutions are calculated concurrently as we move along with the 'fluid elements' in the hydrodynamical formulation.

1. Introduction

The exact source of quantum mechanical effects in the Schrödinger equation cannot be isolated within the equation itself. Rather, the entire equation is said to be the source of all the quantum effects. Within Bohmian quantum mechanics, however, all the effects originate from a single source of term called the quantum potential. It is by properly adjusting the contribution of the quantum potential that Bohmian mechanics is made applicable to all the possible scales of physical domain. For example, in the mesoscale region, the quantum potential cannot be ignored, but, at the same time, remains relatively small in its contribution. Thus, it can be expanded in a rapidly converging series before its first few terms are summed up to make an effective quantum correction for the region. Then, the disregarded remaining terms of the series constitute a numerical error involved in the approximate scheme. Thus, this gives chemists and engineers a powerful numerical scheme to continuously apply their dynamical models from the macroscopic to the microscopic domain.

2. Ontological and Hydrodynamical Formulations

With its classical ontology and determinism, both de Broglie-Bohm ontological and related Madelung-Bohm-Takabayasi hydrodynamical interpretation of quantum mechanics provide a continuous transition from the quantum domain up into the nanoscale. In principle, this transition can have varying degrees of adjustments from the appropriate corrections of the quantum potential, covering the full-scale spectrums of the nanoscale. It is possible because the single isolated term, the quantum potential, is allegedly responsible for all the quantum mechanical effects. Specifically, in the semi-classical region, the quantum potential is relatively small in its magnitude, thus, the quantum potential can be expanded in series, and then the first few dominating terms can be summed to be an effective quantum correction in the semi-classical domain, while the neglected remaining terms combined can be an calculation error involved in the series expansion.

However, there are some concerns with this series expansion of the quantum potential. For a system with N particles, the quantum potential is defined in a 3N configuration space. In this 3N multi-dimensional space with strong correlations between physical variables, expanding the quantum potential in series itself presents a daunting computational task. Simply taking the first few dominating terms of the series expansion may require a very fast convergence of the series in the first place. This effectively limits the scale domain of its application to be more classical, and the number of particles to be very small. Otherwise, for a larger N system, even in the 'classical' domain of application, the quantum potential is not quite expandable in any sense. In this case, scientists may instead have to use the single particle equation of motion with the quantum potential corresponding to that single particle and a 'mean field approximation' for the rest of the particles involved. This is feasible because for a single particle, the original 3N configuration variables in the quantum potential simply become 3-D variables of a familiar 3-D function. However, taking a mean field approximation for the rest of the particles implies that many of the non-local quantum effects tend to be lost, although the approximation is widely used in the standard quantum mechanical context.

This way of handling many-body problem of interacting electrons in a static external potential with an approximate effective potential (i.e. a mean field approximation) has also been routinely conducted in other successful frameworks including Density

Functional Theory (DFT). For example, in a particular DFT of Kohn-Sham DFT (KS DFT), the so-called "local-density approximation" (LDA) is used to approximate the effective potential of the Coulomb interactions among electrons. In general, DFT is an extremely successful approach for the description of ground state properties of an interacting system of electrons in metals, semiconductors, and insulators. The main idea of DFT is to describe the system via its density and not via its many-body wave function of the standard quantum mechanics. The computational costs of DFT are relatively low when compared to the standard (semi-classical) quantum mechanical calculations such as Hartree-Fock theory from the complicated many-electron wave function. According to Wikipedia, "DFT is now a leading method for electronic structure calculations in chemistry and solid-state physics," but, at the same time, "despite recent improvements, there are still difficulties in using density functional theory to properly describe intermolecular interactions, especially Vander Waals forces (dispersion); charge transfer excitations; transition states, global potential energy surfaces and some other strongly correlated systems; and in calculations of the band gap in semiconductors.[1]

Now, going back to the issue of approximating the quantum potential, rather than expanding the quantum potential, more creatively, under the hydrodynamical formulation, scientists can estimate the quantum potential term by (visually) fitting it to a Gaussian function from the actual positional distribution of 'fluid elements.' More specifically, this fitting procedure takes a couple of steps. First, the positional distribution of fluid elements can be visually determined by using a (Gaussian) fitting function. This is always possible because both each fluid element has a well defined (thus, visually accessible) position in real space in the hydrodynamical formulation. For example, in the simplest case, if the fluid elements are uniformly distributed throughout a given volume of space, then the probability density ρ of finding the fluid elements is unity inside the space and zero outside. Second, the probability density ρ is later translated into the amplitude (R) of the wave function in the Bohmian quantum mechanics from the equation (15) of 3.3 as follows.

