

Diffusion Effect in Quantum Hydrodynamics

Moise Bonilla-Licea ^{1,*}, Dieter Schuch ^{2,†} and Moises Bonilla Estrada ^{3,†}

¹ Department of Physics and Mathematics, Universidad Iberoamericana, Prolongación Paseo de la Reforma 880, Mexico City 01219, Mexico

² Institute of Theoretical Physics, Goethe-University Frankfurt, Max-von-Laue-Str. 1, D-60438 Frankfurt am Main, Germany

³ CINVESTAV-IPN, Control Automático, AP 14-740, Mexico City 07000, Mexico

* Correspondence: mbonilla.19.04@gmail.com

† These authors contributed equally to this work.

Abstract: In this paper, we introduce (at least formally) a diffusion effect that is based on an axiom postulated by Werner Heisenberg in the early days of quantum mechanics. His statement was that—in quantum mechanics—kinematical quantities such as velocity must be treated as complex matrices. In the hydrodynamic formulation of quantum mechanics according to Madelung, the complex Schrödinger equation is rewritten in terms of two real equations—a continuity equation and a modified Hamilton–Jacobi equation. Considering seriously Heisenberg’s axiom, the velocity occurring in the continuity equation should be replaced by a complex one, thus introducing a diffusion term with an imaginary diffusion coefficient. Therefore, in quantum mechanics, there should be a diffusion effect showing up in the dynamics. This is the case in the time evolution of the free-motion wave packet under time reversal. The maximum returns to the initial position; however, the width of the wave packet does not shrink to its initial width. This effect is obvious but—as far as we know—it is not mentioned in any textbook. In our paper, we discuss this effect in detail and show the connection with a complex version of quantum hydrodynamics.

Keywords: diffusion; Madelung equations; Heisenberg quantization

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1. Introduction

A recent paper [1] discussed the formal similarities and differences between the following diffusion (or heat) equation

$$\frac{\partial}{\partial t} T(\vec{r}, t) = D \Delta T(\vec{r}, t) \quad (1)$$

which describes the spatial and temporal change of a **real** distribution function $T(\vec{r}, t)$ due to a random process—where D is a **real** diffusion coefficient and Δ is the Laplace-operator—and the following time-dependent Schrödinger equation (particularly for the free motion, i.e., potential, $V = 0$)

$$\frac{\partial}{\partial t} \psi(\vec{r}, t) = i \frac{\hbar}{2m} \Delta \psi(\vec{r}, t), \quad (2)$$

which describes the same evolution of a **complex** state function $\psi(\vec{r}, t)$ whose absolute value squared, i.e., $\rho(\vec{r}, t) = \psi^* \psi$, is a quantum mechanical probability distribution and $i \frac{\hbar}{2m}$ (with i and the reduced Planck constant $\hbar = \frac{h}{2\pi}$) now being a purely **imaginary** coefficient. Despite the formal similarities, both equations describe very different processes.

The solutions $\psi(\vec{r}, t)$ of Equation (2) are also called wave functions because they behave comparably to solutions of the following wave equation:

$$\frac{\partial^2}{\partial t^2} u(\vec{r}, t) = \frac{c^2}{n^2} \Delta u(\vec{r}, t) \quad (3)$$

for a wave $u(\vec{r}, t)$ that shows properties such as diffraction and dispersion, where n is the diffraction index and c is the speed of light in a vacuum. In contrast with Equation (1), this equation is invariant under time reversal as t appears quadratic on the lhs of (3).

So, although mathematically the Schrödinger equation has a structure similar to that of (1)—i.e., a parabolic differential equation—its solutions behave similarly to those of (3): a hyperbolic differential equation with a second derivative in time. The difference between Equations (1) and (2) is that $\psi(\vec{r}, t)$ is in general a **complex** function and the imaginary unit i appears explicitly in Equation (2). (These fundamental differences and their mathematical and physical consequences were already pointed out explicitly by Schrödinger himself in [2]—see also [3] for an English translation and comments.) However, this is an important—if not the most important—difference between classical and quantum physics, as stressed by C. N. Yang in their lecture on the occasion of Schrödinger’s 100th anniversary (see [4]), since “complex numbers become a conceptual element of the very foundations of physics”. This is reflected by the fact that i occurs explicitly in the fundamental equations of quantum mechanics not only in Schrödinger’s Equation (2), but also in Heisenberg’s commutation relation $pq - qp = -i\hbar$ in their matrix mechanics (with q = position and p = momentum operators).

There are attempts in the literature to turn a complex space into a real space with twice as many dimensions, arguing that complex numbers are just a convenient mathematical tool, but not essential for the quantum mechanical description of nature. However, this is not true, as real and imaginary parts, or amplitude and phase of the complex wave function, are not independent of each other, but are uniquely coupled. This can be seen clearly in the hydrodynamic formulation (see Section 2) where the continuity Equation (6) for the density, ρ , and thus for the amplitude, $\sqrt{\rho}$, contains the phase of the wave function via $\vec{v}_M = \frac{1}{m} \nabla S$; additionally, this is shown in Equation (8) where the phase, S , contains the amplitude via V_{qu} . This is not taken into account by doubling the number of degrees of freedom. The viewpoint that complex quantities are essential for quantum mechanics has also recently been confirmed experimentally (see, e.g., [5,6]).

