Developments of Bohmian Mechanics

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Bohmian mechanics is a deterministic theory of quantum mechanics that is based on a set of \( n \) velocity functions for \( n \) particles, where these functions depend on the wavefunction from the \( n \)-body time-dependent Schrödinger equation. It is well known that Bohmian mechanics is not applicable to stationary states, since the velocity field for stationary states is the zero function. Recently, an alternative to Bohmian mechanics has been formulated, based on a conservation of energy equation, where the velocity fields are not the zero function, but this formalism is only applicable to stationary states with real valued wavefunctions. In this paper, Bohmian mechanics is merged with the alternative to Bohmian mechanics. This is accomplished by introducing an interpretation of the Bohm quantum potential. The final formalism gives dynamic particles for all states, including stationary states. The final main working equation contains two kinetic energy terms and a term that contains a factor that can be interpreted as a pressure. The derivation is a simple \( n \)-body generalization of the recent generalization, or refinement, of the Madelung equations.

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I. INTRODUCTION

Bohmian mechanics\textsuperscript{1,13} is a deterministic theory of quantum mechanics that is based on a set of $n$ velocity functions for $n$ particles, where these functions depend on the wavefunction from the $n$-body time-dependent Schrödinger equation. The two equations of Bohmian mechanics are equivalent to the time-dependent Schrödinger equation. An important function in Bohmian mechanics is the Bohm quantum potential.\textsuperscript{1,2,8} It is well known that Bohmian mechanics is not applicable to stationary states, since the velocity field for stationary states is the zero function. Therefore, as pointed out by Jung,\textsuperscript{12} a resting hydrogen $ns$ electron would have a strong non-zero electric dipole moment, and such a dipole moment would have been measured by experiment, if it existed. This same problem also appears in quantum hydrodynamics.\textsuperscript{8} Recently, an alternative to Bohmian mechanics has been formulated,\textsuperscript{14} based on a conservation of energy equation, where the velocity fields are not the zero function. However, this method is only applicable to stationary states with real valued wavefunctions. In this paper, Bohmian mechanics is merged with the alternative to Bohmian mechanics. This is accomplished by introducing an interpretation of the Bohm quantum potential. The final formalism gives a dynamic particles trajectories for stationary states. The final main working equation contains two kinetic energy terms and a term that can be interpreted as a pressure. The derivation is a simple $n$-body generalization of the recent generalization, or refinement, of the Madelung equations.\textsuperscript{15}

II. QUANTUM ENERGY EQUATION FOR STATIONARY STATES

In this section we review the conservation of energy equation for quantum mechanical stationary states with real valued wavefunctions,\textsuperscript{14} where these equations are an $n$-body generalization of fluid dynamic equations applicable to one-body systems.\textsuperscript{16}

We also give a justification for the interpretation of the kinetic energy. The $n$-body time-independent Schrödinger equation with a normalized, real-valued eigenfunction $R$ can be written

$$-\frac{\hbar^2}{2m} \sum_{i=1}^{n} \left[ R \nabla_i^2 R \right] + \sum_{i=1}^{n} V_i \Upsilon + \frac{1}{2} \sum_{i \neq j}^{n} R_{ij}^{-1} \Upsilon = E \Upsilon,$$

(1)

where

$$\left[ \psi \nabla_i^2 \psi \right](\mathbf{x}) = \psi(\mathbf{x}) \nabla_{r_i}^2 \psi(\mathbf{x}), \quad \mathbf{x} = \mathbf{x}_1, \cdots \mathbf{x}_n,$$
and where the probability distribution is \( \Upsilon = R^2 \); also, the electron coordinate \( \mathbf{x}_i \) is defined by \( \mathbf{x}_i = \mathbf{r}_i, \omega_i \), where \( \mathbf{r}_i \in \mathbb{R}^3 \) and \( \omega_i \in \{-1, 1\} \) are the spatial and spin coordinates, respectively. Furthermore, the \( V_i \) and \( R_{ij}^{-1} \) multiplicative operators are defined by the following:

\[
[V_i \Upsilon](\mathbf{x}) = V(\mathbf{r}_i) \Upsilon(\mathbf{x}), \quad [R^{-1}_{ij} \Upsilon](\mathbf{x}) = |\mathbf{r}_i - \mathbf{r}_j|^{-1} \Upsilon(\mathbf{x}) ;
\]

where the one-body external potential \( V \) is a specified real-valued function with domain \( \mathbb{R}^3 \) such that \( \{ \mathbf{r} \in \mathbb{R}^3 | R(\mathbf{x}) = 0 \} \) has measure zero. This last requirement for \( V \) implies that the division of an equation by \( R \) or \( \Upsilon \) gives an equation that is defined almost everywhere.

