



PAPER

OPEN ACCESS

RECEIVED
23 December 2021REVISED
25 March 2022ACCEPTED FOR PUBLICATION
29 March 2022PUBLISHED
8 April 2022

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A fluid description based on the Bernoulli equation of the one-body stationary states of quantum mechanics with real valued wavefunctions

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E-mail: james.finley@enmu.edu**Keywords:** schrodinger equation, bernoulli equation, madelung fluid, compressible flow, quantum mechanics, fluid dynamics, quantum hydrodynamics

Abstract

A formalism is developed, and applied, that describes a class of one-body quantum mechanical systems as fluids where each stationary state is a steady flow state. The time-independent Schrödinger equation for one-body stationary states with real-valued wavefunctions is shown to be equivalent to a compressible-flow generalization of the Bernoulli equation of fluid dynamics. The mass density, velocity and pressure are taken as functions that are determined by the probability density. The generalized Bernoulli equation describes compressible, irrotational, steady flow with variable mass and a constant specific total energy, i.e. a constant energy *per mass* for each fluid element. The generalized Bernoulli equation and a generalized continuity equation provide a fluid dynamic interpretation of a class of quantum mechanical stationary states that is an alternative to the unrealistic, static-fluid interpretation provided by the Madelung equations and quantum hydrodynamics. The total kinetic energy from the Bernoulli equation is shown to be equal to the expectation value of the kinetic energy, and the integrand of the expectation value of the kinetic energy is given an interpretation. It is also demonstrated that variable mass is necessary for a satisfactory fluid model of stationary states. However, over all space, the flows conserve mass, because the rate of mass creation from the sources are equal to the rate of mass annihilation from the sinks. The following flows are examined: the ground and first excited-states of a particle in a one-dimensional box, the harmonic oscillator, and the hydrogen s states.

1. Introduction

Quantum hydrodynamics [1] is a method that is based on the Madelung equations [2, 3]. This approach incorporates the quantum potential by Bohm [4, 5] and includes developments by Takabayasi [6]. Quantum hydrodynamic theory has been employed to treat systems with single particle wave functions [7–22]. The method has also been generalized to treat many particle systems [23, 24]. Application of this formalism includes the investigation of spin effects [25, 26], Bose–Einstein condensates [27], graphene [28] and plasmas [29–31]. The utilized information from these methods are trajectories of point masses that move with the fluid velocity and trace out pathlines. Essential aspects of fluid dynamics are not part of the method, including a pressure function and the kinematics of fluid-element deformation. The Madelung equations [2, 3] 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 [32] and Sonego [33]. The key aspect of the derivation of the Madelung equations is the definition of the velocity field, taken as $\mathbf{u} = \hbar \nabla S / m$, where the wavefunction ansatz is $\phi = \sqrt{\rho} e^{iS}$. Also important is the identification of the variable mass-density,

defined by $\rho_m = m\rho$, where m is the mass of the system and $\rho = |\phi|^2$ is the probability density. The Madelung equations do not contain a pressure. There are at least two extensions of the Madelung equations [34, 35]. Tsekov [36] derives a complex Navier–Stokes equation using a complex velocity. Vadasz [37] derived an extension of the Schrödinger equation from the Navier–Stokes equation.

Because of the velocity definition mentioned above, the Madelung equations do not provide a reasonable model for quantum mechanical stationary states that have real valued wavefunctions, and, as pointed out by Wyatt [1], quantum hydrodynamic approaches are also not applicable to these stationary states. Such states have a static Madelung fluid with ‘stationary’ trajectories, and this is not in agreement with the usual non-zero kinetic-energy expectation value, suggesting that a satisfactory model should have some motion. Also, as pointed out by Jung [38], 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. While the trajectory methods of Floyd [39] and Faraggi and Matone [40] can treat stationary states, these methods are not based on the Madelung equations, and they do *not* contain a fluid dynamic component.

There are at least two fluid dynamics formulations of quantum mechanical systems where the velocity definition \mathbf{u}_\pm , given by

$$\mathbf{u}_\pm = \pm \frac{\hbar}{2m} \frac{\nabla \rho}{\rho} \quad (1)$$

is obtained by making an interpretation of a derived fluid-dynamic equation. Salesi [41] obtains a Lagrangian function that is equivalent to the Madelung equations, and this function contains the term $\rho_m |\mathbf{u}_\pm|^2 / 2$, where \mathbf{u}_\pm is defined by (1). He interprets $\rho_m |\mathbf{u}_\pm|^2 / 2$ as the kinetic energy per volume in the center of mass coordinate frame with velocity \mathbf{u}_\pm . Also, the function $\varrho_m |\mathbf{u}_\pm|^2 / 2$, with \mathbf{u}_\pm also *replaced* by the rhs of (1), is a term of the Hamiltonian functional of the generalized fluid-dynamics formalism by Broer [42], where the Hamiltonian functional is derived from the time-dependent Schrödinger equation, and ϱ_m satisfies $\varrho_m = 2\rho_m$. These two alternatives suggest an opportunity to model, or represent, certain quantum mechanical systems as an irrotational, compressible fluid with velocity \mathbf{u}_\pm .

In this paper (in section 2), 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, where the variable mass-density ρ_m is defined in the same way as for a Madelung fluid. As in the Salesi development [41], the fluid velocity \mathbf{u}_\pm is defined by equation (1), and there are two possible velocities directions, \mathbf{u}_+ and \mathbf{u}_- . Also, the integration of the kinetic-energy per volume $\rho_m |\mathbf{u}_\pm|^2 / 2$ over all space is shown to be equal to the kinetic energy expectation-value of the corresponding quantum state, giving an additional justification for the interpretation of equation (1) as a velocity definition.

The generalized Bernoulli and a continuity equations provide a method that is an alternative to quantum hydrodynamics for the treatment of steady states with real valued wavefunctions, where quantum hydrodynamics is not applicable. In contrast to the approaches that employ the Madelung equations, including quantum hydrodynamics [1], the velocity choice gives *nonstatic* steady flows for quantum mechanical stationary states. Also in contrast to quantum hydrodynamics [1], the presented formalism contains essential fluid-dynamic elements, including a pressure function and the kinematics of fluid-element deformation. The presented formalism also has the advantage of providing equations that are very easy to solve compared to the ones mentioned above.

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 each quantum-mechanical stationary-state represented by a one-body real-valued wavefunction, there is a unique solution of the generalized Bernoulli equation. This relationship provides a physical correspondence, or analogy, between certain quantum states and fluid flows. Furthermore, the generalized Bernoulli equation and a generalized continuity equation can provide a fluid dynamic interpretation of a class of quantum mechanical stationary states that is an alternative to the static fluid interpretation provided by the Madelung equations [2, 3].

In this paper, the developed formalism is used to describe quantum mechanical systems as fluids where each stationary state is a steady flow state. The following flows are examined: states of a particle in a one-dimensional box (4.1), the ground and first excited-states of the harmonic oscillator (4.2), and the hydrogen 1s (2.3) and 2s (4.3) states. Each flow can be partitioned into segments (or regions) where matter does not enter or leave by convection. A typical segment has an unstable equilibrium point where the fluid is moving away from this point. These steady flows are stabilized by a continuous creation and annihilation of matter. Also, in the limit of a fluid particle reaching a node—a region of space of measure zero—the particle has infinite speed and zero mass, i.e., the fluid elements ‘burn out’ at the nodes where the mass is exhausted.

Also, in this paper, interpretations are made in the form of assigning physical meaning to functions (in section 2). Besides the fluid velocity \mathbf{u}_\pm defined by equation (1), the pressure function is identified from the generalized Bernoulli equation, and the pressure as a function of the radial coordinate is calculated for the

hydrogen 1s state. Furthermore, the *integrand* of the quantum-mechanical expectation value of the kinetic energy is given as a sum of two terms: One term is interpreted as the kinetic energy per volume and the other one is the pressure, and the kinetic energy interpretation agrees with an interpretation given by Salesi [41]. Elsewhere [43] an extension of these interpretations are used to extend the applicability range of the Madelung equations.

Also, in this paper (in section 3), it is demonstrated that for many quantum mechanical stationary states, including the hydrogen atom s states, local mass conservation is incompatible with steady-flow. In other words, the non-classical element of variable mass is necessary for a satisfactory fluid model. Fortunately, the velocity and mass-density definitions mentioned above yield a generalization of the steady-flow continuity equation (3) 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, because the rate of mass creation from the sources are equal to the rate of mass annihilation from the sinks.

Furthermore, the generalized continuity equation, mentioned above, is distinct from the one implied by the Schrödinger equation, and that well known continuity equation is unchanged and is satisfied by the quantum mechanical states that satisfy the generalized Bernoulli equation.

2. A Bernoullian equation for quantum systems

2.1. The theoretic foundation

In this paper, we have one type of quantum mechanical state and one type of fluid flow. For convenience, temporary terminology is introduced to refer to these states.

Definitions. A quantum 1 (Q1) wavefunction ϕ is a real-valued eigenfunction of a one-body time-independent Schrödinger equation. A Q1 probability state is a state represented by a quantum 1 wavefunction ϕ .

Let ϕ be a Q1 wavefunction that is a solution of the one-body Schrödinger equation with external potential V and mass m :

$$-\frac{\hbar^2}{2m}\nabla^2\phi + V\phi = \bar{E}\phi. \quad (2)$$

We next show that the probability density $\rho = \phi^2$ is a solution of the following:

$$\frac{1}{2}m\mathbf{u}^2 + p\rho^{-1} + V = \bar{E}, \quad (3)$$

where

$$\mathbf{u}_{\pm} = \pm \frac{\hbar}{2m} \frac{\nabla\rho}{\rho}, \quad (4)$$

$$p = -\frac{\hbar^2}{4m}\nabla^2\rho, \quad (5)$$

and $u^2 = |\mathbf{u}_{\pm}|^2$. Equation (3) is a compressible-flow generalization of the Bernoulli equation [44, 45] 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 streamlines, called uphill and downhill flow, respectively.