Even though Heisenberg and Schrödinger arrived from different starting points, they share the same guideline: the relation between classical and quantum mechanics should be mediated via the mean value which is the principle of correspondence [7] and mathematically expressed by the so-called Ehrenfest theorem [8]. As Heisenberg pointed out, the difference lies in the treatment of kinematic quantities, such as position and velocity, while Heisenberg associates them with time-dependent complex matrices; for Schrödinger, the time-dependence was contained in the complex wave function. However, in the beginning, Schrödinger did not consider the imaginary unit in their first communication [9] where, in the definition of their wave function via the action S according to $S = K \ln \psi$, the constant K is chosen to be $K = \hbar$ and the wave function itself is assumed to be real. It was after some correspondence with Lorentz (see, e.g., [10]), he had to admit that their wave function is complex. So, in [11]—published a few months later—he uses a complex form for the wave function in Equation (2), and below Equation (4) he explicitly uses ... “komplexe Wellenfunktion Ψ ”.

The importance of i in quantum mechanics and Schrödinger’s struggle with complex quantities in wave mechanics has also been discussed recently in the literature [12–14]. It is not only the wave function, but also the operators—essential to Schrödinger’s wave mechanical form of quantum mechanics—which can be complex or imaginary, such as the momentum operator in position representation, $\hat{P} = \frac{\hbar}{i} \nabla$ (with ∇ = Nabla operator).

What about the time reversal invariance of the Schrödinger Equation (2)? As pointed out, even recently in several articles on this subject [15–19], a simple replacement of t by

$-t$ would change the form of (2) as in the case of the diffusion equation. Time reversal in classical physics also means that velocity or momentum change sign (magnetic fields are not included in our discussion), but the time, t , does not occur explicitly in the quantum mechanical operator, \hat{P} ; however, a change of sign can be achieved by taking the conjugate complex of this operator. This is sometimes used as an explanation for the so-called Wigner time-reversal invariance. (A more precise formulation requires the time inversion operator to be anti-linear. Wigner actually used more appropriately the terminology “reversal of motion” instead of “time reversal” [20].) In other words, in quantum mechanics, it is not only t that has to be changed to $-t$, but the conjugate complex also has to be taken; meaning $\psi(\vec{r}, t) \rightarrow \psi^*(\vec{r}, -t)$ and $i\frac{\hbar}{2m} \rightarrow -i\frac{\hbar}{2m}$. In this case, the form of Equation (2) remains invariant under this transformation.

However, considering the latter condition for the time reversal, it is actually only the phase of the complex wave function—when written in polar form as $\psi(\vec{r}, t) = \sqrt{\rho(\vec{r}, t)} \exp\left[\frac{i}{\hbar}S(\vec{r}, t)\right]$ —that is affected by this transformation, not the amplitude, $\sqrt{\rho}$, providing that t occurs in ρ in an even power. Does this mean that the time-dependent Schrödinger equation contains an element of broken time-reversal invariance as the (real) diffusion equation does? If so, how can this formally be seen in the equations?

To answer these questions, we consider the Gaussian wave packet solution of Equation (2) (in one dimension), where the probability density, $\rho(x, t)$, also Gaussian, can be written in the following form:

$$\rho(x, t) = \frac{1}{\sqrt{2\pi\sigma_x^2(t)}} \exp\left[-\frac{(x - \langle x \rangle)^2}{2\sigma_x^2(t)}\right] \tag{4}$$

where $\langle x \rangle$ is the mean value of position and $\sigma_x(t) = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ describes the position uncertainty and, in this case, the width of the Gaussian function. It is well known that a Gaussian function is completely determined by its maximum—here $\langle x \rangle$ (position mean value)—and its width—here σ_x —where, in our case, both parameters can be time-dependent. In the case of the free motion, $V = 0$, the width is spreading quadratically in time according to

$$\sigma_x^2(t) = \sigma_0^2 \left[1 + \left(\frac{\hbar t}{2m\sigma_0^2}\right)^2\right]. \tag{5}$$

Let us consider an initial wave packet with its maximum at $\langle x \rangle(t = 0) = \langle x \rangle_0$ that follows the classical trajectory, moving with the (constant) velocity $\langle v \rangle = \frac{1}{m}\langle p \rangle = \frac{1}{m}p_0 = v_0$ and having the initial width $\sigma_x(t = 0) = \sigma_0$. After a time interval, τ , the maximum has reached the following position: $\langle x \rangle(\tau) = v_0\tau$. Now, applying time reversal, the maximum fulfills that which Lohschmidt described in their argument against Boltzmann’s \mathcal{H} -function, i.e., the system will go (in configuration space) through the same states as before, only in reverse order. So, after another time interval, τ , the maximum of the Gaussian will reach the following initial position: $\langle x \rangle(2\tau) = \langle x \rangle_0$.