Elsewhere\(^{14}\) it is demonstrated that the Schrödinger equation (1), with the restriction \( \Upsilon(\mathbf{x}) \neq 0 \), is equivalent to

\[
\sum_i \frac{1}{2} m u_i^2 + \Upsilon^{-1} \sum_i P_i + \sum_i V_i + \frac{1}{2} \sum_{i \neq j} R_{ij}^{-1} = \bar{E} \tag{2}
\]

where

\[
u_{i \pm} = \pm \frac{\hbar}{2m} \nabla_i \Upsilon, \tag{3}
\]

\[
P_i = -\frac{\hbar^2}{4m} \nabla^2_i \Upsilon \tag{4}
\]

and \( u_i^2 = |u_{i \pm}|^2 \). For the configuration \( \mathbf{x} = \mathbf{x}_1, \cdots \mathbf{x}_n \), where one electron is at \( \mathbf{x}_1 \), another one is located at \( \mathbf{x}_2 \), and so on, the function

\[
\frac{1}{2} m [u_i(\mathbf{x}_1, \mathbf{x}_2, \cdots \mathbf{x}_i, \cdots \mathbf{x}_n)]^2
\]

is interpreted as the kinetic energy of the \( i \)th particle, i.e., the particle located at \( \mathbf{x}_i \), where this particle has velocity \( \mathbf{u}_{i \pm} \) or \( \mathbf{u}_{i-} \). Equation (2) can be interpreted as a classical energy equation with a Hamiltonian function that depends on the probability distribution \( \Upsilon \) and the potential energy functions \( V_i \) and \( R_{ij} \).

For later use, we compare (1) and (2), giving

\[
-\frac{\hbar^2}{2m} \sum_{i=1}^n [R \nabla^2_i R] = \sum_i \frac{1}{2} \Upsilon m u_i^2 + \sum_i P_i \tag{5}
\]

For each Cartesian coordinate \( \alpha_i \in \{x_i, y_i, z_i\}, i = 1, \cdots n \), we require that the wavefunction satisfy

\[
\lim_{\alpha_i \to \pm \infty} R(\mathbf{x}) = \lim_{\alpha_i \to \pm \infty} \frac{\partial R}{\partial \alpha_i} = 0
\]
Hence
\[ \int_{-\infty}^{\infty} \frac{\partial^2 \Upsilon}{\partial \alpha_i^2} d\alpha_i = \frac{\partial \Upsilon}{\partial \alpha_i} \bigg|_{-\infty}^{\infty} = 2 R \frac{\partial R}{\partial \alpha_i} \bigg|_{-\infty}^{\infty} = 0 \]
and therefore
\[ \int_{\mathbb{R}^3} \nabla_i^2 \Upsilon \, dr_i = 0 \]
This result combined with (4) gives
\[ \int P_i(r_i, \omega_i) \, dr_i = 0 \]
and it follows that the $P_i$ terms do not contribute to the expectation value of the kinetic energy, denoted $\langle T \rangle$. Using the above equality for $P_i$, and integrating $\mathbb{P}$ over the $3n$ spatial coordinates and summing over the $n$ spin coordinates, we have
\[ \langle T \rangle = -\frac{\hbar^2}{2m} \sum_{i=1}^{n} \langle R | \nabla_i^2 | R \rangle = \sum_{i=1}^{n} \frac{1}{2} m \langle R | \omega_i^2 | R \rangle \] (6)
where Dirac notation and the definition $\Upsilon = R^2$ are used. This result supports the interpretations given above for the kinetic energy and velocity.

