Quantum corrections to classical trajectories

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Abstract. A consistent formalism with quantum mechanics, different from Bohmian mechanics, which describes the quantum corrections to classical trajectories, is developed. The quantum potential of Bohmian mechanics is part of the kinetic energy in our formalism. The difficulties of the Bohmian mechanics formalism are pointed out.

1. Introduction

David Bohm \cite{1} in 1952 has suggested a causal interpretation of quantum mechanics by introducing the concept of quantum potential. Bohm started with the one-particle Schrödinger equation,

\[ i\hbar \partial \psi / \partial t = -(\hbar^2 / 2m)\nabla^2 \psi + V (x) \psi, \]  
\( (1) \)

assuming the wave function \( \psi \) can be expressed as,

\[ \psi = R \exp (iS/\hbar), \]  
\( (2) \)

where \( R \) and \( S \) are real functions of spatial coordinates and time. Substituting Eq.(2) in Eq.(1) we obtain,

\[ i\hbar \partial \psi / \partial t = \hbar (\partial / \partial t) (R \exp(iS/\hbar)) = \exp(iS/\hbar) [i\hbar (\partial R/\partial t) - R \partial S/\partial t], \]  
\( (3) \)

and

\[ [-\psi^* (\hbar^2 / 2m) \nabla^2 \psi + V (x) \psi] / (\psi^* \psi) = \]
\[ = \left( -\frac{\hbar^2 \nabla^2 R}{R} - 2i\hbar (\nabla R) (\nabla S) - i\hbar (\nabla^2 S + (\nabla S)^2) \right) / (2m) + V (x). \]  
\( (4) \)

Substituting Eq.(3) and Eq.(4) into Eq.(1) we obtain,

\[ -R \partial S/\partial t + i\hbar (\partial R/\partial t) = \]
\[ = \left( -\frac{\hbar^2 \nabla^2 R - 2i\hbar (\nabla R) (\nabla S) - i\hbar (\nabla^2 S) R + R (\nabla S)^2}{(2m)} \right) + V (r) R. \]  
\( (5) \)
The real part of Eq.(5) is,
\[
-\partial S/\partial t = H = -\hbar^2 \nabla^2 R / (2mR) + (\nabla S)^2 / (2m) + V(r).
\]
where \(H\) is the Hamiltonian. Let us denote by \(Q\) the quantum potential,
\[
Q(R) = -\hbar^2 \nabla^2 R / (2mR),
\]
then the real part is
\[
-\partial S/\partial t = H = (\nabla S)^2 / (2m) + V(r) + Q(r).
\]
The imaginary part of Eq.(5) is,
\[
\partial R/\partial t = -2(\nabla R) (\nabla S) - (\nabla^2 S) R / (2m).
\]
In the classical Hamilton-Jacobi equation (see Appendix) the momentum \(p(x)\) and the Hamiltonian \(H\) are coordinate dependent [9], and given by,
\[
p(x,t) = \nabla S, \quad \partial S/\partial t = -H(x,p,t)
\]
while in classical mechanics the momentum is coordinate independent. Bohm found that the phase \(S\) of the wavefunction \(\psi\) of Eq(2) has similar properties to the action of the Hamilton-Jacobi equation.

Bohm interpreted Eq.(8) as the classical Hamilton-Jacobi equation with the quantum correction, the quantum potential \(Q\), Eq(7). In his formalism the trajectories are subjected to boundary conditions and are not related to quantum probabilities.

2. Dirac’s work

Dirac [2], already in 1955 has observed that the phase of the wavefunction \(S\), of Eq(2), has similar properties to the action of the Hamilton-Jacobi Equation, (see Appendix). In his seminal book [3] he further developed these relations, which inspired Richard Feynman [4] to develop his path integral approach to quantum mechanics.

3. Ehrenfest’s theorem

Ehrenfest theorem [6] states, that the expectation values of the position and momentum operators \(\hat{x}\) and \(\hat{p}\) are related to the force \(F = -V'(x)\), where \(V(x)\) is the scalar potential as,
\[
m \frac{d}{dt} <\hat{x}> = <\hat{p}> , \quad \frac{d}{dt} <\hat{p}> = - <V' <\hat{x}> >.
\]
Ehrenfest theorem was generalized by Heisenberg. For an operator \(\hat{A}\)
\[
\frac{d}{dt} <\hat{A}> = \frac{1}{i\hbar} <[\hat{A}, \hat{H}] > + < \frac{\partial \hat{A}}{\partial t} >.
\]
Clearly, the expectation values do not satisfy Newtons equations exactly, though they do reproduce the quantum equations Eq(12). [8].

In the next section we suggest to apply quantum expectation values of the quantum operators to evaluate quantum corrections to classical trajectories.
4. Observables at points along trajectories

Influenced by the works of Dirac, Feynman, Ehrenfest and Bohm. We consider the summation of all points on the trajectories including their quantum probabilities.