However, what happens to the width? Starting the time-reversed evolution with the width, $\sigma_x(\tau) = \sigma_0\sqrt{1 + \left(\frac{\hbar\tau}{2m\sigma_0^2}\right)^2} = \sigma_\tau$, the Gaussian wave packet will continue spreading according to $\left(\frac{-\hbar t}{2m\sigma_0^2}\right)^2 = \left(\frac{\hbar t}{2m\sigma_0^2}\right)^2$ and will arrive after a second period, τ , with an even broader width, $\sigma_x(2\tau) = \sigma_\tau\sqrt{1 + \left(\frac{\hbar\tau}{2m\sigma_0^2}\right)^2} \neq \sigma_0$ at the initial position—i.e., the wave packet will **not shrink** to its initial width. (It should be pointed out that this continuation of the spreading is not connected with any perturbation due to the interaction with an environment that might be assumed to take place in order to reverse the motion. The time reversal is purely a “Gedankenexperiment”, where no interaction with any environment is taken into account, only the Schrödinger equation for an isolated system is considered.) $\sigma_0!$

Obviously, the amplitude of the wave function, and thus the density, $\rho(x, t)$, behaves differently from the phase of the wave function that is affected by the time reversal, similar to velocity in classical physics. Can this different behavior also somehow be expressed in

the corresponding equations of motion for amplitude and phase—bearing in mind that Heisenberg’s kinematic quantities, in particular velocity, are to be considered complex?

For this purpose, we apply Madelung’s hydrodynamic formulation of quantum mechanics [21] that allows us to separate the time-dependent Schrödinger equation into two (coupled) equations: one continuity equation for the amplitude and a modified Hamilton–Jacobi equation for the phase. This corresponds to an Euler-type equation for a velocity field. However, the continuity equation does not contain any irreversible diffusion current. In the following, this problem is solved by introducing complex kinematic quantities, inspired by Heisenberg’s original idea. This naturally causes the appearance of a diffusive current in the continuity equation with an already known diffusion coefficient. The reason that the diffusive current is absent in the Madelung approach is that it cancels with the imaginary part of the now-complex velocity field.

The paper is organized as follows: In Section 2, a short overview of the current hydrodynamic formulation of quantum mechanics is presented and the inconsistencies related to the diffusion process are specified. To solve this problem, in Section 3.1, a complex notation of kinematic quantities is introduced and applied in Section 3.2 to obtain the missing diffusion term in the continuity equation. Using the Gaussian wave packet solutions of the time-dependent Schrödinger equation as example, in Section 3.3, the relation between the real and imaginary parts of the introduced complex velocity field and phase and amplitude of the wave function is demonstrated. Section 3.4 shows that the introduction of the complex velocity field does not change the form of the Euler equation for the phase of the wave packet, in agreement with the correct evolution of the wave packet maximum. Finally, in Section 4, the results are summarized and our conclusions are drawn.

2. Conventional Quantum Hydrodynamics

Shortly after Schrödinger published their papers on wave mechanics, Madelung showed [21] that the **complex** Schrödinger equation is equivalent to a set of **two real** hydrodynamic equations.

A continuity equation for the density, ρ , has the following form:

$$\frac{\partial}{\partial t}\rho + \nabla(\rho\vec{v}_M) = 0 \quad (6)$$

where \vec{v}_M denotes a velocity field related with the action S in the phase of the wave function via

$$\vec{v}_M = \frac{1}{m}\nabla S. \quad (7)$$

The second hydrodynamic equation is obtained from the following evolution of the phase:

$$\frac{\partial}{\partial t}S + \frac{1}{2m}(\nabla S)^2 + V + V_{\text{qu}} = 0, \quad (8)$$

that is a modified Hamilton–Jacobi Equation. (Note that the real Equations (6) and (8) are invariant under time reversal, if t is replaced by $-t$ and S , by $-S$, leading to $-\vec{v}_M$ using (7).) Taking its gradient yields

$$\rho\left(\frac{\partial}{\partial t} + \vec{v}_M \cdot \nabla\right)\vec{v}_M = -\rho\frac{1}{m}\nabla(V + V_{\text{qu}}), \quad (9)$$

showing formal similarity with the Euler equation

$$\rho\left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla\right)\vec{v} = -\rho\vec{f} - \nabla P, \quad (10)$$

with \vec{f} being the force density per mass and P the thermodynamic pressure. Comparison suggests the connection between the so-called “quantum potential” $V_{\text{qu}} = -\frac{\hbar^2}{2m^2} \frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}$ and the pressure P via

$$\nabla P = \rho \frac{1}{m} \nabla V_{\text{qu}} = \frac{\rho}{m} \nabla \left(-\frac{\hbar^2}{2m} \frac{\Delta\sqrt{\rho}}{\sqrt{\rho}} \right). \tag{11}$$

As Takabayasi points out in [22], there should be a stress tensor rather than a pressure term, what makes sense in particular for $\nabla \cdot \vec{v} \neq 0$ (such as for a spreading wave packet in quantum mechanics), as in this case these two quantities are not identical. However, in our quantum mechanical case, a proper explanation of V_{qu} in terms of the complex quantities—introduced in the next Section—will be given.

