Refined Madelung Equations

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Abstract

The Madelung equations are two equations that are equivalent to the one-body time-dependent Schrödinger equation. In this paper, the Madelung equation, whose gradient is an Euler equation, is refined by introducing interpretations of functions that are shown to depend only on the real-part of the complex-valued wavefunction. These interpretations are extensions of functions from the recently derived generalized Bernoulli equation, applicable to real-valued quantum-mechanical stationary states. In particular, the velocity and pressure definitions are extended so that they depend on the real-part of a time-dependent complex-valued wavefunction. The Bohn quantum potential is then interpreted as the sum of two terms, one involving the kinetic energy and the other involving the pressure. Substituting the interpreted quantum-potential into the Madelung equation gives a refined equation containing two kinetic energy terms, a pressure term, and the external potential. It is easily demonstrated that the refined Madelungen equation, applied to the hydrogen atom states with a nonzero magnetic quantum number, gives a fluid velocity that contains both a radial component and a free vortex. Hence, the fluid particles have angular momentum and move on streamlines that terminate at infinity. It is also demonstrated that the two velocities from the refined Madelung equation are related: One is the real component and the other is the imaginary component of a complex velocity. Furthermore, an Euler equation for quantum mechanical systems is derived by taking the gradient of the refined Madelung equation.

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I. INTRODUCTION

The Madelung equations \[1, 2\] are two equations that are equivalent to the one-body time-dependent Schrödinger equation, and these equations are very similar to the Euler equations of fluid dynamics. The Madelung equations provide an alternate “perspective” of quantum mechanics compared to the conventional one via the Schrödinger equation, and the possibility of a quantum-mechanical foundation based on the Madelung equations is investigated by Wilhelm \[3\] and Sonego \[4\]. The Madelung equations do not contain a pressure. There are at least two extensions of the Madelung equations \[5, 6\].

Because of the velocity definition, the Madelung equations do not provide a reasonable model for quantum mechanical stationary states that have real valued wavefunctions. Such states have a static Madelung fluid, and this is not in agreement with the usual non-zero kinetic-energy expectation value, suggesting that a satisfactory model should have some motion. This shortcoming is also pointed out by Wyatt \[7\] for quantum hydrodynamics \[8–24\], a method that is based on the Madelung equations.

Recently, a compressible-flow generalization of the Bernoulli equation of fluid dynamics is shown to be equivalent to the time-independent Schrödinger equation for one-body stationary states with real-valued wavefunctions \[25\]. The generalized Bernoulli equation describes compressible, irrotational, steady flow with a constant specific total energy, i.e., a constant energy per mass for each fluid elements. For the formalism, the velocity and mass-density definitions yield a generalization of the steady-flow continuity equation where mass is not locally conserved, and where the pressure is proportional to the mass creation rate per volume, yielding sources and sinks. However, over all space, the flows conserve mass.

The generalized Bernoulli equation, mentioned above, and a generalized continuity equation provide a fluid dynamic interpretation of a class of quantum mechanical stationary states that is an alternative to the interpretation provided by the Madelung equations \[1, 2\]. Furthermore, the integrand of the quantum-mechanical expectation value of the kinetic energy is given as a sum of two terms, and one term is interpreted as the kinetic energy per volume and the other one is the pressure. In additional, speed of speed of equations are derived from the generalized continuity equation and a derived variable-mass Euler equation. Applications of the formalism is applied to a fluid (or particle) in a one-dimensional box, the
ground and first excited-state of the one-dimensional harmonic oscillator, and the hydrogen
1s and 2s states.

