Bohm’s Quantum Potential as an Internal Energy

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Abstract

We pursue our discussion of Fermi’s surface initiated in Dennis, de Gosson and Hiley and show that Bohm’s quantum potential can be viewed as an internal energy of a quantum system. This gives further insight into the role it played by the quantum potential in stationary states. It also allows us to provide a physically motivated derivation of Schrödinger’s equation for a particle in an external potential.

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1 Introduction

The time evolution of a quantum system with wavefunction \( \psi = \psi(\mathbf{r},t) \) in physical space, \( \mathbb{R}^3 \), is governed, in non-relativistic quantum mechanics, by the Schrödinger equation

\[
i\hbar \frac{\partial \psi}{\partial t}(\mathbf{r},t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r},t) + V(\mathbf{r},t)\psi(\mathbf{r},t). \tag{1}\]

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Writing the wavefunction in polar form \( \psi(r, t) = R(r, t)e^{iS(r, t)/\hbar} \), this equation is mathematically equivalent to the system of real equations:

\[
\frac{\partial S}{\partial t}(r, t) + \frac{1}{2m}(\nabla_r S(r, t))^2 + Q(r, t) + V(r, t) = 0 \quad (2)
\]

\[
\frac{\partial \rho}{\partial t}(r, t) + \nabla_r \cdot \left( \rho(r, t) \frac{\nabla_r S}{m}(r, t) \right) = 0. \quad (3)
\]

Equation (2) can be regarded as a Hamilton–Jacobi equation derived, not from the classical Hamiltonian, but from the \( \psi \)-dependent Hamiltonian

\[
H^{\psi}(r, p, t) = \frac{1}{2m}|p|^2 + Q(r, t) + V(r, t).
\]

Equation (3) can be viewed as a continuity equation for the probability \( \rho(r, t) = R^2(r, t) \). We are going to show that the additional term \( Q(r, t) \) (the “quantum potential”) can be interpreted as an internal energy associated with a certain region of phase space, absent in classical mechanics, but arising in quantum mechanics from the uncertainty principle. In order to explain how this internal energy arises we must first return to consider arguments outlined in our recent paper \[5\] where we investigated the consequences of Fermi’s idea \[7\] which associated every quantum state with a certain geometric curve or, more generally, a hypersurface in phase space.

## 2 The Fermi Hamiltonian

Consider a wavefunction \( \psi_0(r) = R_0(r)e^{iS_0(r)/\hbar} \), which we assume represents a particle with mass \( m \) in physical space \( \mathbb{R}^3 \) at the initial time \( t = 0 \); here \( r = (x, y, z) \) is the position vector. At this point we do not consider an explicit time dependence of \( \psi_0 \). We assume that \( R_0(r) > 0 \) and that \( R_0 \) is twice continuously differentiable, and that the phase \( S_0 \) is real and continuously differentiable. It is easily verified that the function \( \psi_0 \) satisfies the second-order partial differential equation

\[
\left[ \frac{1}{2m} \left(-i\hbar \nabla_r - \nabla_r S_0(r) \right)^2 + \frac{\hbar^2}{2m} \frac{\nabla^2_r R_0(r)}{R_0(r)} \right] \psi_0(r) = 0; \quad (4)
\]

this can be done by a direct calculation, or by noting that a change of gauge making \( S_0 = 0 \), immediately gives

\[
-\frac{\hbar^2}{2m} \left[ \nabla^2_r - \frac{\nabla^2_r R_0(r)}{R_0(r)} \right] R_0(r) = 0.
\]
We can rewrite equation (4) more concisely as \( \hat{H}_F \psi = 0 \) where \( \hat{H}_F \) is the “Fermi operator”

\[
\hat{H}_F = \frac{1}{2m} (-i\hbar \nabla_r - \nabla_r S_0(r))^2 - Q_0(r). 
\]  

(5)

The function \( Q_0 \) is given by

\[
Q_0(r) = -\frac{\hbar^2}{2m} \frac{\nabla_r^2 R_0(r)}{R_0(r)}. 
\]  

(6)