Madelung’s formulation of wave mechanics was also later independently used by David Bohm in their deterministically inspired version of quantum mechanics [23,24] where he claimed the existence of real paths of (quantum) particles that can be obtained by integration of Equation (7). As we have shown recently [25], this deterministic viewpoint is incorrect and has to be replaced by a probabilistic one that differs from the usual probabilistic viewpoint taken in quantum mechanics. Nevertheless, Bohmian mechanics can still be helpful in the treatment of quantum systems, e.g., tunneling problems, particularly when performing numerical simulations [26,27].

Looking at Madelung’s fluid as a classical one, it can be associated with an irrotational, inviscid and compressible one with no obvious quantum effects at first sight. One may argue that these effects are embedded in the term related to the “quantum potential”, V_{qu} . However, apart from this rather misleading terminology (V_{qu} actually originates from the kinetic energy operator, as will be shown below, and is not a potential at all), the corresponding term has still a more classical meaning, only indicating that the fluid is compressible, since V_{qu} depends on the density. As mentioned above, there is the well-known diffusive effect of the wave packet spreading; however, there is no diffusive current in the continuity Equation (6), only a convective one.

On the other hand, from a fundamental point of view, it should be expected that the (kinetic) quantities in a hydrodynamic formulation of quantum mechanics would be of a complex nature, unlike the classical counterpart. As Heisenberg [28] wrote in their pioneering paper of 1925:

“The Einstein–Bohr frequency condition (which is valid in all cases) already presents such a **complete departure** from classical mechanics, or rather (using the viewpoint of wave theory) **from the kinematics underlying this mechanics**, that even for the simplest quantum theoretical problems the velocity of classical mechanics simply cannot be maintained.”

This was a milestone for future quantization methods—i.e., mappings onto classical-like equations: only kinematic quantities should be of a different nature than their classical counterparts. From this viewpoint, the mapping of a quantum system onto hydrodynamical equations should be of the following form:

$$\frac{\partial}{\partial t} \rho + \nabla \cdot \vec{j} = 0 \tag{12}$$

$$\rho \left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) \vec{v} = -\rho \frac{1}{m} \nabla V - \nabla P, \tag{13}$$

where the flow, \vec{v} , and the density current, \vec{j} , should be of a **complex** nature, since their origin is kinematic, whilst ρ , not being of a kinematic quantity, must remain a positive real quantity.

It is important to emphasize that we are not claiming that the hydrodynamical Equations (6) and (9) are inaccurate, but rather that they are only one perspective of the quantization principle. Therefore, the explanation of the diffusive effects of wave packets is unanswered within the current hydrodynamic formulation due to the absence of a diffusive

current in the continuity equation. We will now show how this can be taken into account in a complex formulation.

3. Complex Hydrodynamical Formulation

3.1. Notation

Characteristic of Madelung’s approach is the splitting of the complex Schrödinger equation into two real equations for the amplitude and the phase of the complex wave function (which are coupled due to the appearance of i in the Schrödinger equation, see also [29]). However, as mentioned in Section 2, the fundamental kinematic quantities such as velocity should—according to Heisenberg—be of a complex nature in quantum mechanics. Let us therefore consider such a complex formulation in position representation (as also used in [29]), defined via the complex wave function, $\langle \vec{r} | \psi(t) \rangle = \psi(\vec{r}, t)$, and the quantum mechanical operators, e.g., $\langle \vec{r} | \hat{P} | \psi(t) \rangle = \frac{\hbar}{i} \nabla \psi(\vec{r}, t)$, according to

$$\vec{v}(\vec{r}, t) \doteq \frac{\langle \vec{r} | \frac{1}{m} \hat{P} | \psi(t) \rangle}{\langle \vec{r} | \psi(t) \rangle} \tag{14}$$

$$T(\vec{r}, t) \doteq \frac{\langle \vec{r} | \frac{1}{2m} \hat{P}^2 | \psi(t) \rangle}{\langle \vec{r} | \psi(t) \rangle} \tag{15}$$

$$H(\vec{r}, t) \doteq \frac{\langle \vec{r} | \hat{H} | \psi(t) \rangle}{\langle \vec{r} | \psi(t) \rangle}, \tag{16}$$

where the conventional Dirac notation has been used.

With the polar ansatz, $\psi(\vec{r}, t) = \sqrt{\rho(\vec{r}, t)} \exp\left[\frac{i}{\hbar} S(\vec{r}, t)\right]$, these quantities can be expressed as

$$\vec{v}(\vec{r}, t) = \frac{\nabla S}{m} - i \frac{\hbar}{2m} \frac{\nabla \rho}{\rho} = \vec{v}_R(\vec{r}, t) + i \vec{v}_I(\vec{r}, t) \tag{17}$$

$$T(\vec{r}, t) = \frac{1}{2m} \vec{v}^2 - i \frac{\hbar}{2} \nabla \cdot \vec{v} \tag{18}$$

$$H(\vec{r}, t) = -\frac{\partial S}{\partial t} + i \frac{\hbar}{2} \frac{\partial \rho}{\partial t} \tag{19}$$

where, in the last relation, the Hamiltonian has been taken equal to the energy operator $H_{op} = E_{op} = i\hbar \partial / \partial t$.