Let us start with the quantum formula for the expectation value of the operator \( \hat{A} \),

\[
< \hat{A} > = \int \int \int \psi^*(x,y,z) \hat{A} \psi(x,y,z) \, dx \, dy \, dz,
\]

where \( \psi \) is the wave function satisfying the normalization condition,

\[
\int \int \int \psi^*(x,y,z) \psi(x,y,z) \, dx \, dy \, dz = 1.
\]

We may rewrite Eq.(13) as,

\[
< \hat{A} > = \int \int \int \left[ \psi^*(\vec{r}) \chi(\vec{r}) \right] \psi^*(\vec{r}) \hat{A} \psi(\vec{r}) \, d^3\vec{r} = \int \int \int A(\vec{r}) \, d^3\vec{r},
\]

where

\[
P(\vec{r}) = \left[ \psi(\vec{r})^* \psi(\vec{r}) \right]
\]

is the probability at the point \( \vec{r} \), and \( d^3\vec{r} = dx \, dy \, dz \). Let us define \( A(\vec{r}) \),

\[
A(\vec{r}) = \frac{\psi^*(\vec{r}) \hat{A} \psi(\vec{r})}{\left[ \psi^*(\vec{r}) \psi(\vec{r}) \right]},
\]

as the value of the operator \( \hat{A} \) at a point \( \vec{r} \).

We may now interpret Eq.(15) following Feynman’s path integral \([4,5]\) as a sum of all possible trajectories weighted with their quantum probabilities.

Let us consider important examples:

**Kinetic energy**

From Eq.(17) for the kinetic energy operator one obtains,

\[
E_{\text{kin}}(\vec{r}) = \frac{\psi^*(\vec{r}) (-i \hbar \nabla)^2 \psi(\vec{r})}{2m \left[ \psi^*(\vec{r}) \psi(\vec{r}) \right]}
\]

\[
= \left( -\hbar^2 \left( \nabla^2 R \right) / R + (\nabla S)^2 \right) / (2m) + i \hbar \left( \partial R / \partial t \right) / R.
\]

With \( \psi(\vec{r}) \) being a solution of the Schrödinger equation, we have the relation Eq(9)

\[
\partial R / \partial t = -2 (\nabla R) (\nabla S) - (\nabla^2 S) R / (2m),
\]

and we can write,

\[
E_{\text{kin}}(\vec{r}) = \frac{(\nabla S)^2}{2m} + Q(r) + i \hbar \frac{(\partial R / \partial t)}{R}.
\]

Now Eq.(8) can be rewritten as, \( Q(R) = -\hbar^2 \nabla^2 R / (2mR)\),

\[
-\partial S / \partial t = H = (\nabla S)^2 / (2m) + V(r) + Q(r) = E_{\text{kin}}(\vec{r}) + V(\vec{r}),
\]

where the quantum potential \( Q(r) \) is given by Eq.(7) and \( E_{\text{kin}}(\vec{r}) \) is given by Eq.(21).
5. Momentum

For the momentum we find,

\[ p(\vec{r}, t) = \frac{R \exp \left(-\frac{iS}{\hbar}\right)(-i\hbar \nabla) R \exp \left(i\frac{S}{\hbar}\right)}{R^2} = \nabla S - i\hbar \frac{\nabla R}{R} \]  

(23)

The importance of the imaginary parts

Above, both the kinetic energy and the momentum have imaginary parts due to non-vanishing partial time derivative and gradient of the function \( R \). These are necessary for allowing bound states and resonance solutions.

6. Summary and conclusions

We have suggested in this paper a formalism of quantum corrections to classical trajectories, which is consistent with Feynman’s ideas that between two points all classical trajectories are possible, restricted to their quantum probabilities. We were also influenced by Ehrenfest’s ideas of the relations between quantum expectation values and classical trajectories. We have assumed that,

the expectation value of an operator \( \hat{A} \) as given by,

\[ < \hat{A} > = \int \int \int P(\vec{r}) A(\vec{r}) d^3 \vec{r}, \]  

(24)

where \( P(\vec{r}) \) is the quantum probability,

\[ P(\vec{r}) = |\psi(\vec{r}, t)|^2, \]  

(25)

where \( \psi(\vec{r}) \) is the normalized wave function, and \( A(\vec{r}) \) represent the classical observable along the trajectory. We followed the interesting idea of P.A.M. Dirac and of David Bohm that the phase of the wavefunction has similar properties to Hamilton’s action.

Our work is not yet complete; we have to better understand what is the role of the imaginary parts of the momentum and kinetic energy.

Appendix A. Hamilton-Jacobi equation

The Hamilton’s principal function

\[ S(q, t) = \int_{(q,t)}^{(q,t)} \mathcal{L} dt, \]  

(A.1)

is the upper limit of the action integral along the minimal action trajectory. \( \mathcal{L} \) is the Lagrangian which satisfies the Euler-Lagrange equation,

\[ \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial \mathcal{L}}{\partial q} \]  

(A.2)
The action $S$ satisfies the Hamilton Jacobi equation [9]

$$\frac{\partial S}{\partial q} = p, \text{ the momentum}$$  \hspace{1cm} (A.3)

where $H$ is the Hamiltonian, and also $H = \frac{\partial \mathcal{L}}{\partial \dot{q}} \dot{q} - \mathcal{L}$.

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