### III. DEVELOPED BOHMIAN MECHANICS

The time-dependent Schrödinger equation is
\[ i\hbar \partial \Psi = -\frac{\hbar^2}{2m} \sum_{i=1}^{n} \nabla_i^2 \Psi + U \Psi = \hat{H} \Psi \] (7)
where
\[ U = \sum_{i \neq j}^{n} |r_i - r_j|^{-1} + \sum_{i=1}^{n} V_i, \] (8)
$\Psi = \Psi(x, t)$ is the $n$-body time-dependent wavefunction, and we use the same notation as in the previous section, e.g., $x_i = r_i, \omega_i$. Let the spin coordinates $\omega_1, \cdots \omega_n$ be specified parameters. Hence, $\Psi = \Psi(r, t)$, where $r = r_1, \cdots r_n$, i.e., we can consider $\Psi$ to be a function of the spatial coordinates and time only. For Bohmian mechanics, the wavefunction ansatz
\[ \Psi = Re^{iSt/\hbar}, \] (9)
where $R$ and $S$ are time-dependent real-valued functions, is substituted into the time-dependent Schrödinger equation (7), which, after significant manipulations, yields the following two equations:

\[
\partial \Upsilon + \sum_{i=1}^{n} \nabla \cdot (\Upsilon \mathbf{u}_i) = 0 \tag{10}
\]

\[
-R \partial S = \sum_{i=1}^{n} \left( \frac{1}{2m} R \nabla \cdot \mathbf{u}_i \right) + UR, \tag{11}
\]

where the probability distribution is $\Upsilon = \Psi \Psi^* = R^2$ and $\partial S(x,t) = \partial S(x,t)/\partial t$. Equation (10) is called the continuity equation. In the special case of a one-body system, with $\Upsilon = \rho$, this equation has the same form as the continuity equation from fluid dynamics,$^{19,20}$ where the mass density is $m\rho$. Bohmian mechanics, also defines the following two functions:

\[
\mathbf{v}_i = \frac{\nabla \mathbf{u}_i}{m}, \tag{12}
\]

\[
Q = -\frac{1}{R} \frac{\hbar^2}{2m} \nabla^2 R = \Upsilon^{-1} \left( -R \frac{\hbar^2}{2m} \nabla^2 R \right), \tag{13}
\]

where $\mathbf{v}_i(x_1, x_2, \cdots x_i, \cdots x_n)$ is interpreted as the velocity of the $i$th particle, i.e., the velocity of the particle located at $x_i$ for the configuration $x = x_1, \cdots x_n$. Also, $Q$ is known as the Bohm quantum potential.$^{1,2,8}$ Substituting these two definitions into (11), and dividing by $R$, we get

\[
- \partial S = \sum_i \frac{1}{2} m v_i^2 + Q + U \tag{14}
\]

where $v_i^2 = |\mathbf{v}_i|^2$.

Note that Eq. (5) is an equality holding for two times differentiable real-valued functions, where $u_i^2 = |u_{\pm}|^2$ and $P_i$ are given be Eq. (3) and (4), respectively. Next we extend the interpretation of (5) to the real part of time-dependent wavefunctions $\Phi$, given by ansatz (9). Making this interpretation and substituting Eq. (5) into (13), we discover

\[
Q = \sum_i \frac{1}{2} m u_i^2 + \Upsilon^{-1} \sum_i P_i \tag{15}
\]

The first term is a kinetic energy term. It is not necessary to interpret the second term. However, one interpretation is the following: $P_i(x_1, x_2, \cdots x_i, \cdots x_n)$ is the pressure experienced by the $i$th particle, i.e., the particle located at $x_i$, for the configuration $x = x_1, \cdots x_n$. Substituting (13) into (14) gives the desired result

\[
- \partial S = \sum_i \frac{1}{2} m v_i^2 + \sum_i \frac{1}{2} m u_i^2 + \Upsilon^{-1} \sum_i P_i + U \tag{16}
\]
This equation is a further development of (14), containing two kinetic energy terms, a 
“compression” energy term $\Upsilon^{-1} \sum_i P_i$, and the external potential $U$, given by (8). The 
right-hand-side of this equation can be interpreted as the time dependent total energy, 
i.e., a Hamiltonian function. For the left-hand side, from (12), $S$ can be interpreted as a 
momentum potential that is a sum of momentums from all $n$ particles, but only including 
the $v_i$ portion of the total velocity $u_{i\pm} + v_i$.