Elsewhere [43] an extension of the interpretations given in this work are used to refine, and further develop, the Madelung equations. In particular, equation (3) is modified by the addition of a kinetic energy term $m\mathbf{v}^2/2$ and the replacement of \bar{E} by the time t derivative term $-\partial S/\partial t$, where the Madelung equations use the wavefunction ansatz $\phi = \sqrt{\rho}e^{iS}$ and the velocity definition $\mathbf{v} = \nabla S/m$, and where $S = S(\mathbf{r}, t)$. The formalism retains the vortex motion from the Madelung equations for the hydrogen-atom stationary-states with nonzero magnetic quantum numbers and, in addition, adds an additional velocity component that yield streamlines that terminate at a node or infinity.

(Furthermore, elsewhere [46], an N -body generalization of (3), based on the N -body generalization of (2), is derived. Also, elsewhere [47] it is demonstrated that Q1 flows satisfy an Euler equation for variable mass, implying that Q1 flow has variable mass and is steady, irrotational, inviscid, and compressible. In the same work, speed of sound equations are derived and applied to the same one-body quantum systems considered here.)

For the proof below, the external potential V is required to be a function such that the subspace $\{\mathbf{r} \in \mathbb{R}^3 | \rho(\mathbf{r}) = 0\}$ has measure zero and the eigenfunctions of (2) are three times continuously differentiable. Hence, the condition $\rho(\mathbf{r}) \neq 0$ for (3) implies that ρ satisfies the equation almost everywhere (a.e.), since $\{\mathbf{r} \in \mathbb{R}^3 | \rho(\mathbf{r}) = 0\}$ has measure zero.

The proof involves first obtaining the following:

$$-\frac{1}{2}\phi\nabla^2\phi = \frac{1}{8}\rho^{-1}\nabla\rho \cdot \nabla\rho - \frac{1}{4}\nabla^2\rho. \quad (6)$$

To show that this is an identity, we obtain two other auxiliary identities. The first one, given by

$$-\frac{1}{2}\phi\nabla^2\phi = \frac{1}{2}\nabla\phi \cdot \nabla\phi - \frac{1}{4}\nabla^2\rho, \quad (7)$$

is obtained from the result of

$$\frac{1}{2}\nabla^2\rho = \frac{1}{2}\nabla \cdot \nabla(\phi\phi) = \nabla \cdot (\phi\nabla\phi) = \nabla\phi \cdot \nabla\phi + \phi\nabla^2\phi.$$

For the second one,

$$\nabla\phi \cdot \nabla\phi = \frac{1}{4}\rho^{-1}\nabla\rho \cdot \nabla\rho, \quad (8)$$

we take the vector dot product $\nabla\rho \cdot \nabla\rho$, where

$$\nabla\rho = \nabla(\phi^2) = 2\phi\nabla\phi,$$

giving an equation that is equivalent to (8):

$$\nabla\rho \cdot \nabla\rho = 4\phi^2\nabla\phi \cdot \nabla\phi = 4\rho\nabla\phi \cdot \nabla\phi.$$

Substituting (8) into (7) gives (6). Multiply (2) by ϕ and using (6), we have

$$\frac{\hbar^2}{8m}\rho^{-1}\nabla\rho \cdot \nabla\rho - \frac{\hbar^2}{4m}\nabla^2\rho + V\rho = \bar{E}\rho.$$

Multiplying by ρ^{-1} we obtain

$$\frac{\hbar^2}{8m} \frac{\nabla\rho}{\rho} \cdot \frac{\nabla\rho}{\rho} - \frac{\hbar^2}{4m}(\nabla^2\rho)\rho^{-1} + V = \bar{E}.$$

Substituting definitions (4) and (5) into this one gives (3). Hence, if ϕ is a solution of (2), then $\rho = \phi^2$ satisfies (3). It is easily seen that the derivation is reversible giving the following: If ρ is a solution of (3), then a three times continuously differentiable function ϕ such that $\rho = \phi^2$, satisfies (2). We indicate this state of affairs by stating that (2) and (3) are equivalent. Note that the function $|\phi| = +\sqrt{\rho}$ satisfies (2) a.e, since the subspace $\{\mathbf{r} \in \mathbb{R}^3 | \rho(\mathbf{r}) = 0\}$ has measure zero, where $|\phi|$ is not necessarily differentiable.

For later use for systems with a (total) charge $q \neq 0$, we write (3) as

$$\frac{1}{2}mu^2 + p\rho^{-1} + q\Phi = \bar{E} \quad (9)$$

where Φ is defined by $V = q\Phi$, and the charge density is $q\rho$.

Note that it follows from definition (4) that the direction of \mathbf{u}_+ and \mathbf{u}_- on a streamline are towards increasing and decreasing density ρ , respectively. The velocity field definition (4) also indicates that Q1 flow states are irrotational. To obtain the velocity potential ω from (4), and avoid taking the natural logarithm of a dimensioned quantity, both densities are replaced by the dimensionless density $\tilde{\rho} = a_0^3\rho$, where a_0 is the Bohr radius, giving

$$\omega = \pm \frac{\hbar}{2m} \ln \tilde{\rho}. \quad (10)$$

It follows from (4) that the potential of the momentum density $\rho_m \mathbf{u}_\pm$ is $\pm(\hbar/2)\rho$. As in the Bernoulli equation for irrotational flow [44, 45], equation (3) holds for the entire flow field with one constant \bar{E} , instead of a different constant for each streamline.

Definitions. A Q1 density ρ is a real valued solution of the Bernoullian (3), where the velocity and pressure are given by (4) and (5), respectively. A Q1 flow state is a state represented by a Q1 density ρ .

Next we show that there are *no* static Q1 flow state. Consider a Q1 static flow where V is not a constant scalar field. Since, \mathbf{u}_\pm is the zero function, equation (4) indicates that ρ is uniform. Hence, from equation (5), it follows that the pressure p is the zero function. Therefore, (3) has no solutions. (equation (2) only has the trivial solution, which is not an eigenfunction.) It is easily shown that if V is a constant function and there are no boundary condition imposed in \mathbb{R}^3 , then there is no *real-valued* eigenfunction of (2). Since (2) and (3) are equivalent, (3) also has no solutions if V is constant. Hence, there is *not* a static Q1 flow state.

2.2. Interpretations of the fields

Dividing equation (9) by the mass of the system m , we have

$$\frac{1}{2}u^2 + p\rho_m^{-1} + \frac{q}{m}\Phi = \frac{\bar{E}}{m}$$

where the function $u^2/2$ is the kinetic energy per mass, also called the specific kinetic energy. Hence, this equation is a statement of the conservation of the *specific* (total) energy \bar{E}/m . Since the total mass m is a known quantity for a given system, $mu^2/2$ has the same information as $u^2/2$. We call $u^2/2$ and $mu^2/2$ the open and

closed specific kinetic energies, respectively, where $mu^2/2$ is closed with respect to the dimension of energy. For convenience, the pressure p is also called the compression energy per volume or the compression energy density. Hence, $p\rho_m^{-1}$ is the open specific compression energy, and $p\rho_m^{-1} \times m = p\rho^{-1}$ is the closed specific compression energy, and this term also appears in (9). Furthermore, the scalar fields Φ and $q\Phi$ are the open and closed specific electrostatic potential-energies, respectively; these are also called the potential-energy per charge and per amount, respectively. Similarly, $mu^2/2$ is also called the kinetic energy per amount. For a one-electron atom with atomic number Z , the external potential V can be written

$$V = (-e)\Phi, \quad \Phi(r) = \frac{Z}{4\pi\epsilon_0} \frac{e}{r} \quad (11)$$

where $(-e)$ and e are the electron and proton charges, respectively. The scalar field Φ is the classical electrostatic-potential of a point source with charge Ze ; Φ is the open specific potential energy, or the potential energy per charge. Hence, $(-e)\Phi = V$ —the external potential from the Schrödinger' (2)—is the closed specific potential energy for Q1 flow states of hydrogenic electronic systems. Equation (9), where \bar{E} is uniform, is a statement of the conservation of the closed *specific* (total) energy \bar{E} , an intensive variable with an energy unit. In other words, the scalar field \bar{E} is a constant of motion for each fluid element. However, equation (9) is *not* a statement of the (non-specific) conservation of energy for the fluid elements. As a trivial analogy, consider a (uniform) thermodynamics system with total energy E , where half of the system is removed by a process that does not change the intensive variables, both the pressure and the temperature. Hence, E become $E/2$, but the total specific energy, the total energy per mass, does not change. This is analogous to what happens to fluid elements that satisfy equation (9), except that \bar{E} is the specific total energy \bar{E}/m times the fixed electron mass m —a constant.

In order to make an interpretation of the Laplacian term from the Schrödinger equation (2), consider the following two equations: (1) The equation obtained by multiplying the Schrödinger equation (2) by ϕ and then followed by substituting $\rho = \phi^2$; and, (2) the Bernoullian equation (3) multiplied by ρ . Subtracting these two equations gives

$$-\frac{\hbar^2}{2m}\phi\nabla^2\phi = \frac{1}{2}\rho_m u^2 + p. \quad (12)$$

Hence, the *integrand* of the expectation value of the kinetic energy for a Q1 probability state is the sum of the kinetic-energy density and the compression-energy density of the corresponding Q1 flow state.

Next we show that the pressure cannot be a non-negative function. For each Cartesian coordinate $\alpha \in \{x, y, z\}$ we require the wavefunction to satisfy

$$\lim_{\alpha \rightarrow \pm\infty} \phi(\mathbf{r}) = \lim_{\alpha \rightarrow \pm\infty} \frac{\partial\phi}{\partial\alpha} = 0.$$

Hence

$$\int_{-\infty}^{\infty} \frac{\partial^2\rho}{\partial\alpha^2} d\alpha = \frac{\partial\rho}{\partial\alpha} \Big|_{-\infty}^{\infty} = 2\phi \frac{\partial\phi}{\partial\alpha} \Big|_{-\infty}^{\infty} = 0$$

and therefore

$$\int_{\mathbb{R}^3} \nabla^2\rho d\mathbf{r} = 0.$$

This result combined with (5) gives

$$\int_{\mathbb{R}^3} p d\mathbf{r} = 0. \quad (13)$$

The result implies that, if p is not the zero function a.e., then it cannot be nonnegative or nonpositive a.e. Hence, the pressure from quantum flows differ in this regard from classical flows where the pressures are required to be thermodynamic pressures, and such pressures are nonnegative.

