Quantum corrections to clasical trajectories.

Alexander Gersten and Amnon Moalem
Department of Physics, Ben Gurion University of the Negev
Beer Sheva, Israel

May 31, 2020

Abstract

A consistent formalism with quantum mechanics, different from Bohmian mechanics, which describes the quantum corrections to classical trajectories, is developed. Our theory is based on Ehrenfest theorem and Feynman's path integrals.The quantum potential of Bohmian mechanics is part of the kinetic energy in our formalism. The difficulties of of the formalism of Bohmian mechanics are pointed out.

1 Introduction

David Bohm[1] in 1952 has suggested a causal interpretation of quantum mechanics by introducing the concept of quantum potential.

Bohm started with the one-particle Schroedinger equation,

$$i\hbar\partial\psi/\partial t = -(\hbar^2/2m)\nabla^2\psi + V(\boldsymbol{x})\,\psi, \tag{1}$$

assuming the wave function ψ can be expressed as

$$\psi = R\exp\left(iS/\hbar\right), \tag{2}$$

where R and S are real functions of spatial coordinates and time.

Substituting Eq.(2) in Eq.(1) , we obtain,

$$i\hbar\partial\psi/\partial t = i\hbar\left(\partial/\partial t\right)\left(R\exp(iS/\hbar)\right) = \exp(iS/\hbar)\left[i\hbar\left(\partial R/\partial t\right) - R\partial S/\partial t\right], \tag{3}$$

and

$$\left[-\psi^*(\hbar^2/2m)\nabla^2\psi + V(\boldsymbol{x})\,\psi\right]/\left(\psi^*\psi\right) =$$

$$= \left(\frac{-\hbar^2\nabla^2 R}{R} - \frac{2i\hbar\left(\nabla R\right)\left(\nabla S\right)}{R} - i\hbar\left(\nabla^2 S\right) + \left(\nabla S\right)^2\right)/(2m) + V(\boldsymbol{x}). \tag{4}$$

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

$$-R\partial S/\partial t+i\hbar\left(\partial R/\partial t\right)=$$

$$=\left(-\hbar^2\nabla^2 R-2i\hbar\left(\nabla R\right)\left(\nabla S\right)-i\hbar\left(\nabla^2 S\right)R+R\left(\nabla S\right)^2\right)/(2m)+V\left(\boldsymbol{x}\right)R \quad (5)$$

The real part of Eq.(5) is,

$$-\partial S/\partial t=H=-\hbar^2\nabla^2 R/(2mR)+\left(\nabla S\right)^2/(2m)+V\left(\boldsymbol{x}\right). \quad (6)$$

where H is the Hamiltonian.
Let us denote by Q the quantum potential,

$$Q\left(R\right)=-\hbar^2\nabla^2 R/(2mR), \quad (7)$$

then the real part is

$$-\partial S/\partial t=H=\left(\nabla S\right)^2/(2m)+V\left(\boldsymbol{x}\right)+Q. \quad (8)$$

The imaginary part of Eq.(5) is,

$$\partial R/\partial t=\left(-2\left(\nabla R\right)\left(\nabla S\right)-\left(\nabla^2 S\right)R\right)/(2m). \quad (9)$$

In the classical Hamilton-Jacobi equation the momentum $\mathbf{p}(\mathbf{x})$ and the Hamiltonian H are coordinate dependent[8], given by,

$$\mathbf{p}(\mathbf{x})=\nabla S,\quad \frac{\partial S}{\partial t}=-H, \quad (10)$$

while in classical mechanics the momentum is coordinate independent.

Bohm interpreted Eq.(6) 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 Ehrenfest's theorem[4],

Ehrenfest theorem[5],[6],[7] 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,

$$m\frac{d}{dt}<\hat{x}>=<\hat{p}>,\ \frac{d}{dt}<\hat{p}>=-<V'<\hat{x}>>. \quad (11)$$

$$m\frac{d\boldsymbol{x}}{dt}=\frac{\nabla S}{2m}-i\hbar\frac{\nabla R}{2mR}$$

Ehrenfest theorem was generalized by Heisenberg. For an operator $\hat{A}$

$$\frac{d}{dt} < \hat{A} >= \frac{1}{i\hbar} < [\hat{A}, \hat{H}] > + < \frac{\partial \hat{A}}{\partial t} > . \tag{12}$$

Clearly, the expectation values do not satisfy Newtons equations exactly, though they do reproduce the quantum equations Eq(12).[7].

In the next section we sugggest to apply quantum expectation values of the quantum operators to evaluate quantum corrections to classical trajectories.

