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Short-time quantum propagator and Bohmian trajectories ☆

Maurice de Gosson [a,*], Basil Hiley [b]

[a] Universität Wien, Fakultät für Mathematik, NuHAG, Wien 1090, Austria
[b] University of London, Birkbeck College, Theoretical Physics Unit, London WC1E 7HX, United Kingdom

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ABSTRACT

We begin by giving correct expressions for the short-time action following the work Makri–Miller. We use these estimates to derive an accurate expression modulo Δt^2 for the quantum propagator and we show that the quantum potential is negligible modulo Δt^2 for a point source, thus justifying an unfortunately largely ignored observation of Holland made twenty years ago. We finally prove that this implies that the quantum motion is classical for very short times.

1. Introduction

In exploring the WKB limit of quantum theory, Bohm [2] was the first to notice that although one starts with all the ambiguities about the nature of a quantum system, the first order approximation fits the ordinary classical ontology. By that we mean that the real part of the Schrödinger equation under polar decomposition of the wave function becomes the classical Hamilton–Jacobi equation in the limit where terms involving $\hbar$ are neglected. In contrast to this approach, in this Letter we show that the classical trajectories arise from a short-time quantum propagator when terms of $O(\Delta t^2)$ can be neglected. This fact was actually already observed by Holland some twenty years ago: In page 269 of his book [6] infinitesimal time intervals are considered whose sequence constructs a finite path. It is shown that along each segment the motion is classical (negligible quantum potential), and that it follows that the quantum path may be decomposed into a sequence of segments along each of which the classical action is a minimum. The novel contribution of the present Letter is an improved proof of Holland's result using an improved version of the propagator due to Makri and Miller [9,10]. (See also de Gosson [3] for a further discussion.)

Now it is well known that explicit approximate expressions for the short-time action already play an essential role in various aspects of quantum mechanics (for instance the Feynman path integral, or semi-classical mechanics), and so does the associated Van Vleck determinant. Unfortunately, as already observed by Makri and Miller [9,10], these expressions, while giving the correct results for long time behavior, are not accurate enough to allow us to explore the short-time propagator rigorously. It is actually worse, the literature seems to be dominated by formulas which Makri and Miller show are wrong even to the first order of approximation!

These results have enabled us to provide precise estimates for the short-time Bohmian quantum trajectories for an initially sharply located particle. We will see that these trajectories are classical to the second order in time, due to the vanishing of the quantum potential for small time intervals.

In this Letter we sidestep the philosophical and ontological debate around the "reality" of Bohm's trajectories and rather focus on the mathematical issues.

2. Bohmian trajectories

Consider a time-dependent Hamiltonian function

$$H(x,p,t)=\sum_{j=1}^{n}\frac{p_j^2}{2m_j}+U(x,t) \tag{1}$$

and the corresponding quantum operator

$$\widehat{H}(x,-i\hbar\nabla_x,t)=\sum_{j=1}^{n}\frac{-\hbar^2}{2m_j}\frac{\partial^2}{\partial x_j^2}+U(x,t). \tag{2}$$

* Corresponding author. Tel.: +43 0 6767877995.
E-mail addresses: maurice.degosson@gmail.com, maurice.de.gosson@univie.ac.at (M. de Gosson).

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The associated Schrödinger equation is

$$i\hbar\frac{\partial\Psi}{\partial t}=\widehat{H}(x,-i\hbar\nabla_x,t)\Psi,\qquad \Psi(x,0)=\Psi_0(x). \tag{3}$$

Let us write Ψ in polar form $Re^{iS/\hbar}$; here $R=R(x,t)\geqslant 0$ and $S=S(x,t)$ are real functions. On inserting $Re^{iS/\hbar}$ into Schrödinger's equation and separating real and imaginary parts, one sees that the functions R and S satisfy, at the points (x,t) where $R(x,t)>0$, the coupled system of non-linear partial differential equations

$$\frac{\partial S}{\partial t}+\sum_{j=1}^{n}\frac{1}{2m_j}\left(\frac{\partial S}{\partial x_j}\right)^2+U(x,t)-\sum_{j=1}^{n}\frac{\hbar^2}{2m_jR}\frac{\partial^2 R}{\partial x_j^2}=0, \tag{4}$$

$$\frac{\partial R^2}{\partial t}+\sum_{j=1}^{n}\frac{1}{m_j}\frac{\partial}{\partial x_j}\left(R^2\frac{\partial S}{\partial x_j}\right)=0. \tag{5}$$

The crucial step now consists in recognizing the first equation as a Hamilton–Jacobi equation, and the second as a continuity equation. In fact, introducing the quantum potential

$$Q^{\Psi}=-\sum_{j=1}^{n}\frac{\hbar^2}{2m_jR}\frac{\partial^2 R}{\partial x_j^2} \tag{6}$$

(Bohm and Hiley [2]) and the velocity field

$$v^{\Psi}(x,t)=\left(\frac{1}{m_1}\frac{\partial S}{\partial x_1},\ldots,\frac{1}{m_n}\frac{\partial S}{\partial x_n}\right) \tag{7}$$