Let the summed kinetic-energy (over all space) of the Q1 flow state represented by ρ be defined by

$$\int_{\mathbb{R}^3} \left(\frac{1}{2}mu^2\right)\rho d\mathbf{r}, \quad (14)$$

where $mu^2/2$ is the closed specific kinetic-energy of the Q1 flow state. Analogous summed energies are also defined for the other terms from equation (3). Since the scalar field \bar{E} is uniform and ρ is normalized, the summed total energy E satisfies

$$E = \int_{\mathbb{R}^3} \bar{E}\rho d\mathbf{r} = \bar{E}. \quad (15)$$

Hence, the summed total energy E of the Q1 flow state is equal to the closed specific total-energy \bar{E} , where \bar{E} is also the energy of the corresponding Q1 probability state that satisfies (2). Note that \bar{E} is a scalar field and E is not a scalar field.

Let $S \in \mathbf{R}^3$. The kinetic energy over the subspace S (of the state represented by ρ) is given by (14) with \mathbf{R}^3 replaced by S . A similar definition is used for the other energy-dimensional scalar fields. For example, the compression energy over the subspace S is

$$\int_S (p\rho^{-1})\rho \, d\mathbf{r} = \int_S p \, d\mathbf{r},$$

and (13) indicates that the summed compression energy (over all space) is zero.

The potential energy over S satisfies

$$\int_S \phi^* V \phi \, d\mathbf{r} = \int_S V \rho \, d\mathbf{r}.$$

With $S = \mathbf{R}^3$, the above equation indicates that the expectation value of the potential energy for a Q1 probability state is equal to the summed potential energy of the corresponding Q1 flow state. Except for special cases, the kinetic energy satisfies

$$\int_S \left(-\frac{\hbar^2}{2m} \phi \nabla^2 \phi \right) d\mathbf{r} \neq \int_S \left(\frac{1}{2} \rho_m u^2 \right) d\mathbf{r}.$$

By setting $S = \mathbf{R}^3$, and using (12) and (13), we find that

$$\int_{\mathbf{R}^3} \phi \hat{T} \phi \, d\mathbf{r} = \frac{1}{2} \int_{\mathbf{R}^3} \rho_m u^2 \, d\mathbf{r}, \quad \hat{T} = -\frac{\hbar^2}{2m} \nabla^2. \quad (16)$$

Hence, the expectation value of the kinetic energy for a Q1 probability state is equal to the summed kinetic energy of the corresponding Q1 flow state. This result gives some justification for the interpretation that $\rho_m u^2/2$ as the kinetic energy per volume for a fluid with velocity \mathbf{u}_\pm , and this identification is in agreement with the interpretation given by Salesi [41].

It would be interesting to explore the radial momentum for fluid flows and compare this property with the corresponding one for quantum-mechanical states, e.g., the hydrogen s states that provide spherical flows. Unfortunately, the radial momentum operator of quantum mechanics, the one derived by Dirac [48], is not self adjoint in the Hilbert space $L^2(\mathbf{R}^3)$ [49], suggesting that the radial momentum is not an observable. However, if transforming the wavefunction into the form as $\Psi = r^{-1/2} u(r) Y(\theta, \varphi)$ where Y is the spherical harmonic function, the radial momentum operator is self adjoint for the Hilbert space $L^2[0, +\infty)$ of $u(r)$.

2.3. The ground state of hydrogenic atoms

Next we examine the velocity, pressure and the energy terms within (9) for the 1s state of the hydrogenic atom with atomic number Z . The flow is spherical, where a given radial unit-vector $\hat{\mathbf{r}}$ of spherical coordinates is tangent to a streamline, and the direction of downhill and uphill flow are $\hat{\mathbf{r}}$ and $-\hat{\mathbf{r}}$, respectively. When examining the results, it is useful to be aware that the derived Hartree atomic units of velocity, pressure and energy are

$$\frac{\hbar}{ma_0}, \quad \frac{\hbar^2}{ma_0^5}, \quad \text{and} \quad \frac{\hbar^2}{ma_0^2}.$$

respectively, where m is the electron mass, and the Bohr radius a_0 is 0.5292×10^{-10} meters to four figures. Since all the energy terms considered are closed, the word ‘closed’ is suppressed.

In spherical coordinates, the probability density for hydrogenic 1s states [50], is

$$\rho(r) = \frac{Z^3}{a_0^3} \pi^{-1} e^{-2Zr/a_0}. \quad (17)$$

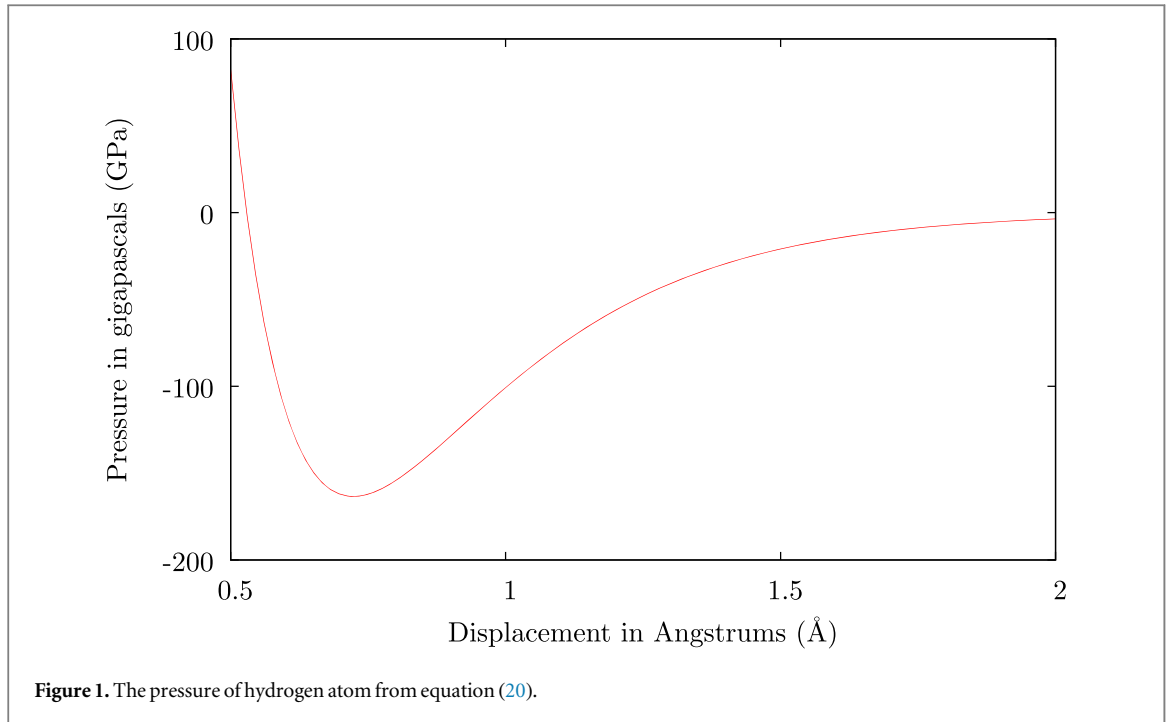
The velocity field is

$$\mathbf{u}_\pm = \pm \frac{\hbar}{2m} \frac{\nabla \rho}{\rho} = \pm \frac{\hbar}{2m} \rho^{-1} \frac{\partial \rho}{\partial r} \hat{\mathbf{r}} = \pm \frac{\hbar}{2m} \rho^{-1} (-2Z/a_0) \rho \hat{\mathbf{r}}.$$

In other words,

$$\mathbf{u}_\pm = \mp \frac{Z\hbar}{ma_0} \hat{\mathbf{r}}, \quad \frac{1}{2} m u^2 = \frac{1}{2} \frac{Z^2 \hbar^2}{ma_0^2}. \quad (18)$$

Hence, the speed $|\mathbf{u}_\pm|$ is constant. For the hydrogen atom $Z = 1$, we have $|\mathbf{u}_\pm| = \hbar/ma_0$, and this constant is both the derived Hartree unit of velocity and the speed of the electron in the first Bohr orbit of hydrogen [50]. The



second equation from (18), for use below, is the specific kinetic energy, and u can be chosen to be $|\mathbf{u}_{\pm}|$, but there are other choices, e.g., $u = \mathbf{u}_{\pm} \cdot \hat{\mathbf{r}}$.

Let $\bar{z} = Z/a_0$. Next we calculate the pressure p and the compression energy per amount $p\rho^{-1}$, starting with the Laplacian of ρ :

$$\nabla^2 \rho = r^{-2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \rho}{\partial r} \right) = -2\bar{z}r^{-2} \frac{\partial}{\partial r} (\rho r^2) = -2\bar{z}r^{-2} (-2\bar{z}r^2 \rho + 2r\rho) = 4\bar{z}^2 \rho - 4\bar{z}r^{-1} \rho.$$

The pressure p , defined by (5), is

$$p(r) = -\frac{1}{4} \frac{\hbar^2}{m} \nabla^2 \rho = \left(-\frac{\hbar^2}{m} \bar{z}^2 + \frac{\hbar^2}{a_0 m} Z r^{-1} \right) \rho(r). \quad (19)$$

Using $\bar{z} = Z/a_0$, this equation can also be written

$$p(r) = \left(\frac{\hbar^2}{a_0 m} Z r^{-1} - \frac{\hbar^2}{a_0 m} \frac{Z^2}{a_0} \right) \rho(r) = \frac{Z \hbar^2}{a_0 m} \left(\frac{1}{r} - \frac{Z}{a_0} \right) \rho(r).$$

Substituting (17) for ρ gives

$$p(r) = \frac{Z^4 \hbar^2}{a_0^4 m} \left(\frac{1}{r} - \frac{Z}{a_0} \right) \pi^{-1} e^{-2Zr/a_0}.$$

Finally we express the pressure in a manner so that it is clearly dependent on r/a_0 :

$$p(r) = Z^4 \frac{\hbar^2}{m a_0^5} \left(\frac{a_0}{r} - Z \right) \pi^{-1} e^{-2r/a_0}, \quad (20)$$

where $\hbar^2/m a_0^5$ is the derived Hartree unit of pressure. For the hydrogen atom, the pressure is zero at $r = a_0$; it is positive and negative for $r < a_0$ and $r > a_0$, respectively. The pressure is plotted for the hydrogen atom in Figure 1 for a calculation with a_0 in the Angstrom unit and $\hbar^2/m a_0^5$ in the Pascal unit.