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

From this, the amplitude R leads to the quantum potential itself. This entire fitting method within the hydrodynamical formulation is one of the main parts of the quantum trajectory method.

Furthermore, since both the ontological and the hydrodynamical interpretations of quantum mechanics conceptually embrace both classical and quantum mechanics with no abrupt conceptual 'quantum leap' in between, they can be used to work in conjunction with hybrid models. The two interpretations will thus help extend our cognitive capacity directly into the nano domain and, at the same time, give us faster, better and variable numerical corrections with reliable error estimates. In this way, scientists in nano research can have a realistic and deterministic quantum transport theory applicable both in classical and quantum domain. Through this Bohmian classical and deterministic picture of illustrations, researchers can conceive of the nano world being extended from a classical world with an appropriate error correction involved.

3. Tunneling Time Calculation under Ontological Formulation

There exists a conceptual question, nearly impossible to formulate properly within the standard quantum mechanics, but, at the same time, substantially easier to approach under the ontological interpretation. This question concerns tunneling. Tunneling is a quantum mechanical effect in which a given incoming particle has some probability of appearing on the other side of a potential barrier even though it has less energy than the potential barrier. Classically, it lacks the energy necessary to go through or over the barrier. Within the standard quantum mechanics, no dynamical process can be given in explaining tunneling. Instead, physicists simply state that such a particle has some "intrinsic" chance either to reflect back by or to tunnel into the barrier. The inability in providing an answer for tunneling time is mainly due to the fact that time is not an observable physical quantity in the standard quantum mechanics.

However, under the ontological interpretation, tunneling is nothing but a simple dynamical motion of a particle. Here, the particle actually goes over the barrier with some additional boost from the quantum potential. In this dynamical picture, each particle has a definite trajectory of motion with a well-defined momentum on every position. Thus, for each very small segment of the trajectory, actual flight-time can be calculated and then time can be summed up for the entire path, giving rise to a tunneling time (e.g. Dewdney *et al.* 1992; Leavens 1990a, 1990b). This is all possible because the visual trajectory is readily available to provide some clear cognitive (i.e. visual and intuitive) understanding of the actual dynamical process for tunneling.

There are questions related to time-dependent understanding of quantum transport phenomena that are only answerable by de Broglie-Bohm interpretation of quantum mechanics. One such question is "how much time does a quantum particle spend in a potential barrier when tunneling through it?" Here, a particle with lower kinetic energy can 'tunnel through' a potential barrier with higher energy. Given a potential barrier of a certain width, the barrier will have greater potential energy than an incoming

[1] The foundations of DFT were developed not by physicists, but by chemists for chemists, and now its success provides new and important experimental (and computational) works in chemistry, which nowadays easily cross the traditional boundary of being pure theoretical or experimental. In this respect, those (often simulated) experimental works motivated by DFT can be called 'synthetic.' So, DFT is an example that successful numerical computability can lead to a prolific generation of empirical outcomes. This point will be emphasized for the hydrodynamical interpretation of Bohmian quantum mechanics. However, DFT that offers an improved computational scheme does not necessarily offers better visualization on quantum dynamical processes than the standard (semi-classical) approach. On the other hand, Bohmian quantum mechanics with quantum trajectories, in this respect, not only provides an effective computational scheme but also offers functional (and visual) illustrations and metaphors on quantum dynamical processes. (For further discussions on DFT, see, for example, an on-line article, "A bird's-eye view of density-functional theory", by Klaus Capelle from arXiv:cond-mat/0211443v5.).

particle, e.g. an electron. Here, two detectors are placed on the particle's one-dimensional path before and after the barrier with known separation between them. Classically, of course, the particle cannot possibly go through the barrier to be detected on the other side of it. However, due to the tunneling effect, the particle has a certain degree of probability either to be reflected back to the first detector, or to be detected by the second detector on the other side of the barrier.