Considering the complex velocity (17), it is obvious that the real part is identical with Madelung’s velocity field, $\vec{v}_R \doteq \vec{v}_M$. The imaginary part, \vec{v}_I , is that which—in [1]—Mita calls dispersive velocity. (The real part of (17), \vec{v}_R , corresponds to Mita’s current velocity. In [1], he essentially discusses the equation of motion of this velocity, their Equation (39), that corresponds to our Equation (41), derived from the modified Hamilton–Jacobi Equation (8), in Mita’s case (26), by taking its gradient. The subject of our present paper is the other of the two hydrodynamic equations, the continuity equation and the possibility to manifest a diffusion effect in this equation.) Through inserting the complex velocity (17) into the expression for the complex kinetic energy (18), it becomes obvious that the real part of this quantity does not only contain the contribution, $\frac{1}{2m} (\nabla S)^2 = \frac{m}{2} v_R^2$, that appears in the modified Hamilton–Jacobi Equation (8), but a contribution from \vec{v}_I also occurs:

$$-\left[\frac{m}{2} v_I^2 - \frac{\hbar}{2} \nabla \cdot \vec{v}_I \right] = -\frac{\hbar^2}{8m} \left(\frac{\nabla \rho}{\rho} \right)^2 - \frac{\hbar^2}{4m} \nabla \cdot \left(\frac{\nabla \rho}{\rho} \right) = -\frac{\hbar^2}{2m} \frac{\Delta \sqrt{\rho}}{\sqrt{\rho}} = V_{qu}, \tag{20}$$

that shows that the “quantum potential” is not really a potential, but entirely depends on the imaginary part of our complex velocity (17).

At this point, a few remarks seem necessary, to avoid confusion with complexified trajectories derived from complex velocity or momentum fields as they appear in various forms of complex Bohmian mechanics [30–40] (for a more detailed review and further

references, see also [26]). Most of these approaches write the wave function in terms of a complex action function, which actually goes back to Schrödinger’s original definition [9]. From there, a complex momentum (or velocity) field arises. To date, there is formal similarity with our approach.

However, in the abovementioned approaches, in view of the fact that the velocity is complex, it is incorrectly concluded that the (independent) position variable must also be complex. Various attempts have been made to accomplish this. Either by integrating the complex velocity (in position space), or by replacing the independent position variable by a complex one in the Schrödinger equation, leading to a different physical situation than that described by the original Schrödinger equation—which is already complex due to the complexity of the wave function, ψ .

3.2. Continuity Equation

The notation introduced in Section 3.1 shows directly how to solve the problem of the missing diffusion term in the continuity Equation (6). Following the logic of quantization advocated by Heisenberg, the kinematic quantity velocity in the current $\rho\vec{v}_M$ should be replaced by $\rho\vec{v}$ using the complex velocity as defined in (17). This replacement introduces an additional term proportional to the imaginary part, $i\vec{v}_I$, that is not present in Madelung’s continuity Equation (6). In order to regain this (real) form of the continuity equation that is usually applied in quantum mechanics, one has to (formally) compensate the contribution of $i\vec{v}_I$. This can be carried out by adding a diffusion current, $-D\nabla\rho$, with the **imaginary** diffusion coefficient, $D = -\hbar/2m$, leading to an equation that has the form of an irreversible Fokker–Planck-type equation, in a position space of a so-called Smoluchowski equation:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho\vec{v} - D\nabla\rho) = \frac{\partial}{\partial t}\rho + \nabla(\rho\vec{v}) - D\Delta\rho = 0 \tag{21}$$

with a complex convection current, $\rho\vec{v}$, and an imaginary diffusion current, $-D\nabla\rho$. In other words, comparing Equation (21) with Equations (12) and (6) shows that the conventional continuity Equation (6) can be regained from the complex Equation (12) that takes into account Heisenberg’s request, if the imaginary contribution in $\vec{j} = \rho\vec{v}$ is eliminated by an imaginary term that has the form of a diffusion current.

Again, to avoid confusion, a few remarks concerning Equations (17) and (21) are necessary. There are equations formally looking similar to (21) in a quantum mechanical context in the literature, most familiar probably from Nelson’s stochastic mechanics [41] or a more recent review article by Bohm and Hiley [42] and several others that can be traced back to a paper by Fürth [43]—who tried to establish a formal connection between the Schrödinger and the diffusion equation. Unlike in Fürth’s paper—where it is explicitly stressed that a corresponding diffusion coefficient in Schrödinger’s case has to be imaginary (a fact that has correctly been taken into account by Fényes [44], even quoting passages of Schrödinger’s original comment, mentioned in the first parenthesis of page 2)—in the work of Nelson, Bohm, Hiley, and others, only real diffusion currents/velocities with the real diffusion coefficient $D = \hbar/2m$ are taken into account; this is essentially different from our approach, with an entirely imaginary diffusion current/velocity.