Returning to the equation (19), the specific compression energy $p\rho^{-1}$ is

$$p\rho^{-1} = -\frac{\hbar^2}{m} \bar{z}^2 + \frac{\hbar^2}{a_0 m} Z r^{-1}.$$

Using the definition [50]

$$\frac{\hbar^2}{a_0 m} = \frac{e^2}{4\pi\epsilon_0}$$

where e is the proton charge, we obtain the desired form:

$$p\rho^{-1} = -\frac{\hbar^2}{m}\bar{z}^2 + \frac{e^2}{4\pi\epsilon_0}Zr^{-1}. \quad (21)$$

Adding the second equation from (18) to equations (21) and (11), we get

$$\frac{1}{2}mu^2 + p\rho^{-1} + (-e)\Phi_p(r) = \frac{1}{2}\frac{Z^2\hbar^2}{a_0^2m} - \frac{\hbar^2}{m}\bar{z}^2 + \frac{e^2}{4\pi\epsilon_0}Zr^{-1} - \frac{Z}{4\pi\epsilon_0}\frac{e^2}{r}.$$

In other words,

$$\frac{1}{2}mu^2 + p\rho^{-1} + (-e)\Phi_p(r) = -\frac{1}{2}\frac{Z^2\hbar^2}{ma_0^2}.$$

Comparing this result with (9) for $q = -e$, we obtain

$$\bar{E} = -\frac{1}{2}Z^2\frac{\hbar^2}{ma_0^2} = -\frac{e^2}{(4\pi\epsilon_0)a_0}\frac{Z^2}{2}.$$

The second form of the energy is obtained from $1/(a_0m) = e^2/(4\pi\epsilon_0\hbar^2)$. As expected, \bar{E} is the eigenvalue of the Schrödinger equation (2) for the 1s ground state with atomic number Z [50].

For use below, we compute $(p\rho^{-1} + (-e)\Phi)$, a constant function, using (21) and (11):

$$p\rho^{-1} + (-e)\Phi = -\frac{Z^2\hbar^2}{a_0^2m}. \quad (22)$$

It is also convenient to write (9) as

$$\frac{1}{2}mu^2 + P\rho^{-1} = \bar{E}, \quad (23)$$

where the effective pressure P is defined $P = p + q\rho\Phi$, which for all $\mathbf{r} \in \mathbf{R}^3$ such that $\rho(\mathbf{r}) \neq 0$, can be written

$$P\rho^{-1} = p\rho^{-1} + q\Phi, \quad (24)$$

and $P\rho^{-1}$ is the specific effective compression-energy or the (total) specific potential-energy. For hydrogenic 1s flow, $P\rho^{-1}$ can be obtained by combining (24) and (22) with $q = -e$:

$$P\rho^{-1} = -\frac{Z^2\hbar^2}{ma_0^2}. \quad (25)$$

Hence, the hydrogen ground-state has both a constant specific potential-energy $P\rho^{-1}$ and, from (18), a constant specific kinetic-energy $mu^2/2$.

An equation of state for a Q1 flow, when it exists, for the pressure p and the effective pressure P , are equations that define the maps $\rho(\mathbf{r}) \rightarrow p(\mathbf{r})$ and $\rho(\mathbf{r}) \rightarrow P(\mathbf{r})$, respectively, where the maps hold for $\text{Range}(\rho)$.

Equation (25), which defines the function P with $P(\rho) = -Z^2\hbar^2/(ma_0^2)\rho$, is an effective pressure equation of state for the ground-states of hydrogenic atoms.

3. The Continuity equation for quantum systems

For the hydrogen ns states, where $n = 1, 2, \dots$, since the wavefunctions of these states are spherically symmetric and quantum mechanics predicts a zero angular momentum, a satisfactory model should have spherical flow, where each fluid element is restricted to a ray with the end point at the nucleus. In addition, since the time dependence of the wavefunctions of stationary states only involves a constant phase factor, these flows should be steady. Since spherical and steady flow without a source and sink requires an infinite mass of fluid to satisfy the two conditions, these two requirements are incompatible. Hence, to provide a reasonable fluid representation, these zero angular-momentum states must have mass that is *not* locally conserved. However, over all space the flows conserve mass. Also, it is reasonable to expect some nonclassical elements of a model of quantum states, so variable mass is just one of those elements. Finally, the variable mass is not only necessary, it is desirable, since it permits a very simple model with few assumptions. This follows because the Bernoullian equation (3) requires the velocity and pressure to satisfy (4) and (5), and these two conditions imply variable mass, since, in general, $\nabla \cdot (\rho_m \mathbf{u}_\pm) \neq 0$. This argument is easily extended to steady flows that cross a node or terminate at a node with zero velocity, where ρ vanishes, since such steady flows must, locally, have variable mass.

The differential and integral forms of the continuity equations for steady flows are [44, 45]

$$\nabla \cdot \rho_m \mathbf{u} = 0 \quad (26)$$

$$\int_S \rho_m \mathbf{u} \cdot \hat{\mathbf{n}} dS = 0 \quad (27)$$

where $\nabla \cdot \rho_m \mathbf{u}$ is the mass creation-rate per volume. For the quantum flows under consideration, a generalization of the differential form of the continuity equation (26) for steady flows is obtained by multiplying the velocity definition (4) by the mass density ρ_m and then taking the divergence of the result:

$$\nabla \cdot \rho_m \mathbf{u}_{\pm} = \pm \frac{\hbar}{2} \nabla^2 \rho. \quad (28)$$

Hence, for this steady-flow generalization of the continuity equation (26), mass is not locally conserved. Using $\nabla^2 \rho = \nabla \cdot \nabla \rho$ with the divergence theorem, we obtain a generalization of (27) for steady flows:

$$\int_S \rho_m \mathbf{u}_{\pm} \cdot \hat{\mathbf{n}} dS = \pm \frac{\hbar}{2} \int_S \nabla \rho \cdot \hat{\mathbf{n}} dS. \quad (29)$$

Reversing the order of (28), followed by multiplying the equations by $\pm \hbar/(2m)$, and using $\rho_m/m = \rho$, we have

$$\frac{\hbar^2}{4m} \nabla^2 \rho = \pm \frac{\hbar}{2} \nabla \cdot (\rho \mathbf{u}_{\pm}).$$

Comparing this result with the pressure definition (5) gives

$$p = \mp \frac{\hbar}{2} \nabla \cdot \rho \mathbf{u}_{\pm}. \quad (30)$$

Hence, the pressure is proportional to the mass creation rate per volume $\nabla \cdot \rho_m \mathbf{u}$. Note that both velocity vectors \mathbf{u}_{\pm} give the same pressure scalar field, but their formulas differ. The previous equation can also be written

$$\nabla \cdot \rho_m \mathbf{u}_{\pm} = \mp \frac{2m}{\hbar} p. \quad (31)$$

Since for downhill flow \mathbf{u}_- the plus sign is taken, mass is created in regions of positive pressure and destroyed in regions of negative pressure. Using (31) and (13), the total mass-creation rate $\dot{M}(\mathbf{R}^3)$ over all space is

$$\dot{M}(\mathbf{R}^3) = \int_{\mathbf{R}^3} \nabla \cdot \rho_m \mathbf{u}_{\pm} d\mathbf{r} = \mp \frac{2m}{\hbar} \int_{\mathbf{R}^3} p d\mathbf{r} = 0.$$

Hence, over all space, mass is conserved. Elsewhere, for the hydrogen 1s state, the (summed) mass creation rate from the region of positive pressure for downhill flow is calculated [47].

4. Applications

Using (4), the component u_{\pm} of the velocity \mathbf{u}_{\pm} on a streamline with a fluid velocity direction of $\hat{\mathbf{z}}$ is

$$u_{\pm} = \mathbf{u}_{\pm} \cdot \hat{\mathbf{z}} = \pm \frac{\hbar}{2m} \rho^{-1} \nabla \rho \cdot \hat{\mathbf{z}} = \pm \frac{\hbar}{2m} \rho^{-1} \partial \rho \quad (32)$$

where $\partial \rho \doteq \nabla \rho \cdot \hat{\mathbf{z}}$, the directional derivative of ρ in the direction $\hat{\mathbf{z}}$. For uniform, one-dimensional models, and spherical flow, $\partial \rho$ is an ordinary or partial derivative, in a bases set where $\hat{\mathbf{z}}$ is the positive direction.

Elsewhere [47] it is demonstrated that the Mach speed (Ma) is 1 where the momentum density ρu_{\pm} is an extremum on a streamline, and for uniform flow, it is demonstrated that $p(r) = 0$ implies $\text{Ma}(r) = 1$. Because of their importance, the points such that $\partial[\rho u_{\pm}] = 0$, are represented by vertical lines in the following plots.

In order to improve efficiency, imperative sentences are used for some derivations that start and end with a large vertical line. All calculations are done with atomic units with the mass m equal to the electron mass, giving $m = a_0 = 1$.

4.1. A fluid (or particle) in a one-dimensional box

For a particle, or fluid, in a one-dimensional box of length ℓ , let ℓ be the Bohr radius a_0 , giving $\ell = 1$ for atomic units. Let $\partial \rho \doteq d\rho/dr$, where $r \in \mathbf{R}$ is the position variable.

