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Schrödinger's equation as a diffusion equation

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Schrödinger's equation can be considered as a diffusion equation with a diffusion coefficient $\beta^2 = \hbar/2m$. In this article, we explore the implications of this view. Rewriting the wave function in a polar form and transforming Schrödinger's equation into two real equations, we show that one of them reduces to the continuity equation, and the other, a nonlinear dynamical equation for the probability density. Considering these two equations as if they were the basic equations of quantum mechanics, we apply them to several one-dimensional quantum systems. We show the dispersive properties in the probability densities of stationary states of a particle in a rigid box and in harmonic potential; quasi-classical Gaussian probability densities of a free particle; and coherent states and squeezed states of the harmonic oscillator. We also present the soliton as a quantum mechanical representation of a free particle. We discuss the meaning of the diffusion coefficient β^2 for each quantum system using a density plot. © 2021 Published under an exclusive license by American Association of Physics Teachers. https://doi.org/10.1119/10.0002765

I. INTRODUCTION

In the course of their studies, physics students encounter two important partial differential equations. One of them is the one-dimensional wave equation

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2},\tag{1}$$

where u is a scalar function representing the physical quantity that depends on space x and time t, and v is the phase speed of the wave. The other is the diffusion equation

$$\frac{\partial T}{\partial t} = \gamma \frac{\partial^2 T}{\partial x^2}.$$
 (2)

Random physical processes resulting in the diffusion of a given quantity T may be described in Eq. (2), where the constant γ is the diffusion coefficient. If T is the temperature, Eq. (2) is called the heat equation. We here consider one-dimensional cases.

What about Schrödinger's equation? Is it a wave equation or a diffusion equation? To answer this question, let us look at the free particle Schrödinger's equation for the wave function ψ ,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}.$$
 (3)

Comparing Eq. (3) with Eq. (1) or Eq. (2), we are compelled to say that it looks more like a diffusion equation than a wave equation, contrary to our common understanding.

Let us rewrite Eq. (3) in the form

$$\frac{\partial \psi}{\partial t} = i\beta^2 \frac{\partial^2 \psi}{\partial x^2},\tag{4}$$

where

$$\beta^2 = \frac{\hbar}{2m}.\tag{5}$$

Comparison of Eq. (4) with Eq. (2) suggests that β^2 might be regarded as the diffusion coefficient. This point will be

justified in Sec. II (Eq. (9)). The appearance of the imaginary unit i in the right-hand side of Eq. (4) reflects the fact that the wave function ψ is complex,² while u and T are real functions of x and t.

Of course, propagating waves are solutions of Eq. (3). Then, how can we show the diffusive nature of Eq. (3)? Let us note that a plane wave cannot represent a free particle for well-known reasons:³ It is not normalizable and its phase velocity is half the velocity of the corresponding classical particle. Thus, in order to obtain a proper quantum mechanical representation of a free particle, we take a linear combination (the Fourier transform) of plane waves to construct a wave packet, usually in the Gaussian form. Then, the wave packet can be normalized and the particle is well localized, satisfying the uncertainty principle. But the dispersion of the wave packet comes into play, as the component plane waves disperse at different phase velocities. This results in the dispersion of the probability density with the coefficient β^2 , as we will see. In this article, we examine the dispersion of the probability densities for a Gaussian wave packet as well as for other quantum systems.

Dispersion processes of probability densities were previously examined by this author through the integrand of the expectation value of the momentum operator. In the present work, we go further and initiate the discussion starting from Schrödinger's equation. We do so by expressing the wave function in a polar form. Then Schrödinger's equation, being a complex equation, gets split into two real equations. One of them is the continuity equation of the probability density and the other a nonlinear dynamical equation of "the probability fluid," a concept that we will explain in detail throughout this paper. The derivation of these equations is done in Sec. II.

In Secs. III–V, we consider these two equations as if they were the basic equations of quantum mechanics. We solve the nonlinear dynamical equation for various quantum systems with the continuity equation as a subsidiary condition. We also give our probability fluid interpretation for each quantum system, paying special attention to the role the coefficient β^2 plays. We will examine stationary states for a particle in the rigid one-dimensional box (Sec. III) and in the harmonic potential. We then discuss the general properties

of quasi-classical states represented by the Gaussian probability densities (Sec. IV). As concrete applications of Gaussian probability densities, we analyze the free particle and the coherent and squeezed states of the harmonic oscillator. These Gaussian quasi-classical states exhibit varied dispersive behaviors depending on the potential in which the particle is confined, or the lack of it.

Since our dynamic equation is nonlinear, we will examine if this nonlinearity can be counter-balanced by the dispersion of the probability density for a given potential. We will see that such a potential can be found and the soliton appears as the solution of the equation. This soliton probability density, maintaining a constant degree of the particle's localization, would be the quantum mechanical representation closest to a classical free particle. A discussion of the free particle soliton is presented in Sec. V. Concluding remarks are given in Sec. VI.