Equation (21) shows that, in quantum mechanics, there is an inherently diffusive effect involved which becomes apparent in the spreading behavior of the wave packet. This is, however, not obvious in the usual description in terms of a real continuity equation as the diffusion current is compensated by the imaginary part of the convection current, $i\rho\vec{v}_I = -i(\hbar/2m)\nabla\rho$.

One could argue that this reasoning is just rhetoric or semantics. After all, the imaginary part of v does not contribute to the mean value of v given that its mean value for square integrable functions, $\psi(\vec{r}, t)$, always vanishes as these functions go to zero for $\vec{r} \rightarrow \pm\infty$. Therefore, \vec{v}_I does not contribute to the equation of motion for the mean values that, according to Ehrenfest [8], should obey the corresponding classical equation.

However, as in the classical Langevin theory of Brownian motion where the fluctuating stochastic force vanishes on average, the square of this force still makes a physically significant contribution to the energy of the Brownian particle. Therefore, we will make an excursion to consider quantities where the square of v_I (or its derivative) is of physical significance. One such situation can be found in the momentum uncertainty σ_p^2 and the corresponding uncertainty product that must fulfil Heisenberg’s requirement.

The momentum uncertainty σ_p^2 ,

$$\sigma_p^2 = \langle \psi(t) | \hat{P}^2 | \psi(t) \rangle - \langle \psi(t) | \hat{P} | \psi(t) \rangle^2 \tag{22}$$

can be written in terms of our complex velocity (in one dimension) as

$$\sigma_p^2 = \int \rho \left(m^2 v^2 - i \hbar m \frac{\partial v}{\partial x} \right) dx - \left[\int \rho (mv) dx \right]^2 \tag{23}$$

leading to

$$\sigma_p^2 = \int \rho \left(m^2 v_R^2 - m^2 v_I^2 + \hbar m \frac{\partial v_I}{\partial x} \right) dx - \left[\int \rho (mv_R) dx \right]^2 \tag{24}$$

because the imaginary parts of the integrals vanish (as discussed in detail in [45]).

This expression can be divided into two contributions—one $\sigma_{p,ph}^2$ depending only on the phase of ψ via v_R , the other $\sigma_{p,am}^2$ depending just on the amplitude via v_I , as follows:

$$\begin{aligned} \sigma_p^2 &= m^2 (\langle v_R^2 \rangle - \langle v_R \rangle^2) - m^2 (\langle v_I^2 \rangle - \frac{\hbar}{m} \langle \frac{\partial}{\partial x} v_I \rangle) \\ &= \sigma_{p,ph}^2 + \sigma_{p,am}^2 \end{aligned} \tag{25}$$

where the integrations are indicated by the pointed brackets. So, the second contribution, $\sigma_{p,am}^2$, depends entirely on the imaginary part of v and thus on the diffusion current in (21), which can actually also be connected to the quantum potential in the Euler Equation (see below).

This contribution, $\sigma_{p,am}^2$, is also the one providing the minimum uncertainty in Heisenberg’s relation that does not vanish even if, e.g., the wave packet does not spread. To demonstrate this, we consider the example of a Gaussian wave packet solution of the time-dependent Schrödinger equation.

3.3. Example

As can be found in detail, e.g., in [46], a Gaussian wave packet solution of the time-dependent Schrödinger equation can be written (in one dimension) as

$$\psi(x, t) = N(t) \exp \left[- \frac{(x - \langle x \rangle)^2}{4\sigma_x^2} + \frac{i}{\hbar} \left(\frac{m}{4} \frac{d}{dt} \sigma_x^2 (x - \langle x \rangle)^2 + \langle p \rangle (x - \langle x \rangle) + K(t) \right) \right], \tag{26}$$

where the normalization coefficients $N(t)$ and $K(t)$ are purely time-dependent functions and not relevant to the following: $\langle p \rangle = m \frac{d}{dt} \langle x \rangle$ is the classical momentum.

From the corresponding probability density

$$\rho(x, t) = \frac{1}{\sqrt{2\pi\sigma_x^2(t)}} \exp \left[- \frac{\tilde{x}^2}{2\sigma_x^2(t)} \right] \tag{27}$$

with $\tilde{x} = x - \langle x \rangle$ and $\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \langle \tilde{x}^2 \rangle$ follows with

$$v_I = - \frac{\hbar}{2m} \frac{\partial}{\partial x} \ln \rho = \frac{\hbar}{2m} \frac{\tilde{x}}{\sigma_x^2} \tag{28}$$

that

$$(\sigma_{p,am})^2 = -m^2(\langle v_I^2 \rangle - \frac{\hbar}{m} \langle \frac{\partial}{\partial x} v_I \rangle) = \frac{\hbar^2}{4} \frac{1}{\sigma_x^2}. \tag{29}$$