Eqs. (4) and (5) become

$$\frac{\partial S}{\partial t}+H(x,\nabla_x S,t)+Q^{\Psi}(x,t)=0, \tag{8}$$

$$\frac{\partial\rho}{\partial t}+\operatorname{div}(\rho v^{\Psi})=0,\quad \rho=R^2. \tag{9}$$

The main postulate of the Bohmian theory of motion is that particles follow quantum trajectories, and that these trajectories are the solutions of the differential equations

$$\dot{x}_j^{\Psi}=\frac{\hbar}{m_j}\operatorname{Im}\frac{1}{\Psi}\frac{\partial\Psi}{\partial x_j}. \tag{10}$$

The phase space interpretation is that the Bohmian trajectories are determined by the equations

$$\dot{x}_j^{\Psi}=\frac{1}{m_j}p_j^{\Psi},\qquad \dot{p}_j^{\Psi}=-\frac{\partial U}{\partial x_j}(x^{\Psi},t)-\frac{\partial Q^{\Psi}}{\partial x_j}(x^{\Psi},t). \tag{11}$$

It is straightforward to check that these are just Hamilton's equations for the Hamiltonian function

$$H^{\Psi}(x,p,t)=\sum_{j=1}^{n}\frac{p_j^2}{2m_j}+U(x,t)+Q^{\Psi}(x,t) \tag{12}$$

which can be viewed as a perturbation of the original Hamiltonian H by the quantum potential Q^{Ψ} (see Holland [7,8] for a detailed study of quantum trajectories in the context of Hamiltonian mechanics).

The Bohmian equations of motion are *a priori* only defined when $R\neq 0$ (that is, outside the nodes of the wave function); this will be the case in our constructions since for sufficiently small times this condition will be satisfied by continuity if we assume that it is case at the initial time.

An important feature of the quantum trajectories defined above is that they cannot cross; thus there will be no conjugate points like those that complicate the usual Hamiltonian dynamics.

3. The short-time propagator

The solution Ψ of Schrödinger's equation (3) can be written

$$\Psi(x,t)=\int K(x,x_0;t)\Psi_0(x_0)\,dx_0 \tag{13}$$

where the kernel K is the quantum propagator:

$$K(x,x_0;t)=\langle x|\exp(-i\widehat{H}t/\hbar)|x_0\rangle. \tag{14}$$

Schrödinger's equation (3) is then equivalent to

$$i\hbar\frac{\partial K}{\partial t}=\widehat{H}(x,-i\hbar\nabla_x,t)K,\qquad K(x,x_0;0)=\delta(x-x_0) \tag{15}$$

where δ is the Dirac distribution. Physically this equation describes an isotropic source of point-like particle emanating from the point x_0 at initial time $t_0=0$. We want to find an asymptotic formula for K for short time intervals Δt. Referring to the usual literature (see, e.g., Schulman [11]), such approximations are given by expressions of the type

$$K(x,x_0;\Delta t)=\left(\frac{1}{2\pi i\hbar}\right)^{n/2}\sqrt{\rho(x,x_0;\Delta t)}\exp\left(\frac{i}{\hbar}S(x,x_0;\Delta t)\right)$$

where $S(x,x_0;\Delta t)$ is the action along the classical trajectory from x_0 to x in time Δt and

$$\rho(x,x_0;\Delta t)=\det\left(-\frac{\partial^2 S(x,x_0;\Delta t)}{\partial x_j\partial x_k}\right)_{1\leqslant j,k\leqslant n}$$

is the corresponding Van Vleck determinant. We will need precise short-time behavior of the action. In this regard Makri and Miller [9,10] have shown that the asymptotic expression for the generating function is given by

$$S(x,x_0;\Delta t)=\sum_{j=1}^{n}\frac{m_j}{2\Delta t}(x_j-x_0)^2-\widetilde{U}(x,x_0)\Delta t+O(\Delta t^2) \tag{16}$$

where $\widetilde{U}(x,x_0,0)$ is the average value of the potential over the straight line joining x_0 at time t_0 to x at time t with constant velocity:

$$\widetilde{U}(x,x_0)=\int_0^1 U(\lambda x+(1-\lambda)x_0,0)\,d\lambda. \tag{17}$$

For instance when

$$H(x,p)=\frac{1}{2m}(p^2+m^2\omega^2x^2)$$

is the one-dimensional harmonic oscillator formula (16) yields the correct expansion

$$S(x,x_0;t)=\frac{m}{2\Delta t}(x-x_0)^2-\frac{m\omega^2}{6}(x^2+xx_0+x_0^2)\Delta t+O(\Delta t^2), \tag{18}$$

the latter can of course be deduced directly from the exact value

$$S(x,x_0;t,t_0)=\frac{m\omega}{2\sin\omega\Delta t}\left((x^2+x_0^2)\cos\omega\Delta t-2xx_0\right) \tag{19}$$

by expanding $\sin\omega\Delta t$ and $\cos\omega\Delta t$ for $\Delta t\to 0$.

Introducing the following notation,

$$\widetilde{S}(x,x_0;\Delta t)=\sum_{j=1}^{n}m_j\frac{(x_j-x_0)^2}{2\Delta t}-\widetilde{U}(x,x_0)\Delta t, \tag{20}$$