One immediately recognizes that \( Q_0 \) is the quantum potential at time \( t = 0 \). The operator \( \hat{H}_F \) is the quantization (in any reasonable quantization scheme) of the Hamiltonian function

\[
H_F(r, p) = \frac{1}{2m} |p - \nabla_r S_0(r)|^2 - Q_0(r). 
\]  

(7)

Let us consider the energy hypersurface

\[
\Sigma_F : H_F(r, p) = 0, 
\]  

(8)

and assume that this hypersurface is the boundary of a phase space set \( \Omega_F \). Following Fermi, we can then identify \( \Omega_F \) with the quantum particle described by the wavefunction \( \psi_0 \). One can show that this identification is compatible with the uncertainty principle in the following sense: in quantum mechanics, the notion of a particle existing at a point in phase space does not make sense.

The set \( \Omega_F \) may therefore be viewed as the “blow-up” of such a point, in fact the smallest entity unfolded from a point allowed by the uncertainty principle. This blow-up requires energy, and this energy is the quantum potential \( Q_0 \). We view it as an internal energy associated with the quantum particle, whose total energy is thus given by

\[
E = E_{\text{kin}} + Q_0 + E_{\text{pot}}. 
\]  

(9)

Note that both \( E_{\text{kin}} \) and \( Q_0 \) are internal energies, as opposed to \( E_{\text{pot}} \) which is energy coming from an external source.

The case of a real bound quantum state is particularly instructive and will be illustrated in the next section in the case of the harmonic oscillator. Assume \( S_0 = 0 \) and that

\[
\left[ -\frac{\hbar^2}{2m} \nabla_r^2 + V(r) \right] \psi_0(r) = E\psi_0(r). 
\]
Using (5) we also have
\[
\left[ -\frac{\hbar^2}{2m} \nabla_r^2 - Q_0(r) \right] \psi_0(r) = 0.
\]
Hence, by subtracting these equations, we find the total energy is given by
\[
E = V(r) + Q_0(r). \tag{10}
\]
It follows that the classical force \( F_c = -\nabla_r V(r) \) and \( F_Q = -\nabla_r Q(r) \) sum up to zero: \( F_c + F_Q = 0 \). This is perfectly in accordance with the fact that in Bohm’s theory of quantum motion, the particle in a bound real state is at rest since \( E_{\text{kin}} = 0 \). Let us probe this counter-intuitive result further.

3 Example: the Isotropic Harmonic Oscillator

Let us illustrate the above conclusions with a simple but instructive example. Choose for \( \psi_0 \), the coherent state
\[
\psi_0(r) = e^{-m\omega|\mathbf{r}|^2/2\hbar}
\]
where \( |\mathbf{r}|^2 = x^2 + y^2 + z^2 \). A straightforward calculation yields
\[
Q_0(r) = -\frac{1}{2} m\omega^2 |\mathbf{r}|^2 + \frac{3\omega \hbar}{2}.
\]
Hence the Fermi operator is \( \hat{H}_F = \hat{H}_0 - \frac{3}{2}\omega \hbar \) where
\[
\hat{H}_0 = -\frac{\hbar^2}{2m} \nabla_r^2 + \frac{1}{2} m\omega^2 |\mathbf{r}|^2.
\]
One thus recovers the fact that \( \psi_0 \) is the ground state of the three-dimensional isotropic harmonic oscillator. The corresponding Fermi function is
\[
H_F = \frac{1}{2m} |\mathbf{p}|^2 + \frac{1}{2} m\omega^2 |\mathbf{r}|^2 - \frac{3\omega \hbar}{2}
\]
with \( |\mathbf{p}|^2 = p_x^2 + p_y^2 + p_z^2 \); the Fermi hypersurface \( \Sigma_F \) is here the constant energy set
\[
H_0 = \frac{1}{2m} |\mathbf{p}|^2 + \frac{1}{2} m\omega^2 |\mathbf{r}|^2 = \frac{3\omega \hbar}{2}
\]
for the classical Hamiltonian \( H_0 \). The Bohm momentum \( \mathbf{p} = \nabla_r S \) is zero since \( \psi_0 \) is real, and the state’s internal quantum potential energy is
\[
Q(r) = \frac{3\omega \hbar}{2} - \frac{1}{2} m\omega^2 |\mathbf{r}|^2. \tag{11}
\]
This is just the ground state energy $3\omega h/2$ minus the potential energy. Equivalently, all the energy $3\omega h/2$ is obtained by adding the classical and quantum potential energy. Observe that the quantum force is here