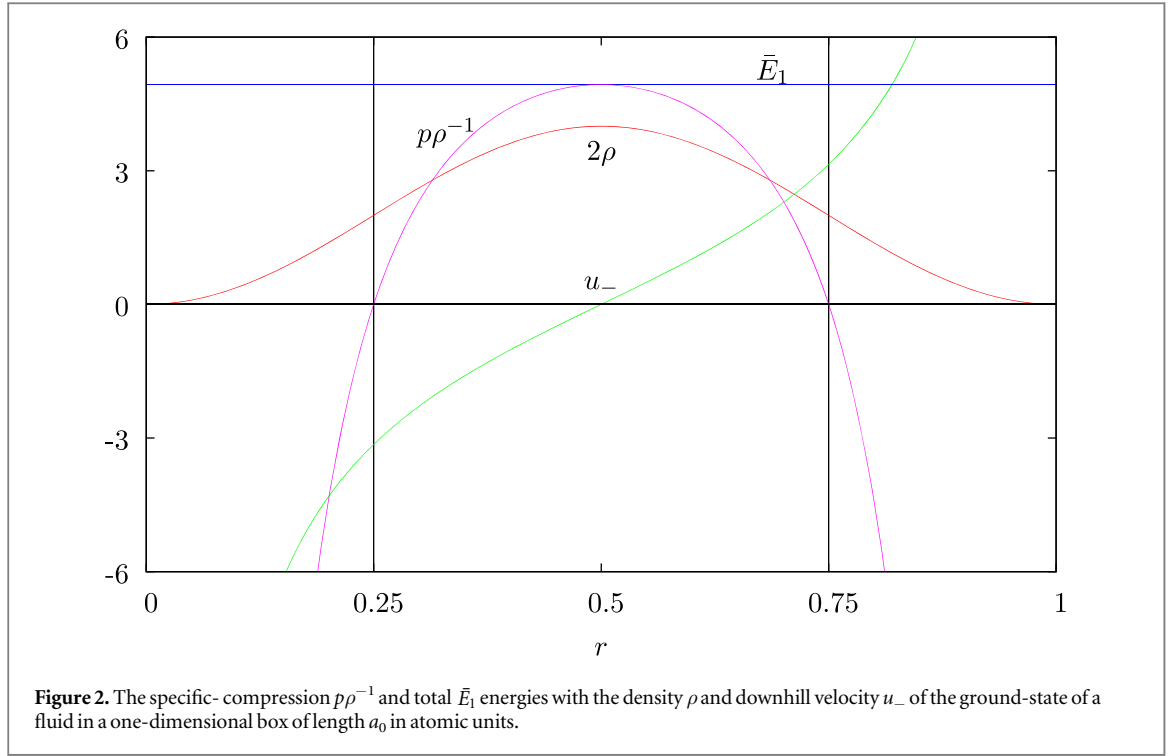
| Start with the well known density ρ [51, 52] with domain $[0, 1]$ and quantum number ($n = 1, 2, \dots$) for the Q1 probability states and compute the velocity-component u_{\pm} using (32), the momentum density ρu_{\pm} , and the Laplacian:

$$\rho(r) = 2 \sin^2(n\pi r)$$

$$\partial \rho(r) = 4n\pi \sin(n\pi r) \cos(n\pi r) \quad (33)$$

$$u_{\pm}(r) = \pm n\pi \cot(n\pi r) \quad (34)$$

$$\rho u_{\pm}(r) = \pm 2n\pi \sin(n\pi r) \cos(n\pi r) \quad (35)$$



$$\partial^2\rho(r) = 4n^2\pi^2[\cos^2(n\pi r) - \sin^2(n\pi r)]. \quad (36)$$

Substitute $(\cos^2(n\pi r) = 1 - \sin^2(n\pi r))$ into (36) and use (5), i.e., $p = -\partial^2\rho/4$, to calculate the pressure:

$$p(r) = -n^2\pi^2[1 - 2\sin^2(n\pi r)]. \quad (37)$$

Use $\rho^{-1}(r) = \csc^2(n\pi r)/2$ and $\csc^2 x = 1 + \cot^2 x$ to calculate the specific compression energy $p\rho^{-1}$:

$$\begin{aligned} [p\rho^{-1}](r) &= -\frac{1}{2}n^2\pi^2[\csc^2(n\pi r) - 2] \\ [p\rho^{-1}](r) &= -\frac{1}{2}n^2\pi^2 \cot^2(n\pi r) + \frac{1}{2}n^2\pi^2. \end{aligned} \quad (38)$$

Calculate the specific kinetic-energy $mu^2/2$ using (34) and the well known total energy \bar{E}_n using the formula for the specific total-energy (23), given by $\bar{E}_n = mu^2/2 + p\rho^{-1}$:

$$\frac{1}{2}[mu_{\pm}^2](r) = \frac{1}{2}n^2\pi^2 \cot^2(n\pi r) \quad (39)$$

$$\bar{E}_n = \frac{1}{2}n^2\pi^2. \quad (40)$$

Using (35), we have

$$\partial[\rho u_{\pm}](r) = 2n\pi[\cos^2(n\pi r) - \sin^2(n\pi r)].$$

Hence, the extremums of momentum density ρu_{\pm} , which satisfy $\partial[\rho u_{\pm}] = 0$, occur at $r \in \{1/4, 3/4\}$ for the $n = 1$ ground state. Figure 2 presents a plot of the specific-compression $p\rho^{-1}$ and the total \bar{E}_1 -energies with the density ρ and the downhill velocity u_- of the ground-state flow in a one-dimensional box of length a_0 in atomic units. The points of extremums of momentum density ρu_{\pm} are represented by vertical lines in the plot, where the pressure is also zero. The specific kinetic $mu^2/2$ energy can be approximated from the figure by noting that $mu^2/2 = \bar{E}_1 - p\rho^{-1}$. The point $r = 0.5$ is an unstable equilibrium point. The maximum density is also at $r = 0.5$ where the velocity is zero. For $r > 0.5$, and downhill flow, the fluid particles are moving and accelerating to the right, in other words, they move downhill with respect to the 'density hill,' so to speak; for $r < 0.5$ they move and accelerate to the left. In the limit of a fluid particle reaching a node, i.e., $r \rightarrow 0$ or $r \rightarrow 1$, the particle have infinity speed and zero mass. From (31), given by $\partial(\rho_m u_{\pm}) = \mp 2p$ for one-dimension and atomic units, it follows that for downhill flow, the streamline segments $(0.25, 0.75)$, where the pressure is positive, is the creation zone, or the source, and $(0, 0.25)$ and $(0.75, 1)$, where the pressure is negative, are the annihilation zones, or the sink. Figure 3 presents a plot of the same variables for the first excited state for $r \in [0, 0.5]$, where the extremums of the momentum density occur at $r \in \{0.125, 0.375\}$. The same general behavior as the ground state is observed, but with an unstable equilibrium point of 0.25 and nodes at 0 and 0.5. For downhill flow, the source is $(0.125, 0.375)$ and the sinks are $(0, 0.125)$ and $(0.375, 0.5)$. The plot from $r \in [0.5, 1]$ can be obtained from figure 3 using the

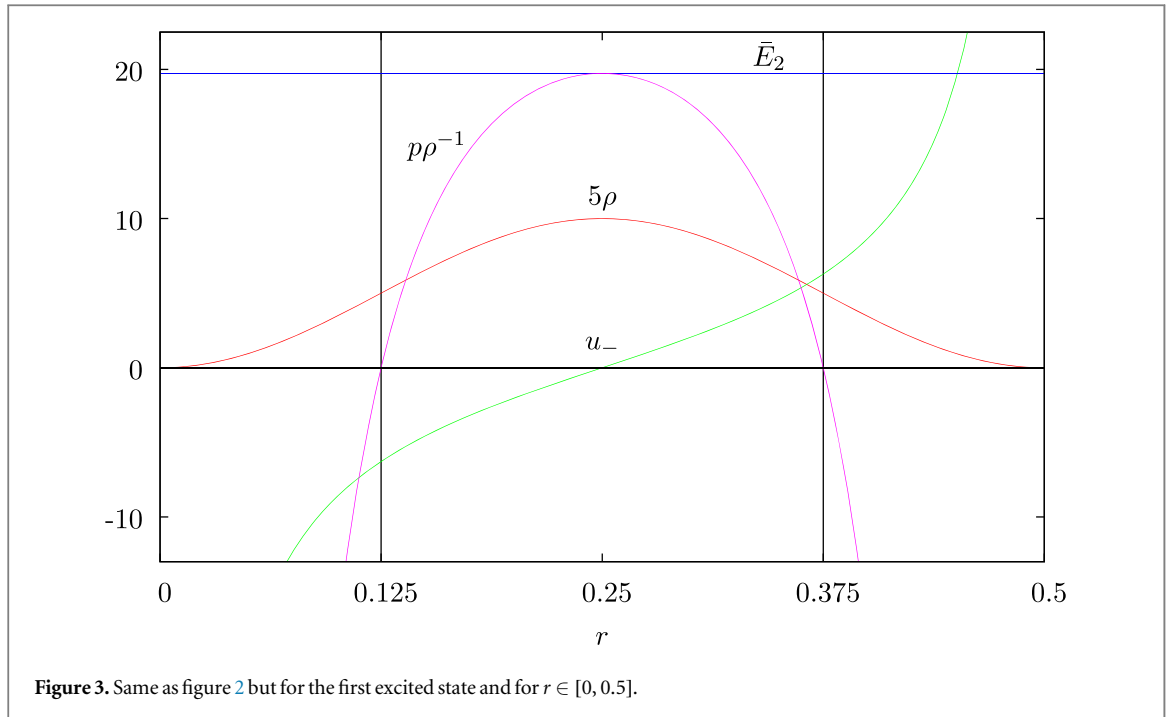


Figure 3. Same as figure 2 but for the first excited state and for $r \in [0, 0.5]$.

periodic property $f(x + 0.5) = f(x)$ for $x \leq 0.5$. Hence, the other unstable equilibrium point is 0.75 and the nodes are 0, 0.5 and 1.

Combining (37) with $\rho = 2 \sin^2(n\pi r)$ gives the pressure equation of state for all flow states in a one-dimensional box:

$$p(\eta) = -n^2\pi^2(1 - \eta),$$

and p is an affine function of $\eta = \rho(r)$.