In recent years, the invention of various high-speed devices based on tunneling in semiconductors has brought new urgency to this question. At first, calculating the tunneling time seems simple, but this simplicity is deceptive. An understanding of the time-dependent aspects of tunneling is clearly required for the construction of a kinetic transport theory for such systems. This time-dependent understanding of tunneling phenomena, however, simply cannot be done outside the Bohmian interpretation (Cushing 1994, p.53). The first major difficulty is that time in quantum mechanics is simply a mathematical parameter. In the standard quantum mechanics, to find the average value of an observable, one usually computes the expectation value of the corresponding Hermitian operator. This cannot be done to find an average value for transit time since time cannot be represented by a Hermitian operator. Therefore, an attempt to calculate the expectation value of time cannot be physically meaningful in the first place. In addition, in the standard formulation of quantum mechanics, a particle does not have a well-defined trajectory in any quantum processes. There is thus no well-defined meaning to any transit time spent by an individual particle between any two points in space. Furthermore, the meaning of probability remains to be unclear in the standard formulation. What does having a certain degree of probability of 'going through' the barrier mean in the first place? Could this mean that some percentage of particles in an ensemble can go through the barrier while the others can't? Then, for a single particle, does the probability mean that it has a certain chance of tunneling if the same experiment is repeated multiple times? (A standard textbook in quantum mechanics will not say much here, except for the claim that there is no actual process of particles' going through the barrier.)

Nevertheless, several unsuccessful attempts under the usual quantum formalism have been proposed to define a sort of 'time' through some physical processes related to tunneling (Hauge and Støvneng, 1989). However, all of these approaches have been rejected by the authors themselves due to serious conceptual flaws in all of them. Their attempts include the followings from [1] to [6].

- In the method of the 'phase times' (and the closely related 'extrapolated phase time), a group velocity is measured following the peaks of the transmitted and the reflected wave packets, since the tunneling process causes spatial and temporal delays in the wave packets. However, the packets are too distorted during the tunneling process to give a definite group velocity. Therefore, the 'phase times' are essentially applicable only asymptotically in character (i.e. the packets are very far away to each other.). Then, with a sufficiently large interval of wave packets, the (extrapolated) phase times no longer represent the time spent in the small barrier region.
- In the method of the Stevens procedure, the group velocity of a wave packet is measured following the front of the wave packet. This is better than the method in [1], because the position of the front remains recognizable and moves through the barrier. However, once the wave packet gets inside of the barrier, no distinct front traveling through the barrier could be detected in numerical simulations.
- In the method of the 'dwell time', the standard statistical interpretation of a wave function is used. For a particle described by a wave packet Ψ (**x**,t), the probability of finding the particle on an arbitrary fixed interval (x_1, x_2) at time t is $P(t; x_1, x_2) = \int_{x1}^{x2} |\Psi(x,t)|^2 \, dx$. Then, the average time spent on (x_1, x_2) by the particle is $\bar{\tau}_D(x_1, x_2) = \int_{x1}^{x2} P(t; x_1, x_2) dt$. This is the 'dwell time' first introduced by Büttiker (1983). However, the 'dwell time' gives the time, averaged over all physical processes in the neighborhood of a barrier (i.e. reflection, self-interference and tunneling), thereby giving no tunneling probability separated from other probabilities. Furthermore, during the approach of the wave packet to the barrier, the incoming part of the wave function already interferes with the reflected part, and thus separating the tunneling probability alone is near impossible even in principle.
- In the method of the local Larmor time, a constant spin precession in a homogeneous magnetic field is utilized to measure the time involved. Here, an infinitesimal magnetic field of $B = B_0 \hat{z}$ in the z- axis covers the entire potential barrier. With the incident spin-1/2 particles polarized in the x direction, the time spent in the field region should be proportional to the averaged y-spin component $< s_y >$ of the particles. The Larmor times, however, have some terms oscillating with kx_1 or, kx_2 where k is a wave vector and the magnetic field covers the (x_1, x_2) interval. Due to this, the y-spin measurement also depends not on the interval but also on the (kinetic) energy of the incoming wave packet. Furthermore, the spin, originally polarized in the x direction, also has a probability of 1/2 of being spin-up or spin-down with respect to the field in the z-axis. This makes the time measurement complicating because the spin-up component will be preferentially transmitted. More seriously, in quantum mechanics, the very statement 'inside/outside' can violate the uncertainty principle. In order to minimize the 'inside/outside' uncertainty, the magnetic field region should sufficiently wide enough to cover the entire potential barrier region. Then, the particle bounces back and forth between the extra regions of the potential barrier and the magnetic field. This unknown number of additional multiple-scatterings can also cause a serious complication to the validity of the procedure.