(The difference between v_R and the classical velocity $\langle v \rangle = \langle p \rangle / m$ is the term depending on $\sigma_x(x, t)$, essentially the position uncertainty, particularly on its time-dependence. It only vanishes in the very particular case of constant σ_x . Since the term is a logarithmic time-derivative, it does not depend on any constant entering σ_x , particularly not on \hbar . Therefore, this term remains also in a limit $\hbar \rightarrow 0$.) From

$$v_R = \frac{1}{m} \frac{\partial}{\partial x} S = \frac{1}{2} \frac{\frac{d}{dt} \sigma_x^2}{\sigma_x^2} \tilde{x} + \frac{\langle p \rangle}{m}, \tag{30}$$

it follows that

$$(\sigma_{p,ph})^2 = m^2(\langle v_R^2 \rangle - \langle v_R \rangle^2) = \frac{m^2}{4} \left(\frac{\frac{d}{dt} \sigma_x^2}{\sigma_x^2} \right)^2 \sigma_x^2 = \frac{\hbar^2}{4} \left(\frac{m}{\hbar} \frac{d}{dt} \sigma_x^2 \right)^2 \frac{1}{\sigma_x^2}. \tag{31}$$

Therefore, the uncertainty product can be written as

$$\sigma_p^2 \sigma_x^2 = (\sigma_{p,am}^2 + \sigma_{p,ph}^2) \sigma_x^2 = \frac{\hbar^2}{4} + \frac{\hbar^2}{4} \left(\frac{m}{\hbar} \frac{d}{dt} \sigma_x^2 \right)^2, \tag{32}$$

i.e., the minimum contribution that also exists for wave packets with a constant width, i.e., for $\frac{d}{dt} \sigma_x^2 = 0$,

$$(\sigma_p^2 \sigma_x^2)_{\min} = \frac{\hbar^2}{4} = \sigma_{p,am}^2 \sigma_x^2 = m^2 |D|^2 \tag{33}$$

depends only on the contribution from the amplitude and thus from the imaginary part of the velocity, v_I , and can be expressed by the absolute value of the diffusion coefficient in v_I .

As the minimum uncertainty, $\hbar^2/4$, is related to the commutation relation of position and momentum—whereas the additional contribution is related to the anti-commutator of these quantities, taking into account their correlation—the following question might come up: are our results valuable for research on the generalized uncertainty principle, as it is discussed in quantum cosmology, where a modification of the commutation relation due to a minimal (Planck) length is considered? In light of the results, such modifications would be essentially connected with the amplitude of the wave function, but more detailed comments need further investigation.

3.4. Euler Equation

The complexified Euler equation corresponding to the Madelung Equation (9) can be obtained easily from Equations (13) and (15)—taking into account that derivatives with respect to position and time commute—leading to

$$m \frac{\partial \vec{v}}{\partial t} = -\nabla H. \tag{34}$$

For a system with a Hamiltonian operator given by $\hat{H} = (1/2m)\hat{P}^2 + V$, it is straightforward to compute

$$m \frac{\partial \vec{v}}{\partial t} = -\nabla \left(\frac{m}{2} \vec{v}^2 - i \frac{\hbar}{2} \nabla \cdot \vec{v} \right) - \nabla V, \tag{35}$$

leading—for a velocity field, \vec{v} , that is irrotational, as in our case—to

$$m \frac{\partial \vec{v}}{\partial t} = -m(\vec{v} \cdot \nabla) \vec{v} + i \frac{\hbar}{2} \nabla (\nabla \cdot \vec{v}) - \nabla V \tag{36}$$

or

$$\rho \left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right) \vec{v} = -\frac{\rho}{m} \nabla (V + V_{qu}) \tag{37}$$

with

$$\rho \vec{v} = \frac{1}{m} \rho \nabla S + D \nabla \rho \tag{38}$$

$$\nabla P = \rho \nabla (D \nabla \cdot \vec{v}), \tag{39}$$

where $D = -i(\hbar/2m)$.

The form of the complexified Euler Equation (37) corresponds to that of the Madelung Equation (9), i.e., unlike in the case of the continuity equation, no additional terms—such as the diffusion term—occur in this equation. It simply reflects the quantization process, confirming the complex nature of kinematic quantities such as the velocity field, as indicated by Heisenberg.

Splitting Equation (37) into real and imaginary parts, yields the real part.

$$\rho \left(\frac{\partial}{\partial t} \vec{v}_R + \vec{v}_R \cdot \nabla \vec{v}_R \right) = -\frac{\rho}{m} \nabla V + \rho \vec{v}_I \cdot \nabla \vec{v}_I - \frac{\rho}{m} \nabla \left(\frac{\hbar}{2} \nabla \cdot \vec{v}_I \right) \tag{40}$$

that can be written, using $V_{qu} = -\frac{m}{2} \vec{v}_I^2 + \frac{\hbar}{2} \nabla \cdot \vec{v}_I = -\frac{\hbar^2}{2m} \frac{\Delta \sqrt{\rho}}{\sqrt{\rho}}$, as

$$\rho \left(\frac{\partial}{\partial t} \vec{v}_R + \vec{v}_R \cdot \nabla \vec{v}_R \right) = \frac{\rho}{m} [-\nabla V - \nabla V_{qu}] \tag{41}$$

which is identical to Madelung’s Equation (9) if v_M is replaced by \vec{v}_R .