If $\Psi$ is a stationary state then $\Psi(x,t) = R(x)e^{-iEt/h}$, so $S(t) = -\bar{E}t$, giving

$$\sum_i \frac{1}{2}mv_i^2 + \sum_i \frac{1}{2}mu_i^2 + \Upsilon^{-1} \sum_i P_i + U = \bar{E}$$

This equation is a generalization of Eq. (2), holding for complex valued wavefunctions.

IV. SUMMARY

The Bohmian equation (11), or (13), with velocities given by (12) and probability distri-
bution $\Upsilon = \Psi\Psi^* = R^2$, is developed by an interpretation the quantum potential, given by 
(15), with velocities given by (3) and $P_i$ defined by (4), giving the result (16), with $U$ de-
finied by (8). The final velocities have been reinterpreted to be $u_{i\pm} + v_i$ instead of just $v_i$. A 
justification for the additional velocity part $u_{i\pm}$ is given by examining the expectation value 
of the kinetic energy (6) in the special case of a real-valued wavefunction $R$ of a stationary 
state. The Lagrangian-function formulation by Salesi\textsuperscript{21} and the generalized fluid-dynamics 
formalism by Broer\textsuperscript{22} come to the same conclusion, interpreting $u_{i\pm}$ as a velocity.

REFERENCES

1D. Bohm, Phys. Rev. 85, 166 (1952).
2D. Bohm, Phys. Rev. 85, 180 (1952).
3R. Tumulka, Entropy 20, 462 (2018), (Special Issue Emergent Quantum Mechanics – David 
Bohn Centennial Perspective).
4A. S. Sanz, Front. Phys 14, 11301 (2019).
5N. Gisin, Entropy 20, 105 (2018), (Special Issue Emergent Quantum Mechanics – David 
Bohn Centennial Perspective).
6A. S. Sanz and S. Miret-Arteş, A Trajectory Description of Quantum Processes. II. Appli-
cations, vol. 831 of Lecture Notes in Physics (Springer, Berlin, 2014).
7D. Dürr and S. Teufel, *Bohmian Mechanics* (Springer, Heidelberg, 2009).
8R. E. Wyatt, *Quantum Dynamics with Trajectories* (Springer, New York, 2005).
9P. K. Chattaraj, ed., *Quantum Trajectories* (CRC Taylor and Francis, New York, 2010).
10K. H. Hughes and G. Parlant, Eds., *Quantum Trajectories* (CCP6, Daresbury, 2011).
11X. Oriols and J. Mompart, Eds., *Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology* (Pan Standford Publishing, Singapore, 2012).
12K. Jung, J. Phys.: Conf. Ser. , 442 (2013).
13K. Renziehausen and I. Barth, Found. Phys. 50, 772–798 (2020).
14J. P. Finley, (2021), *A Quantum Mechanics Conservation of Energy Equation for Stationary States with Real Valued Wave Functions*, the manuscript is available from http://arXiv.org/abs/2107.10311.
15J. P. Finley, (2021), *Refined Madelung Equations*, the manuscript is available from http://arXiv.org/abs/2109.12766.
16J. P. Finley, (2021), *The Fluid Dynamics of the One-Body Stationary States of Quantum Mechanics with Real Valued Wavefunctions*, the manuscript is available from http://arXiv.org/abs/2107.10315.
17I. N. Levine, *Quantum Chemistry*, 5th ed. (Prentice Hall, Upper Saddle Rever, 1991).
18B. H. Bransden and C. J. Joachain, *Physics of Atoms and Molecules* (Longman, London and New York, 1989).
19B. R. Munson, D. F. Young, and T. H. Okiishi, *Fundamentals of Fluid Dynamics*, 5th ed. (Wiley, Hoboken, 2006).
20A. H. Shapiro, *The Dynamics and Thermodynamics of Compressible Fluid Flow*, Vol. 1 (Ronald, New York, 1953).
21G. Salesi, Mod. Phys. Lett. A 11, 1815–1823 (1996).
22L. J. F. Broer, Physica 76, 364–372 (1974).