In this paper, in Sec. II the Madelung equation, whose gradient is an Euler equation, is
refined by introducing interpretations from the generalized Bernoulli equation of functions
that are shown to depend only on the real-part of the complex-valued wavefunction. In
particular, the velocity and pressure definitions, applicable to a real-valued wavefunction,
are extended so that they also hold with the real part of a time-dependent complex-valued
wavefunction. The Bohn quantum potential [7, 26, 27] is then interpreted as the sum of two
terms, one involving the kinetic energy and the other involving the pressure. Substituting
the interpreted quantum potential into the Madelung equation gives a refined equation
containing two kinetic energy terms, a pressure term, and the external potential. It is easily
demonstrated that the refined Madelung equation, applied to the hydrogen atom states
with a non zero magnetic quantum number, gives a velocity that contains both a radial
component and a free vortex. Hence, the fluid particles have angular momentum and move
on streamlines the terminate at infinity.

In Appendix A it is demonstrated that the two velocities from the refined Madelung
equation are related: One is the real component and the other is the imaginary component
of a complex velocity. Also, Appendix B derives an Euler equation for quantum mechanical
systems.

II. REFINED MADELUNG EQUATIONS

Let \( \phi \) be a real-valued eigenfunction of a one-body time-independent Schrödinger equation
with external potential \( V \). Elsewhere [25] it is shown that the following two equations are
equivalent:

\[
\begin{align*}
-\frac{\hbar^2}{2m} \nabla^2 \phi + V \phi &= \bar{E} \phi \\
\frac{1}{2} mu^2 + p \rho^{-1} + V &= \bar{E}
\end{align*}
\]  

(1)  

(2)

The first equation is the one-body time-independent Schrödinger equation. The second
equation, with the definitions,

\[ u_\pm = \pm \frac{\hbar}{2m} \frac{\nabla \rho}{\rho} , \]  

(3)
\[ p = -\frac{\hbar^2}{4m} \nabla^2 \rho, \] (4)

and \( u^2 = |\mathbf{u}_\pm|^2 \), is a steady, compressible-flow generalization of the well known Bernoulli equation \([28, 29]\) with mass density \( \rho_m = m\rho \), velocity \( \mathbf{u}_\pm \) and pressure \( p \). Note that there are two possible velocities \( \mathbf{u}_+ \) and \( \mathbf{u}_- \), giving two possible directions along each streamline, called uphill and downhill flow, respectively. (Elsewhere \([30]\), an \( N \)-body generalization of \((2)\), based on the \( N \)-body generalization of Eq. \((1)\), is derived.)

The velocity \( \mathbf{u}_\pm \) and mass-density \( \rho_m \) definitions above yield a generalization of the steady-flow continuity equation, given by

\[ \nabla \cdot \rho_m \mathbf{u}_\pm = \pm \frac{2m}{\hbar} p \] (5)

where mass is not locally conserved, and where the pressure is proportional to the mass creation rate per volume, yielding sources and sinks. Since mass is not conserved locally, energy also is not conserved locally. Also, since \( u^2/2 \) is the specific kinetic energy, it follows that Eq. \((2)\) (divided by the mass \( m \)) is a statement of the conservation of the specific (total) energy \( \bar{E}/m \) for the fluid particles. Over all space, the flows do conserve mass and energy; the sources and sinks cancel.

For later use, note that the equation

\[ \frac{1}{2} mu^2 + p\rho^{-1} = \rho^{-1} \left( -\frac{\hbar^2}{2m} \phi \nabla^2 \phi \right) \] (6)

follows from comparing \((1)\) and \((2)\). However, it is easily demonstrated that this equation, with \( R \) replacing \( \phi \), is an equality holding for any real valued function \( R \) such that \( R^2 = \rho \). In the derivation below, we extend the definitions \((3)\) and \((4)\) to the cases where \( R \) is the real part of a time-dependent complex-valued wavefunction \( \psi \).

The one-body time-dependent Schrödinger equation is \([31, 32]\)

\[ i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi \] (7)

where \([\partial \psi](t) = \partial \psi / \partial t\). The two Madelung equations, given by \([1, 2, 7]\)

\[ \partial \rho_m + \nabla \cdot (\rho_m \mathbf{v}) = 0 \] (8)

\[ -\partial S = \frac{1}{2m} \nabla S \cdot \nabla S + Q + V \] (9)

are equivalent to the Schrödinger equation, where the wavefunction ansatz is

\[ \psi(x, t) = R(x, t)e^{iS(x, t)/\hbar}, \] (10)
and $R$ is required to be nonnegative. The function $Q$, defined below, is the Bohmian quantum potential. The Madelung equations characterize the flow of a compressible gas with mass density $\rho_m = m|\psi|^2$ and velocity

\[ \mathbf{v} = \frac{\nabla S}{m} \] (11)

Eq. (8) is the continuity equation, a statement of the conservation of mass. The gradient of (9) is very similar to the Euler equation of fluid dynamics.