It can be shown straightforwardly that the imaginary part of Equation (37) vanishes if the continuity equation is fulfilled (for details, see also [29]).

It should also be mentioned that, as in the conventional case, the fluid remains irrotational, inviscid, and compressible.

4. Conclusions

In classical mechanics, time reversal means the following replacements: $t \rightarrow -t$, $v \rightarrow -v$ or $p \rightarrow -p$. According to Loschmidt’s arguments, if a system reaches a certain position in configuration space after a certain period of time, this system will return to its initial position after the same period of time if time reversal is applied according to the abovementioned rules.

Concerning quantum mechanics, the situation is different as time does not appear explicitly in the operator for momentum or velocity, rather it appears as the imaginary unit i . This is related to a major difference between classical and quantum mechanics. According to Wigner [20], one should not talk about “time reversal” in quantum mechanics but about “motion reversal”. The latter, however, is not simply the replacement of t by $-t$, but also involves the application of complex conjugation. This, in turn, affects not just the operators that can contain the imaginary unit, i , but also the complex wave function in the Schrödinger equation. Writing this wave function in polar form, $\psi(x, t) = \sqrt{\rho(x, t)} \exp \left[\frac{i}{\hbar} S(x, t) \right]$ —consistent with Madelung—shows that complex conjugation only affects the phase of the wave function, not its amplitude, $\sqrt{\rho}$.

Looking at the time evolution of the wave packet solution of the time-dependent Schrödinger equation, specifically for free motion, $V = 0$, it is obvious that motion reversal in the abovementioned way does not revert to the initial state after a second period of time evolution. In agreement with the classical trajectory, the maximum of the wave packet reaches its initial position after motion reversal. However, the width does not shrink to its initial one but becomes much broader due to continuing dispersion—such as a diffusion effect—also in the time-reversed segment of the evolution. This irreversible effect should somehow also be manifested in the equation of motion for density, $\rho(x, t)$.

According to Madelung [21], the complex Schrödinger equation can be rewritten as two (coupled) real equations; one for the phase, the other for the amplitude of the wave

function. Using the classical definition of time reversal as mentioned above, both equations seem invariant under this operation. However, the typical quantum mechanical aspect of complex quantities is eliminated in this formulation.

Following Heisenberg, in the quantum theory kinematic quantities, such as velocity, should be replaced by complex ones. Proceeding accordingly in Madelung's (continuity) equation for the density, replacing the real velocity, \vec{v}_M , with the complex, \vec{v} —as defined in (14)—this equation can only be fulfilled if a diffusion term (with imaginary diffusion coefficient) is added to compensate for the contribution from the imaginary part, \vec{v}_I , of the complex velocity, leading to a Smoluchowski-type equation. This additional diffusion term expresses, at least formally, the spreading behavior of the wave packet.

In Madelung's second equation for the phase, the replacement of \vec{v}_M by complex \vec{v} does not change the form of the corresponding Euler equation; this demonstrates that the Wigner "time reversal" also affects the phase of the wave function and therefore leads to a consistent treatment. This is supported by the fact that the maximum of the wave packet—related to the mean value of position following the classical trajectory—returns to its initial position after time inversion and complex conjugation. Complex conjugation of the phase changes the sign of the classical velocity (or momentum) that appears in the phase, thus having the same effect as time reversal in the classical case.

In conclusion, the irreversible behavior of the quantum mechanical wave packet observed under motion reversal formally becomes obvious only if the complex kinematic quantities are applied.

In this sense, Equations (21) and (37) constitute the correct mapping from a quantum system onto a hydrodynamic formulation showing the effects involved more clearly. That does not mean that Madelung's Equations (6) and (9) are incorrect but rather that they display only one aspect of the quantization principle.

Though the mean value of the imaginary part of the complex velocity vanishes, it does not mean \vec{v}_I has no further influence on the quantum system. This becomes obvious when considering the uncertainty product of position and momentum. As has been shown in (32), using (29), the minimum uncertainty ($\hbar^2/4$) depends entirely on \vec{v}_I and its derivative and can be expressed via the absolute value of the (imaginary) diffusion coefficient as $(\hbar^2/4) = m^2|D|^2$.

There are certainly other currents related to quantum mechanics that could be considered from the viewpoint of our approach, but this shall not be the subject of this work.

In this paper, only non-relativistic quantum mechanics and the corresponding currents are considered. Interesting questions might be the following: could the asymmetry in the spreading behavior be related to the absence of Lorentz symmetry? Could a relativistic formulation could resolve this problem? This would require the consideration of Dirac currents and, maybe, a transition from complex numbers to quaternions; this is quite beyond the scope of this work, but might be an interesting target for future investigations.

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