Definitions. Let $L \in \mathbb{R}^3$ be a streamline of a one-dimensional flow, where L is represented by an interval, and the position along the streamline is given by the variable $r \in L$. A *node* $r_{\text{node}} \in L$ on L is a point such that $\rho(r_{\text{node}}) = 0$. An *antinode* $r_{\text{antinode}} \in L$ is a point such that $\partial\rho(r_{\text{antinode}})/\partial r = 0$. A *flow hill* $H(r_b, r_{\text{antinode}}, r_r)$ of L is a interval $(r_b, r_r) \in L$ such that $r_{\text{antinode}} \in (r_b, r_r)$ is an antinode, and r_b , for $i = l, r$, is a node or a point at infinity, and there are no other nodes in H .

The particle in a box of length 1 contains one flow hill, $[0, .5, 1]$, for the ground state, and two flow hills, $[0, .25, .5]$ and $[.5, .75, 1]$, for the first excited state.

4.2. The harmonic oscillator

In this subsection we treat the ground state and first excited state of the harmonic oscillator, with quantum numbers $n = 0, 1$. The Q1 wavefunctions for the ground- and first excited-states of the harmonic oscillator are [51, 52]

$$\phi_0(x) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2}, \quad \phi_1(x) = 2\left(\frac{2\alpha^3}{\pi}\right)^{1/4} x e^{-\alpha x^2} \tag{41}$$

where $\alpha = m\omega/(2\hbar)$, $\omega = \sqrt{k/m}$, and the specific potential-energy is $V(x) = m\omega^2 x^2/2$. We choose $m, k = 1$, giving $\omega = 1$ and $\alpha = 1/2$ in atomic units.

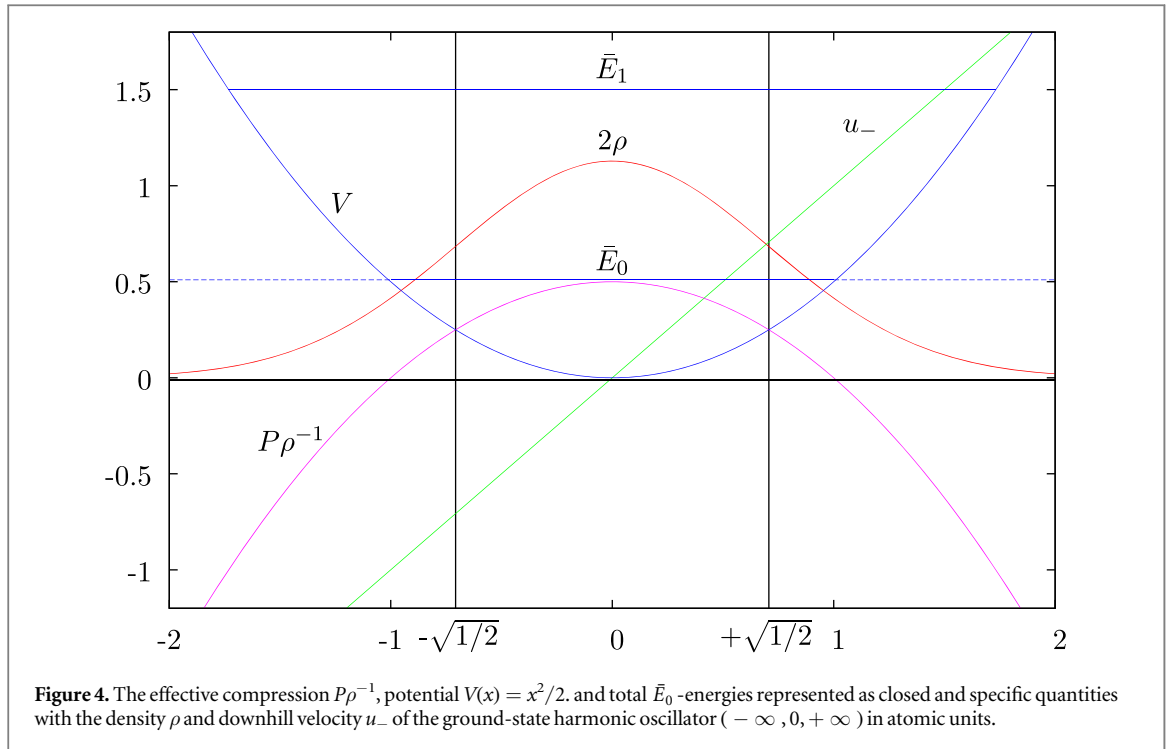
4.2.1. The harmonic oscillator ground state: $(-\infty, 0, +\infty)$

The ground state of the harmonic oscillator has one flow hill $(-\infty, 0, +\infty)$. | Start with the density formula $\rho = \phi_0^2$ and (41) to compute the uphill flow velocity-component using (32), i.e., $u_+ = \partial\rho/(2\rho)$, the momentum density ρu_+ , and the specific kinetic energy $mu_+^2/2$:

$$\begin{aligned} \rho(x) &= \phi_0^2(x) = \pi^{-1/2} e^{-x^2} \\ \partial\rho(x) &= -2x\rho(x) \end{aligned} \tag{42}$$

$$u_+(x) = \frac{1}{2}[\rho^{-1}\partial\rho](x) = -x \tag{43}$$

$$\rho u_+ = -x\pi^{-1/2} e^{-x^2} \tag{44}$$



$$\frac{1}{2}mu^2(x) = \frac{1}{2}x^2. \tag{45}$$

Using (42), compute the second derivative:

$$\partial^2\rho(x) = -2\pi^{-1/2}\partial(xe^{-x^2}) = (-2 + 4x^2)\rho. \tag{46}$$

Compute the pressure p using (46) and (5), i.e., ($p = -\partial^2\rho/4$), the specific compression energy $p\rho^{-1}$, the specific effective-compression energy $P\rho^{-1} = p\rho^{-1} + V$, with $V(x) = x^2/2$, and the well known specific total-energy \bar{E}_0 from (23):

$$p(x) = \left(\frac{1}{2} - x^2\right)\rho \tag{47}$$

$$[p\rho^{-1}](x) = \frac{1}{2} - x^2 \tag{48}$$

$$[P\rho^{-1}](x) = \frac{1}{2} - \frac{1}{2}x^2 \tag{49}$$

$$\bar{E}_0 = \frac{1}{2}mu^2 + P\rho^{-1} = \frac{1}{2}. \tag{50}$$

Figure 4 presents the specific- effective-compression $P\rho^{-1}$, potential $V(x) = x^2/2$, and total \bar{E}_0 energies with the density ρ and downhill velocity u_- of the ground-state harmonic oscillator with $m, k = 1$ in atomic units. The same type of behavior is observed as in the particle in a box states considered, figures 2 and 3, with $x = 0$ being an unstable equilibrium point. In addition, there is flow into the classical forbidden regions, given by the two regions beyond the solid horizontal line at energy \bar{E}_0 , and this behavior corresponds to quantum-mechanical tunneling. Because of the pressure term, the fluid particles do not have negative kinetic energy in the classical forbidden zone, so the zone is not forbidden.

For $p(x) = 0$ we obtain $[P\rho^{-1}](x) = V(x)$. From (47), $p(x) = 0$ is satisfied at $x = \pm\sqrt{1/2}$, and these values agrees with the extremums of the momentum density that satisfies $\partial(\rho u_+) = 0$, where from (44) we have

$$\partial[\rho u_+](x) = -\pi^{-1/2}\partial(xe^{-x^2}) = \pi^{-1/2}(-1 + 2x^2)e^{-x^2}.$$

In the figure $x = \pm\sqrt{1/2}$ are represented by vertical lines where $[P\rho^{-1}](x)$ and $V(x)$ cross. A special case of this same type of crossing appears in figures 2 and 3, where $V(x) = 0$, giving $P\rho^{-1}(x) = p\rho^{-1}(x) = 0$ at the crossing points.

The limits at infinity of the fluid speed are called the speed limits, and there are usually two limits, for $r \rightarrow \pm\infty$. If both limits are equal, the single value is called the speed limit. The speed limit $|u_\infty|$ of the ground state harmonic-oscillator is infinity.

4.2.2. The harmonic oscillator first excited state: $(-\infty, -1, 0]$ and $[0, 1, \infty)$

The first excited state has two flow hills: $(-\infty, -1, 0]$ and $[0, 1, \infty)$, since ρ has maximums (antinodes) at $x = \pm 1$ and a minimum (a node) at $x = 0$. The velocity and momentum density are antisymmetric with respect to the node at $x = 0$, e.g., $u_{\pm}(-x) = -u_{\pm}(x)$. The other functions considered are symmetric with respect to the node. Therefore, we only need to consider the hill $[0, 1, \infty)$, since the behavior of the functions in $(-\infty, -1, 0]$ can be generated from the information from $[0, 1, \infty)$.