II. DISPERSIVE PROPERTIES OF THE PROBABILITY DENSITY IMPLICIT IN SCHRÖINGER'S EQUATION

We will first summarize the dispersive properties of the quantum mechanical probability densities. A more detailed derivation of these can be found in Ref. 4.

Consider the expectation value of the momentum operator

$$\langle \vec{P} \rangle = \int_{V_0} \psi^* \vec{P} \psi d\tau, \tag{6}$$

where $\psi(\vec{r},t)$ is the wave function of a quantum system, $d\tau = dxdydz$ is the infinitesimal volume, and V_0 is the entire space. The integrand of $\langle \vec{P} \rangle$ can be written as

$$\psi^* \vec{P} \psi = m (\vec{J} + i \vec{D}), \tag{7}$$

where

$$\vec{J} = \frac{\hbar}{m} Im (\psi^* \vec{\nabla} \psi) \tag{8}$$

is the probability current density, and

$$\vec{D} = -\beta^2 \vec{\nabla} \rho, \tag{9}$$

with $\rho = \psi^* \psi$ being the probability density of a quantum system. The current density \vec{J} is a familiar quantity appearing in textbooks of quantum mechanics. But the quantity \vec{D} is seldom discussed. Being the negative gradient of a density, \vec{D} has the form of a diffusion current. Depending on the quantum system under consideration, we will see that \vec{D} in fact is a diffusion current density, a part of \vec{J} that satisfies the continuity equation.

Equation (9) has a form of Fick's first law of diffusion, where β^2 is recognized as the diffusion coefficient. Equation (2) is known as Fick's second law of diffusion.⁵

Substituting Eq. (7) into Eq. (6) and noting that $\langle P \rangle$ is real, we have

$$\langle \vec{P} \rangle = m \int_{V_0} \vec{J} d\tau \tag{10}$$

and

$$\int_{V_0} \vec{D} d\tau = 0. \tag{11}$$

Equation (11) states that, at any time t, the total dispersion of the probability density always vanishes.

The kinetic energy of a particle can be decomposed into two parts: A part due to the current density \vec{J} and the other part due to the dispersion density D of the probability density distribution. It can be shown that

$$\left\langle \frac{P^2}{2m} \right\rangle = \int_{V_0} \varepsilon_K d\tau,\tag{12}$$

where

$$\varepsilon_K = \frac{1}{2} m \frac{J^2 + D^2}{\rho} \,. \tag{13}$$

The dispersive properties of usual quantum systems were discussed in Ref. 4.

To go beyond this discussion, let us transform the wave function according to

$$\psi = e^{R+iS},\tag{14}$$

where R and S are scalar functions of position \vec{r} and time t. Let us call this transformation the polar transformation. There are two reasons for this transformation. First, we can rewrite the kinematical variables in a manner more amenable to physical interpretation. Substituting Eq. (14) into Eq. (8), the probability current density can be written as

$$\vec{J} = \rho \vec{\eta},\tag{15}$$

with

$$\vec{\eta} = \beta^2 \vec{\nabla}(2S). \tag{16}$$

The quantity $\vec{\eta}$ has the unit of velocity, and for this reason, let us call it the current velocity. Similarly, the dispersive⁶ density D can be written as

$$\vec{D} = \rho \vec{\xi},\tag{17}$$

with

$$\vec{\xi} = -\beta^2 \vec{\nabla}(2R). \tag{18}$$

We will call $\vec{\xi}$ the dispersive velocity. Note that both $\vec{\eta}$ and $\vec{\xi}$ depend on \vec{r} and t. These are the kinematical parameters of the probability density distribution, the probability fluid.⁷ The constant β^2 then is the dispersion coefficient of this probability fluid. We will see the significance of this coefficient in various examples.

Thanks to Eqs. (15) and (17), Eqs. (10) and (11) can be rewritten as

$$\langle \vec{P} \rangle = \int_{V_0} m \rho \vec{\eta} d\tau \tag{19}$$

$$\int_{\nu_0} m\rho \vec{\xi} d\tau = 0. \tag{20}$$

The quantity $m\rho$ may be thought of as the mass density of the probability fluid. It is as if the mass of the particle m were distributed over this fictitious fluid. Then the quantity $m\rho\bar{\eta}$ in Eq. (19) appears as the momentum density of the transport process of the probability fluid. Furthermore, the quantity $m\rho\bar{\xi}$ may be considered as the momentum density of the dispersive process. Equation (20) states that the sum of the dispersive momentum always vanishes. Also, the kinetic energy density in Eq. (13) can be rewritten as

$$\varepsilon_K = \frac{1}{2} m \rho (\eta^2 + \xi^2), \tag{21}$$

which shows that ε_K does not diverge as $\rho \to 0$, contrary to what may be inferred from Eq. (13). Later, we will see that the first term on the right hand side of Eq. (21) will give rise to the kinetic energy of the corresponding classical particle. The second term yields the purely quantum mechanical kinetic energy due to the dispersive process of the probability fluid.