Using the above velocity definition with $v^2 = u_\pm \cdot u_\pm$, (9) can be written

\[ -\partial S = \frac{1}{2} mv^2 + Q + V \] (12)

The Bohm quantum potential $Q$ is defined by \[7, 26, 27\]

\[ Q = -\frac{\hbar^2}{2mR^2} \nabla^2 R \]

Using $R = \rho^{1/2}$ we have

\[
\nabla^2 R = \nabla \cdot \nabla \rho^{1/2} = \frac{1}{2} \nabla \cdot (\rho^{-1/2} \nabla \rho) = \frac{1}{2} \nabla \rho^{-1/2} \cdot \nabla \rho + \frac{1}{2} \rho^{-1/2} \nabla^2 \rho \\
= -\frac{1}{4} \rho^{-3/2} \nabla \rho \cdot \nabla \rho + \frac{1}{2} \rho^{-1/2} \nabla^2 \rho
\]

Hence,

\[ Q = \frac{\hbar^2}{8m} \rho^{-2} \nabla \rho \cdot \nabla \rho - \frac{\hbar^2}{4m} \rho^{-1} \nabla^2 \rho \]

Next, as discussed above, we extend the velocity and pressure definitions, (3) and (4), so that they hold for $\phi = R$, where $R$ is the real part of the complex valued wavefunction $\psi$, and note that we still have $R^2 = \rho$. Doing this, and using Eq. (9), we obtain

\[ Q = \frac{1}{2} mu^2 + p\rho^{-1} = \rho^{-1} \left( -\frac{\hbar^2}{2m} R \nabla^2 R \right) \], \quad (13)

where $u^2 = \mathbf{u} \cdot \mathbf{u}$. Substituting for $Q$, (12) becomes the desired result:

\[ -\partial S = \frac{1}{2} mv^2 + \frac{1}{2} mu^2 + p\rho^{-1} + V \] (14)

This equation is a refinement of (12), containing two kinetic energy terms, a “compression” energy term $p\rho^{-1}$, and the external potential $V$. The right-hand-side of this equation (divided by $m$) can be interpreted as the time dependent total specific energy, i.e., a Hamiltonian function for specific energy.
If $\psi$ is a stationary state then $\psi(x, t) = R(x)e^{-iEt/\hbar}$, so $S(t) = -\bar{E}t$, giving

$$\frac{1}{2}mv^2 + \frac{1}{2}mu^2 + p\rho^{-1} + V = \bar{E}$$

(15)

This equation is a generalization of (2) holding also for complex-valued one-body stationary states.

For real valued stationary states, since the velocity $u$ satisfies (3), the directions of $u_{\pm}$ is perpendicular to the level surfaces of $\phi$ and $\rho$. Hence, for the hydrogen-atom real-valued states, the streamlines terminate at points at infinity. This behavior also holds for the streamlines from the velocity field $u$ alone, for steady-state complex-valued hydrogen wavefunctions, ignoring $v$. In spherical coordinate, the hydrogen wavefunctions can be written $\psi(r, \theta, \phi) = R(r, \theta)e^{\pm i\ell \phi}$, where $\ell$, an integer, is the magnetic quantum number. From the ansatz (10), we have $S = \pm \hbar \ell \phi$. Hence $v = \pm \hbar \ell (r \sin \theta)^{-1} \dot{\phi}$, so, for $\ell \neq 0$, the flows have a vortex, and the vortex is a free vortex, since $\nabla \times v = 0$. Therefore, the hydrogen atom states with $\ell \neq 0$ have fluid particle with a nonzero angular momentum, and this has some agreement with the angular momentum predictions from quantum mechanics, but the model has nothing to say about the measurement process. Also, using the gradient in spherical coordinates, it follows that $u \cdot v = 0$, giving $|u + v|^2 = u^2 + v^2$.