- In the method of complex time, an action-path integral is performed to calculate the time. This involves the path-integral averaged over an arbitrary path from the initial point to the final one in a region containing the given interval in one dimension. Elegant as it is, this procedure in general generates complex numbers although the duration of a tunneling process must be real numbers.
- In the method of the Büttiker-Landauer time, an oscillating time-dependent potential barrier is used. For tunneling through a rectangular barrier with a small oscillating component added to the height, the incident particles, with energy E, can absorb or emit modulation quanta ħω during the tunneling process, leading to the appearance of sidebands with energies $E + n\hbar\omega$. Then, the relative sideband intensities could be identified with the traversal time for tunneling. In any case, a necessary requirement for a meaningful expression for reflection time τ_R and tunneling time τ_T is $\tau_D = R\tau_R + T\tau_T$, where *T* and *R*=1-*T* are the transmission and reflection probabilities, respectively. This is a direct consequence of the fact that an incident particle ends up either (not both) reflected or transmitted in the one-dimensional tunneling. The Büttiker-Landauer time, however, fails to satisfy this important necessary condition.

All of these methods are designed to indirectly measure some physical duration of processes during, before or after tunneling. However, all have been found to suffer from one flaw to another, "flaws sufficiently serious that they must be rejected" as Hauge and Støvneng themselves admit.

de Broglie-Bohm ontological interpretation, by contrast, can be and has been used to calculate the tunneling times. In the formalism, the transit time of a particle between any two points is conceptually well defined since the motion of a particle is completely deterministic, which provides some cognitive advantages through visualization. When a particle enters a region where the first detector is located, the initial particle momentum at that position is given by the 'guidance condition,' although the initial position is 'hidden'. Through this guidance condition, the particle's momentum is well defined all the time and therefore, the trajectory of the particle can be uniquely calculated. On this causal (and ontological) interpretation, the future behavior of a particle is completely determined by its initial position and also by the state represented by the wave function.

Tunneling occurs when a particle gets an agitation or a boost from the quantum potential determined by its position. Therefore, whether tunneling or reflecting takes place is determined by its guidance condition at the initial position of the particle. After the trajectory is calculated, it can be visualized. Then, for each very small segment of its visualized trajectory, scientists can figure out the time the particle spends on its small segment since both the velocity (momentum) and the length of the segment are readily available. Finally, simply adding the times on each segment through its entire trajectory will give either a reflection or a tunneling time for the particle. Dewdney, for example, has shown graphically the time evolution of the trajectories for a collection of incident particles (Dewdney 1992). Leavens has also done some numerical calculations for the various times related with tunneling (Leavens 1990a, 1990b).

Specifically, in both of their works, the initial position of a particle x_0 gives an initial momentum of $p_0 = \frac{\partial S(x)}{\partial x}\Big|_{x0}$. The time τ spent between x_1 and x_2 is determined from the calculated, thus visualized, trajectory as described above. These initial positions are then distributed according to $|\Psi(x_0)|^2$. The various kinds of τ such as τ_D , τ_R , and τ_T (dwell time, reflection time and tunneling time, respectively) can then be computed as

$$\tau_D = \int \tau(x_0)|\Psi(x_0)|^2 dx_0 ,$$

$$\tau_R = \frac{1}{R}\int_{\{R\}} \tau(x_0)|\Psi(x_0)|^2 dx_0 ,$$

$$\tau_T = \frac{1}{T}\int_{\{T\}} \tau(x_0)|\Psi(x_0)|^2 dx_0 ,$$

while *T* and *R*=1-*T* (the transmission and reflection probability) are

$$R = \int_{\{R\}} |\Psi(x_0)|^2 dx_0 ,$$

$$T = \int_{\{T\}} |\Psi(x_0)|^2 dx_0 .$$

These definitions, of course, satisfy the necessary requirement, $\tau_D = R\tau_R + T\tau_T$, for reflection and tunneling time.

However, this trajectory calculation can be very challenging to actually compute even for one particle system. Due to the quantum potential term, the equations of motion within de Broglie-Bohm ontological formulation involve a notorious set of time-dependent, non-linear, partial differential equations with singularities. In practice, therefore, scientists may need instead a complete solution from the corresponding linear time-dependent Schrödinger equation in connection with a guidance condition to get the trajectory available. However, solving the time-dependent Schrödinger equation alone is still a very demanding task computationally. De Broglie-Bohm ontological formulation does not give us any better way to solve of the equations of motion in

the first place. Rather, it is ontological and deterministic features that give us some cognitive advantages in understanding the quantum mechanical dynamics such as the tunneling process.

The hydrodynamical formulation of quantum mechanics does provide better numerical schemes to solve the equations of motions involved. In this sister formulation, we do not need a complete solution before to get the trajectories started. Instead, the trajectories and the solutions are calculated concurrently as we move along with the 'fluid elements' in the hydrodynamical formulation, while the trajectories themselves provides some up-to-date information for the solutions of the equations, and, at the same, the solutions themselves becomes further information for the progression of the trajectories.

4. References

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