Starting with the open density formula $\rho = \phi_1^2$ and (41), compute the uphill flow velocity-component using (32), i.e., $u_+ = \partial\rho/(2\rho)$, the momentum density ρu_+ , and the specific kinetic energy $mu^2/2$:

$$\rho(x) = \beta x^2 e^{-x^2}, \quad \beta = 2\left(\frac{1}{\pi}\right)^{1/2}$$

$$\partial\rho(x) = 2x\beta e^{-x^2} + (-2x)x^2\beta e^{-x^2} = 2(x - x^3)\beta e^{-x^2} \tag{51}$$

$$u_+(x) = \frac{1}{2}[\rho^{-1}\partial\rho](x) = \frac{1}{2}x^{-2}(2x - 2x^3) = x^{-2}(x - x^3)$$

$$u_+(x) = x^{-1} - x \tag{52}$$

$$[\rho u_+](x) = \beta(x - x^3)e^{-x^2} \tag{53}$$

$$\frac{1}{2}[mu^2](x) = \frac{1}{2}(x^{-1} - x)^2. \tag{54}$$

Using (51), compute the Laplacian of ρ :

$$\beta^{-1}\partial^2\rho(x) = 2\partial[(x - x^3)e^{-x^2}]$$

$$\beta^{-1}\partial^2\rho(x) = 2(1 - 3x^2)e^{-x^2} - 4x(x - x^3)e^{-x^2}$$

$$\partial^2\rho(x) = (2 - 10x^2 + 4x^4)\beta e^{-x^2}. \tag{55}$$

Compute the pressure p using (55) and (4), the specific compression energy $p\rho^{-1}$, the specific effective-compression energy $P\rho^{-1} = p\rho^{-1} + V$, with $V(x) = x^2/2$, and the well known specific total-energy \bar{E}_1 from (23):

$$p(x) = -\frac{1}{2}(1 - 5x^2 + 2x^4)\beta e^{-x^2} = -\frac{1}{2}x^{-2}(1 - 5x^2 + 2x^4)\rho \tag{56}$$

$$[P\rho^{-1}](x) = -\frac{1}{2}x^{-2}(1 - 5x^2 + 2x^4) + \frac{1}{2}x^2$$

$$[P\rho^{-1}](x) = -\frac{1}{2}x^{-2} + \frac{5}{2} - x^2 + \frac{1}{2}x^2 = \frac{5}{2} - \frac{1}{2}x^{-2} - \frac{1}{2}x^2$$

$$\frac{1}{2}[mu^2](x) = \frac{1}{2}(x^{-1} - x)^2 = \frac{1}{2}(x^{-2} + x^2 - 2) = \frac{1}{2}x^{-2} + \frac{1}{2}x^2 - 1$$

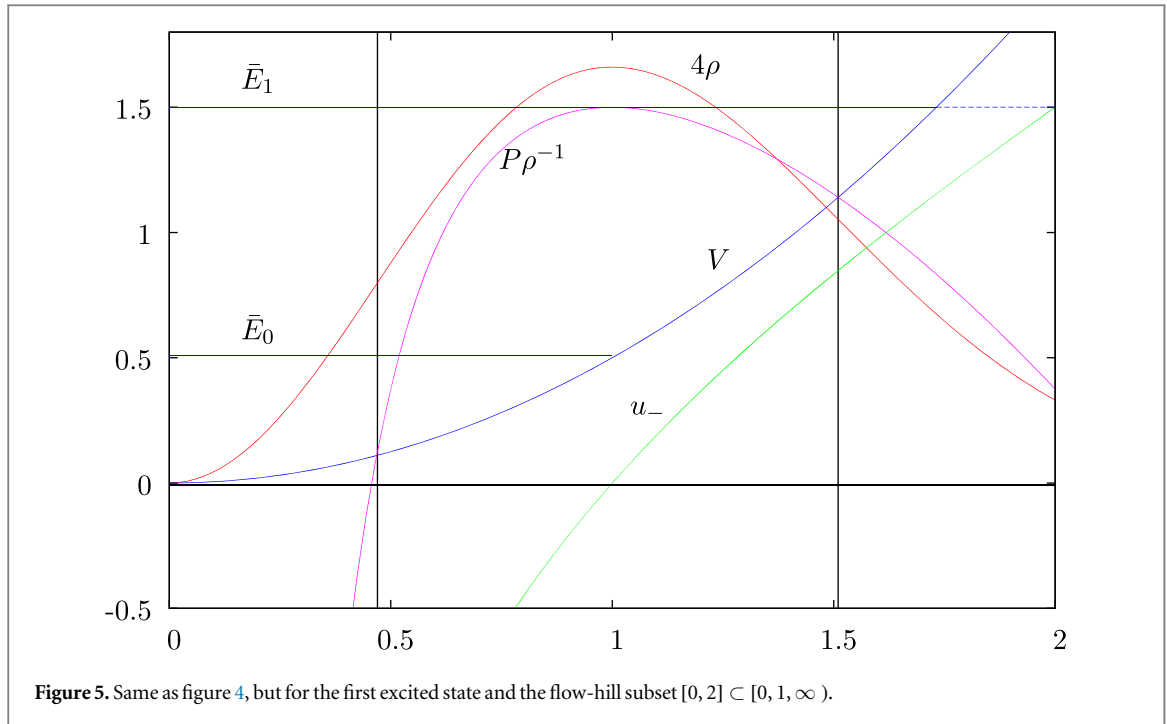
$$\bar{E}_1 = \frac{3}{2}.$$

Figure 5 presents the same functions as in figure 4, for the flow-hill subset $[0, 2] \subset [0, 1, \infty)$ of the first excited state. By examining the pressure p and the momentum density ρu_+ functions, it is easily demonstrated that the points such that $p(x) = 0$ and $\partial[\rho u_{\pm}](r) = 0$ are approximately $x = \pm 0.47$ and $x = \pm 1.51$. These points are represented by vertical lines in the figure. Since $p(x) = 0$ implies $[P\rho^{-1}](x) = V(x)$, the curves for $P\rho^{-1}$ and V cross at the vertical lines, as in the ground state.

Some of the same type of general behavior, as seen in the ground state, is observed, including an unstable equilibrium point at the antinode ($x = 1$). However, unlike the ground state, the functions restricted to $[0, \infty)$ are neither symmetric nor antisymmetric with respect to the antinode (at $x = 1$). The flow hill $[0, 1, \infty)$ is also distinct from the others considered, since it contains both a node (at $x = 0$) and a point at infinity. As in the ground state, the speed limit is ∞ .

Definition. Let $L \subset \mathbf{R}$ be a streamline for a one-dimensional flow, and I an interval such that $I \subset L$. If no matter can enter or leave I by convection, then I is called a closed flow segment of L . If I does not contain a proper subset that is closed, then I is a primitive flow segment of L .

It is easy to prove that flow hills always contain two primitive flow segment. For example, the ground state of the particle in a box has the following two primitive flow segments: $[0, 1/2]$ and $[1/2, 1]$, where at the antinode $r = 1/2$, the velocity is zero, and at the nodes $r = 0, 1$, the density is zero. Hence, there is no convection into or out of the two primitive flow segments.



4.3. The hydrogen 2s state: $[0, 2]$ and $[2, 4, \infty)$

In this subsection we treat the 2s state of the hydrogen atom. In spherical coordinates, since each streamline depends on the radial coordinate r only, the results below hold for any streamline given by a ray $r \in [0, \infty)$, defined by polar and azimuth angles. The 2s state has the primitive flow segment $[0, 2]$ and the flow hill $[2, 4, \infty)$. The segment $[0, 2]$ contains the nucleus $r_{\text{nuc}} = 0$ and the node $r_{\text{node}} = 2$, but it does not contain an antinode. The momentum density is an extremum at the points at 2.59 and 5.41, and these are represented by vertical lines in the following plot.

[Let $h = 1/2$. To calculate the pressure p , note equation (A1) from appendix appendix. Start with the Q1 wavefunction ϕ of the hydrogen 2s state [50–52] and calculate the radial partial derivative in spherical coordinates: $\partial\phi \doteq \nabla\phi \cdot \hat{r} = \partial\phi/\partial r$.

$$\phi(r) = \eta(2 - r)e^{-hr}, \quad \eta = \frac{1}{4\sqrt{2\pi}} \tag{57}$$

$$\partial\phi = \eta[-1 - h(2 - r)]e^{-hr} = \eta(hr - 2)e^{-hr}. \tag{58}$$

Obtain the uphill velocity component u_+ using (A3), given by $u_+ = \partial\phi/\phi$, and the two previous equations, and also compute the kinetic-energy density $mu^2/2$.