3 Observables at points along trajectories

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

$$< \hat{A} >= \int\int\int \psi^*(x, y, z)\hat{A}\psi(x, y, z)dxdydz, \tag{13}$$

where ψ is the wave function satisfying the normalization condition,

$$\int\int\int \psi^*(x, y, z)\psi(x, y, z)dxdydz = 1. \tag{14}$$

We may rewrite Eq.(13) as,

$$< \hat{A} >= \int\int\int [\psi^* (\vec{r})\, \psi (\vec{r})] \frac{\psi^* (\vec{r})\, \hat{A}\psi (\vec{r})}{[\psi^* (\vec{r})\, \psi (\vec{r})]} d^3\vec{r} = \int\int\int P (\vec{r})\, A (\vec{r})\, d^3\vec{r}, \tag{15}$$

where

$$P (\vec{r}) = \left[\psi (\vec{r})^* \psi (\vec{r})\right] \tag{16}$$

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

$$A (\vec{r}) = \frac{\psi^* (\vec{r})\, \hat{A}\psi (\vec{r})}{[\psi^* (\vec{r})\, \psi (\vec{r})]}, \tag{17}$$

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

We may now interprete Eq.(15) following Feynman's path integral[2],[3] as a sum of all trajectories possible between two points wheighted with respect to their quantum probabilities.
Let us consider important examples:

3.1 Kinetic energy

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

$$E_{kin}(\vec{r}) = \frac{\psi^* (\vec{r}) (-i\hbar\nabla)^2 \psi (\vec{r})}{2m [\psi^* (\vec{r}) \psi (\vec{r})]} \tag{18}$$

$$= \left(-\hbar^2(\nabla^2 R)/R + (\nabla S)^2\right)/(2m) + i\hbar(\partial R/\partial t)/R. \tag{19}$$

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

$$\partial R/\partial t = \left(-2 (\nabla R) (\nabla S) - \left(\nabla^2 S\right) R\right)/(2m), \tag{20}$$

and we can write,

$$E_{kin}(\vec{r}) = \frac{(\nabla S)^2}{2m} - \frac{\hbar^2(\nabla^2 R)}{2mR} + i\hbar\frac{(\partial R/\partial t)}{R}. \tag{21}$$

Now Eq.(8) can be rewritten as,

$$-\partial S/\partial t = (\nabla S)^2/(2m) + V(\boldsymbol{x}) + Q = E_{kin}(\vec{r}) + V(\vec{r}), \tag{22}$$

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

4 Momentum

For the momentum we find,

$$\boldsymbol{p}(\vec{r}) = \frac{R\exp(-iS/\hbar)(-i\hbar\nabla) R\exp(iS/\hbar)}{2mR^2} = \frac{\nabla S}{2m} - i\hbar\frac{\nabla R}{2mR} \tag{23}$$

4.1 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 nessesary for allowing bound states and resonances solutions.

5 Summary and conclusions

We have suggested in this paper a formalism of quantum corrections to classical trajectories, which is consistent with Feyman'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 trjectories. We have assumed that,

the expectation value of an operator $\hat{A}$ is given by,

$$< \hat{A} >= \int\int\int P\left(\vec{r}\right) A\left(\vec{r}\right) d^3\vec{r}, \tag{24}$$

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

$$P\left(\vec{r}\right) = \left[\psi\left(\vec{r}\right)^* \psi\left(\vec{r}\right)\right], \tag{25}$$

where $\psi\left(\vec{r}\right)$ is the normalized wave function, and $A(\vec{r})$ represent the classical observable along the trajectory.

Our work is not yet complete, we have to understand better how to perform the summation over all the trajectories and to understand what is the role of the imaginary parts of the momentum and kinetic energy.

References

[1] Bohm D., A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables. I, *Phys. Rev.* **85**, 166-179 (1952).

[2] Feynman R.P., Hibbs A.R., and Styer D.F., *Quantum mechanics and path integrals*, McGraw-Hill, New York (2005).

[3] Chaichian M., and Demichev A., *Path Integrals in Physics, Volume I,* Institute of Physics Publishing, Bristol and Philadelphia (2001).

[4] *Vikipedia*- "Ehrenfest theorem"

[5] Ehrenfest P. (1927) Zeitschrift fúr Physik, **45**, Issue 7-8, pp. 455-457

[6] Hall, Brian C. (2013), Quantum Theory for Mathematicians,*Graduate Texts in Mathematics*, 267, Springer

[7] Bondar, D. et al,(2012) "Operational Dynamic Modeling Transcending Quantum and Classical Mechanics". *Physical Review Letters.* **109**(19)

[8] Gersten A. "Tensor Lagrangians, Lagrangians Equivalent to the Hamilton-Jacobi Equation and Relativistic Dynamics" *Found Phys* (2011) **41**: 88–98