$$F_Q = -\nabla r Q(r) = m\omega^2 r$$

whereas the classical force is $F_C = -m\omega^2 r$ (it is a restoring force, directed towards the equilibrium position), and we thus have $F_Q + F_C = 0$.

4 Stationary States in General

The counter-intuitive result of a stationary particle in the ground state of the harmonic oscillator is not unique. In fact it is clear that a particle in any stationary state described by a real wave function will have zero kinetic energy and will therefore not be moving.

Consider an even simpler case of a particle trapped between infinitely large confinement potentials. A straightforward calculation will show that a stationary particle will occur for all energy eigenstates. Einstein [6], himself, used this example as an objection to the whole approach, claiming that it violated physical intuition. He required the particle to be moving back and forth within the box. If that is the preferred intuition, then there is the problem of how the particle goes through the nodes of the wave functions of the higher energy states. For at the nodes, the quantum potential becomes infinitely repulsive and therefore conservation of energy would be violated if the particles were actually oscillating [3].

What our model is telling us is that, in the quantum domain, we must give up the idea that a particle is represented as a point in phase space. As we remarked earlier, the blow up requires energy and this energy comes from the particle itself – it comes from its kinetic energy. In the extreme case of a particle described by a real wave function, all the kinetic energy is transferred into quantum potential energy, the remaining rest mass is absorbed into the rest of the atom. This situation is reminiscent of the photon where the whole quantum of energy is absorbed by the atom, thereby completely losing its identity. There is a difference, however, in that a lepton cannot lose its identity owing to lepton number conservation.

In the reverse process, the photon emerges at an atomic transition associated with the process of emission. However, the electron only emerges with its full kinetic energy when it escapes the Coulomb potential. This brings out one of the differences in the behaviour of a photon and a lepton (particle), a difference that forces us to treat the electromagnetic field in a
different way [4]. Furthermore it illustrates that the concept of a particle in Bohm’s theory is very different from that of a classical particle [20].

5 Derivation of Schrödinger’s Equation

Let us now return to our general discussion and suppose the wavefunction depends on time under the action of some potential \( V \) (possibly itself time-dependent); the internal energy also becomes time-dependent, and the total Hamiltonian function is thus

\[
H(\mathbf{r}, \mathbf{p}, t) = \frac{\mathbf{p}^2}{2m} + Q(\mathbf{r}, t) + V(\mathbf{r}, t)
\] (12)

where \( Q(\mathbf{r}, t) \) is the quantum potential at time \( t \), derived as above. If we believe that, as in classical physics, the motion of the particle represented by the wavefunction is determined by the action, we see that the latter is a solution of the Hamilton–Jacobi equation

\[
\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla \mathbf{r} S)^2 + Q(\mathbf{r}, t) + V(\mathbf{r}, t) = 0.
\] (13)

Let us now assume, with Born, that \( \rho = \psi^* \psi = R^2 \) represents a probability density; this is consistent with Gleason’s theorem [8]. One way of interpreting Gleason’s theorem is to view it as a derivation of the Born rule from fundamental assumptions about quantum probabilities, guided by quantum theory, in order to assign consistent and unique probabilities to all possible measurement outcomes. Gleason proved that there is no alternative to the Born rule for Hilbert spaces of dimension of at least three. Introducing the associated probability current

\[
\mathbf{j} = \rho \frac{\nabla \mathbf{r} S}{m},
\] (14)

conservation of probability is equivalent to the continuity equation

\[
\frac{\partial \rho}{\partial t} + \nabla \mathbf{r} \cdot \mathbf{j} = 0;
\] (15)

that is to the continuity equation

\[
\frac{\partial \rho}{\partial t} + \nabla \mathbf{r} \cdot \left( \rho \frac{\nabla \mathbf{r} S}{m} \right) = 0.
\] (16)