$$u_+ = (hr - 2)(2 - r)^{-1} = -\frac{1}{2}(r - 4)(r - 2)^{-1}$$

$$\frac{1}{2}mu^2 = \frac{1}{8}(r - 4)^2(r - 2)^{-2}.$$

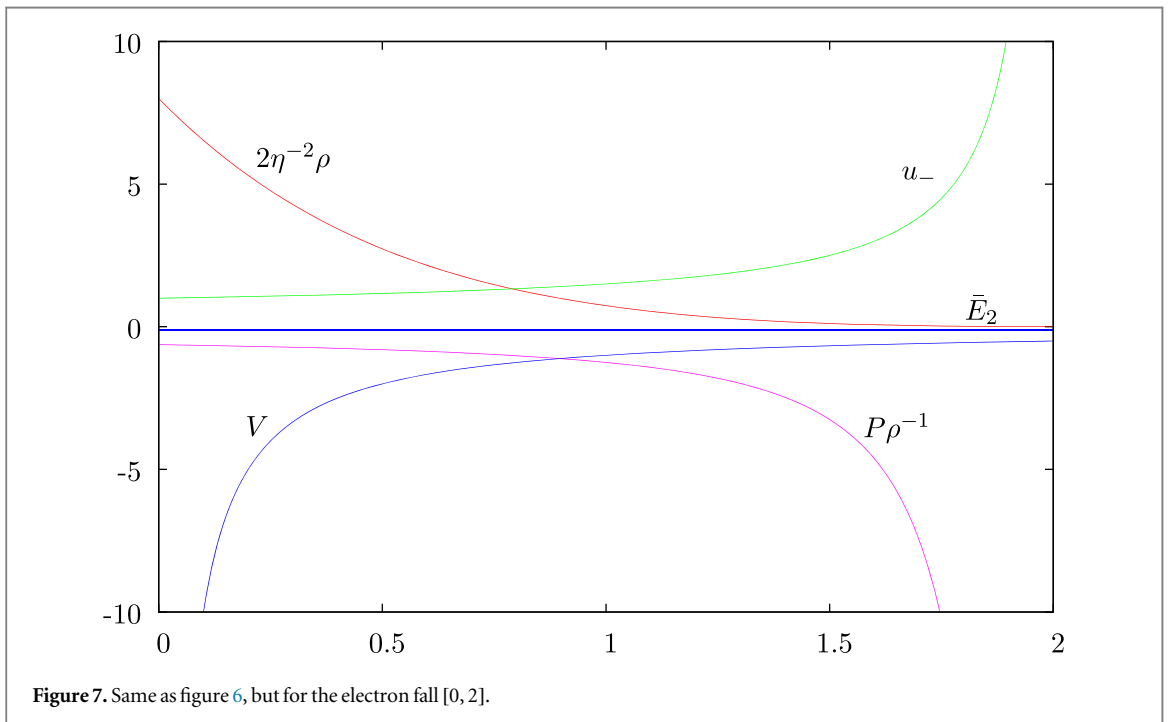
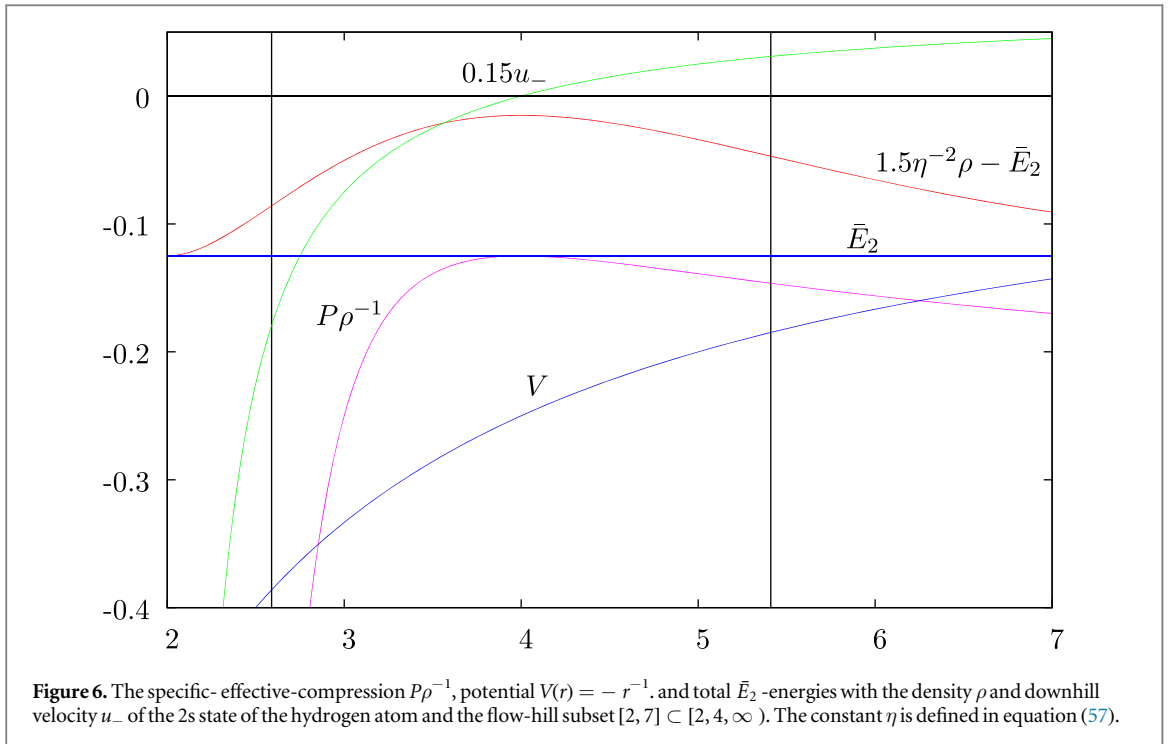
Use this formula for $mu^2/2$, the well known eigenvalue of the Schrödinger equation for the 2s state, $E_2 = -1/8$, and (23), which can be written $P\rho^{-1} = \bar{E} - \frac{1}{2}u^2$, to compute the specific compression-energy $P\rho^{-1}$.

$$P\rho^{-1} = -\frac{1}{8}[1 + (r - 4)^2(r - 2)^{-2}].$$

Elsewhere the pressure p is computed [47] using the orbital expression (A1):

$$p(r) = \frac{1}{2}\eta^2(r - 2)(1 + 3h - 4r^{-1} - h^2r)e^{-r} - \frac{1}{2}\eta^2(hr - 2)^2e^{-r}. \tag{59}$$

Figure 6 presents the same type of specific energy plot as figures 4 and 5 but for the hydrogen 2s state with the flow-hill subset $[2, 7] \subset [2, 4, \infty)$. It follows from the shape of the specific potential-energy $P\rho^{-1}$ that, overall, the absolute value of the acceleration is much greater on the lhs side of the unstable equilibrium point at 4.0 than on the rhs. The lhs of this flow-hill subset resembles the corresponding subset $[0, 2] \subset [0, 1, \infty)$ for the first excited state of the harmonic oscillator flow from figure 5, but the two differ significantly on the rhs of the unstable equilibrium point. Also, unlike the harmonic oscillator flows, the speed limit of $1/2$ is finite. The



momentum extremums, represented by two vertical line, appear on either side of the antinode, as in the other cases considered, but the pressure is not zero there, because spherical flow is not uniform flow, since the *direction* of the unit radial-vector \hat{r} varies with the streamline.

Figure 7 presents the same scalar fields as in figure 6, but for the primitive flow segment $[0, 2]$, where $\mathbf{r} = 0$ is the location of the nucleus. The density restricted to the segment $[0, 2]$ is a strictly decreasing function. Primitive flow segment that do not contain an antinode, like this one, are called fluid falls. The density ρ , velocity component u_{\pm} , and specific- effective-compression $P\rho^{-1}$ have finite values at the nucleus, $r_{\text{nuc}} = 0$. The specific potentials $V = -1/r$ and $P\rho^{-1}P\rho^{-1}$ seem to be approximate mirror images of each other, with respect to the vertical line at about 1.

The behavior of the hydrogen 1s flow, with the single electron fall $[r_{\text{nuc}}, \infty)$ of a given streamline, can be compared to the 2s flow at the limiting points r_{nuc} and r_{∞} . The r_{∞} limit of $|\rho u_{\pm}|$ for the hydrogen 1s state is the

same as the 2s state, and the limit of $|u_{\pm}|$ differ, but they are both finite. Also, all the functions considered, except for the pressure p and the external potential V , have finite limits at the point-charge location, $r_{\text{nuc}} = 0$.

The 1s hydrogenic flow is different from the others considered, because it has a single fall with a point at infinity as an end point; it has no antinode. However, if the external electrostatic potential is modified to take into account mass and volume effects of the nucleus, as in isotope shifts [50], then the external potential should have a minimum at the nucleus. This would change the flow of the hydrogenic 1s state. Also, if the point at infinity are changed to a node at a great distance, to model a hydrogen atom in deep space, the results might also significantly change.

5. Summary

In this paper it is proven that the compressible-flow generalization of the Bernoullian equation (3) is equivalent to the one-body time-independent Schrödinger equation (2) for real-valued wavefunctions ϕ , where the pressure p is defined by (5). The definition of mass density given by $\rho_m = m\rho$, where m is the mass of the system and ρ is the probability density, is a natural choice that is also used in the Madelung equations. Since, the velocity \mathbf{u}_{\pm} , given by (4), satisfies (16), involving the expectation value of the kinetic energy, it is also a natural choice. These mass density ρ_m and velocity \mathbf{u}_{\pm} choices yield compressible, irrotational, variable-mass steady flows that satisfies the generalized continuity equation (28). Since the variable mass choice gives the simplest possible description of a compressible dynamic fluid, described by the Bernoullian equation (3), variable mass is a desirable element of the formalism, especially since nonclassical elements are inevitable. The generalized Bernoulli equation and a generalized continuity equation provide a fluid dynamic interpretation of a class of quantum mechanical stationary states that is an alternative to the unrealistic, static-fluid interpretation provided by the Madelung equations and quantum hydrodynamics.

The developed formalism is applied to flows of a particle (or fluid) in a one-dimensional box, the one-dimensional harmonic oscillator, and the hydrogen 1s and 2s states. A typical example is given by the ground-state harmonic oscillator of figure 4, where the classical potential energy V with a stable equilibrium point is replaced by a potential energy $P\rho^{-1}$ with an unstable equilibrium point. For downhill flow u_- , the system is in perpetual motion and stabilized in a steady flow by mass creation in the region $x < |\sqrt{1/2}|$ and mass annihilation in $x > |\sqrt{1/2}|$.

Also, the integrand of the quantum-mechanical expectation value of the kinetic energy, given by (12), is interpreted as a sum of two terms: The kinetic energy per volume $\rho_m u^2/2$ and the pressure p . Elsewhere [43], an extension of these interpretations are used to refine, and further develop, the Madelung equations, where the quantum potential is replaced by an additional kinetic energy term and a term involving the pressure. The main equation of the formalism reduces to the Bernoullian equation (3) for stationary states with real valued wavefunctions.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix A. Orbital expressions

For every equality and formula involving the density ρ , there is a corresponding one involving orbitals ϕ , since $\rho = \phi^2$. Here we derive some equalities involving orbitals.

Obtain orbital expressions for p by rearranging (7) and using (5).

$$-\frac{1}{4}\nabla^2\rho = -\frac{1}{2}\phi\nabla^2\phi - \frac{1}{2}\nabla\phi \cdot \nabla\phi$$

$$p = -\frac{\hbar^2}{2m}\phi\nabla^2\phi - \frac{\hbar^2}{2m}\nabla\phi \cdot \nabla\phi. \quad (\text{A1})$$

Use $\nabla\rho = 2\phi\nabla\phi$ and (4) to obtain an orbital expression for the velocity \mathbf{u}_{\pm} , the velocity component $u_{\pm} = \mathbf{u}_{\pm} \cdot \hat{\mathbf{z}}$, and the kinetic energy density $mu^2/2$.

$$\mathbf{u}_{\pm} = \pm\frac{\hbar}{2m}(\rho^{-1})\nabla\rho = \pm\frac{\hbar}{m}(\phi^{-2})\phi\nabla\phi$$

$$\mathbf{u}_{\pm} = \pm\frac{\hbar}{m}\frac{\nabla\phi}{\phi} \quad (\text{A2})$$

$$u_{\pm} = \pm \frac{\hbar}{m} \frac{\partial \phi}{\phi} \quad (\text{A3})$$

$$\frac{1}{2} m u^2 = \frac{\hbar^2}{2m} \phi^{-2} \nabla \phi \cdot \nabla \phi. \quad (\text{A4})$$

Obtain the orbital continuity equation from (A2).

$$\nabla \cdot (\phi \mathbf{u}) = \pm \frac{\hbar}{m} \nabla^2 \phi.$$

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