**Appendix A: Equalities for the Velocities**

Next we show that

$$u_{\pm} = \pm \text{Re} \left( \frac{\hbar}{m} \nabla \psi \right), \quad v = \text{Im} \left( \frac{\hbar}{m} \nabla \psi \right)$$

(A1)

The first one is obtained by substituting $\rho = R^2$ into (3):

$$u_{\pm} = \pm \frac{\hbar}{2m} \nabla R^2 = \pm \frac{\hbar}{m} \nabla R = \pm \text{Re} \left( \frac{\hbar}{m} \nabla \psi \right)$$
The second one is proven in the following sequence, starting with the ansatz \( \psi = \text{Re} e^{iS/\hbar} \) and requiring (11) for \( v \) to hold.

\[
\nabla \psi = (\nabla R)e^{iS/\hbar} + i\hbar^{-1}\text{Re} e^{iS/\hbar} \nabla s
\]

\[
\frac{\nabla \psi}{\psi} = (\nabla R)R^{-1} + i\hbar^{-1} \nabla s
\]

\[
\frac{\hbar \nabla \psi}{m \psi} = \frac{\hbar}{m}(\nabla R)R^{-1} + i\frac{\nabla s}{m}
\]

\[
v = \frac{\nabla s}{m} = \text{Im} \left( \frac{\hbar \nabla \psi}{m \psi} \right)
\]

Let \( w = \hbar \nabla \psi / (m \psi) \). Equations (A1) implies that \( w = u + iv \), and \( |w|^2 = u^2 + v^2 \).

**Appendix B: The Euler equation for quantum mechanical systems**

For a fluid of classical mechanics, the Euler equation with variable mass and steady flow is [25]

\[
\frac{1}{2} \rho_m \nabla u^2 + \nabla \cdot (\rho_m u) u + \nabla p + \rho \nabla V = 0 \tag{B1}
\]

Elsewhere [25] it is shown that this equation is equivalent the gradient of (2), which, for \( \rho(\mathbf{r}) \neq 0 \), can be written

\[
\frac{1}{2} \rho_m \nabla u^2 + \rho \nabla \left( \frac{p}{\rho} \right) + \rho \nabla V = 0 \tag{B2}
\]

Comparing the two, we have

\[
\rho \nabla \left( \frac{p}{\rho} \right) = \nabla \cdot (\rho_m u) u + \nabla p \tag{B3}
\]

Taking the gradient of (14) and multiplying the result by \( \rho \) we have

\[
\rho_m \partial v + \frac{1}{2} \rho_m \nabla v^2 + \frac{1}{2} \rho_m \nabla u^2 + \rho \nabla \left( \frac{p}{\rho} \right) + \rho \nabla V = 0 \tag{B4}
\]

Substituting (B3), we obtain

\[
\rho_m \partial v + \frac{1}{2} \rho_m \nabla v^2 + \frac{1}{2} \rho_m \nabla u^2 + \nabla \cdot (\rho_m u) u + \nabla p + \rho \nabla V = 0, \tag{B5}
\]

a Euler equation applicable to quantum mechanical systems. The other two equations being the continuity equations, (8) and (5).
Appendix C: Summary

In this paper, the refined Madelung equation (14) is derived. This equation with the continuity equation (8) are equivalent to the one-body time dependent Schrödinger equation (7). The two velocities, $u_\pm$ and $v$, and the pressure $p$ are defined by Eq. (3), (11) and (4). Equation (14) can be viewed as combination of a Madelung equation (12) and the generalized Bernoullii equation (2), or as a refinement of the corresponding Madelung equation with new interpretations for a pressure $p$ and an additional velocity component $u_\pm$.

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