Summarizing, the time-evolution of the phase \( S \) and the amplitude \( R \) of the wavefunction is determined by the system of coupled partial differential
equations (13) and (16). As is well-known (see e.g. Bohm and Hiley [2], Holland [19]), this system is equivalent to the Schrödinger equation

\[ \text{i} \hbar \frac{\partial \psi}{\partial t}(r, t) = -\frac{\hbar^2}{2m} \nabla^2 r \psi(r, t) + V(r, t) \psi(r, t). \]

Thus we have shown that if we take the internal energy (quantum potential) into account, then the evolution of the wavefunction is governed by the Schrödinger equation. What happens if we ignore this internal energy? Then, as one of us has shown in [9], the wavefunction will satisfy the non-linear partial differential equation

\[ \text{i} \hbar \frac{\partial \psi}{\partial t}(r, t) = - \left( \frac{\hbar^2}{2m} \nabla^2 r + Q(r, t) \right) \psi(r, t) + V(r, t) \psi(r, t). \]

6 Relation to the Uncertainty Principle

In [11] one of us introduced the notion of “quantum blob”, which is the image of a phase space ball with radius \( \sqrt{\hbar} \) by a linear symplectic transformation, and their study was pursued in [12, 14]. A quantum blob is an ersatz for the awkward notion of quantum cell from thermodynamics, and enjoys the pleasant property of symplectic symmetry; its introduction was motivated by the Robertson–Schrödinger (RS) inequalities, and a quantum blob can be viewed as the minimum uncertainty set in phase space that is compatible with these inequalities. Now, the RS inequality

\[ \Delta x^2 \Delta p_x^2 + \text{Cov}(x, p_x)^2 \geq \frac{1}{4} \hbar^2 \]

(and similar relations for the other variables) are expressed in terms of the variances \( \Delta x^2, \Delta p^2 \) and the covariance \( \text{Cov}(x, p_x) \); these are conventional measures of spreading, without any precise physical meaning. For instance, Hilgevoord and Uffink note in [17, 18] that variances only give an adequate physical measurement of the spread of a wavefunction when the probability density is nearly Gaussian. In the present paper, we have associated a quantum system with a much more natural notion, that of Fermi set \( \Omega_F \), which is canonically associated with the state \( \psi \). We have shown in [5] that in the case of one degree of freedom, where \( \Omega_F \) becomes a phase space surface, we have \( \text{area}(\Omega_F) \geq \frac{1}{2} \hbar \), which is compatible with the RS inequalities (de Gosson [10, 11, 13], de Gosson and Luef [16]); for an arbitrary number of degrees of freedom we conjecture that this condition on areas should be replaced with \( c(\Omega_F) \geq \frac{1}{2} \hbar \) for some symplectic capacity \( c \). This property
would imply that every Fermi set $\Omega_F$ contains \textit{de facto} \cite{14} \cite{16} a quantum blob, in accordance with the uncertainty principle. This allows us to define $\Omega_F$ as the quantum-mechanical counterpart of a classical point-like particle, generalising the discussion in Section 4.

Let us illustrate this on the example of the ground state of the three-dimensional isotropic harmonic oscillator. Here the Fermi set is the phase space ellipsoid

$$
\Omega_F : \frac{1}{2m}|p|^2 + \frac{1}{2}m\omega^2|r|^2 \leq \frac{3\omega h}{2}.
$$

An easy calculation shows that the intersection of $\Omega_F$ with any of the conjugate variable planes $x, p_x, y, p_y$, and $z, p_z$ is an ellipse with area $3h/2$. It follows \cite{15} that the symplectic capacity of $\Omega_F$ is

$$
c(\Omega_F) = \frac{3h}{2}.
$$

Hence $\Omega_F$ contains a “quantum blob”. This statement can actually be refined by using the notion of Ekeland–Hofer capacity, which allows the classification of phase space ellipsoids using the action integrals of the periodic orbits on the boundary of the Fermi set $\Omega_F$; we will develop this approach in a forthcoming paper.

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