The other more important reason for the transformation in Eq. (14) is that we can derive two basic equations that describe the behavior of the probability fluid. To this end, let us rewrite Schrödinger's equation for a particle in an external potential V as

$$\frac{\partial \psi}{\partial t} = i\beta^2 \nabla^2 \psi + \frac{V}{i\hbar} \psi. \tag{22}$$

Using Eq. (14), we have

$$\frac{\partial \psi}{\partial t} = \left(\frac{\partial R}{\partial t} + i \frac{\partial S}{\partial t}\right) \psi,\tag{23}$$

and

$$\nabla^2 \psi = \left[(\vec{\nabla} R)^2 - (\vec{\nabla} S)^2 + \nabla^2 R \right] \psi + i \left[2(\vec{\nabla} R) \cdot (\vec{\nabla} S) + \nabla^2 S \right] \psi. \tag{24}$$

Substituting Eqs. (23) and (24) into Eq. (22), the real part of the resulting equation is

$$\frac{\partial R}{\partial t} = -\beta^2 \left[2(\vec{\nabla}R) \cdot (\vec{\nabla}S) + \nabla^2 S \right],\tag{25}$$

and the imaginary part

$$\frac{\partial S}{\partial t} = \beta^2 \left[\left(\vec{\nabla} R \right)^2 - \left(\vec{\nabla} S \right)^2 + \nabla^2 R \right] - \frac{V}{\hbar}.$$
 (26)

Since $\rho = e^{2R}$, we have

$$\frac{\partial R}{\partial t} = \frac{1}{2\rho} \frac{\partial \rho}{\partial t},\tag{27}$$

and

$$\vec{\nabla}R = \frac{1}{2\rho}\vec{\nabla}\rho. \tag{28}$$

Also, from Eqs. (15) and (16),

$$\vec{J} = \rho \beta^2 \vec{\nabla}(2S). \tag{29}$$

Taking the divergence of Eq. (29) and using Eq. (28), we have

$$(\vec{\nabla}R) \cdot (\vec{\nabla}S) = \frac{1}{4\beta^2} \frac{1}{\rho} \vec{\nabla} \cdot \vec{J} - \frac{1}{2} \nabla^2 S. \tag{30}$$

Substituting Eqs. (27) and (30) into Eq. (25), we obtain

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0. \tag{31}$$

Equation (31) is the continuity equation stating local conservation of probability. Again, this shows that the distribution of probability density behaves as it were a fluid.⁸

From the definitions of $\vec{\eta}$ and $\ddot{\xi}$ (Eqs. (16) and (18)), we have

$$\vec{\nabla}S = \frac{1}{2\beta^2}\vec{\eta} \tag{32}$$

and

$$\vec{\nabla}R = -\frac{1}{2\beta^2}\vec{\xi}.\tag{33}$$

The divergence of Eq. (33), then is

$$\nabla^2 R = -\frac{1}{2\beta^2} \vec{\nabla} \cdot \vec{\xi}. \tag{34}$$

Taking the gradient of Eq. (26), in which Eqs. (32)–(34) are inserted, we obtain

$$\frac{\partial \vec{\eta}}{\partial t} + \frac{1}{2} \vec{\nabla} (\eta^2) = \frac{1}{2} \vec{\nabla} (\xi^2) - \beta^2 \vec{\nabla} (\vec{\nabla} \cdot \vec{\xi}) - \frac{1}{m} \vec{\nabla} V.$$
(35)

To simplify Eq. (35), let us take the curl of Eq. (33),

$$\vec{\nabla} \times \vec{\xi} = -2\beta^2 \vec{\nabla} \times (\vec{\nabla}R) = 0. \tag{36}$$

Hence

$$\vec{\nabla} \times (\vec{\nabla} \times \xi) = \vec{\nabla} (\vec{\nabla} \cdot \vec{\xi}) - \nabla^2 \vec{\xi} = 0, \tag{37}$$

for any vector function $\vec{\xi}$. Therefore, it follows that

$$\vec{\nabla} \left(\vec{\nabla} \cdot \vec{\xi} \right) = \nabla^2 \vec{\xi}. \tag{38}$$

Using Eq. (38) in Eq. (35), we finally obtain

$$\frac{\partial \vec{\eta}}{\partial t} + \frac{1}{2} \vec{\nabla} \left(\eta^2 \right) = \frac{1}{2} \vec{\nabla} \left(\xi^2 \right) - \beta^2 \nabla^2 \vec{\xi} - \frac{1}{m} \vec{\nabla} V. \tag{39}$$

Equation (39) describes the balance between the acceleration of the probability current and the one due to the diffusion current. We view this equation as the equation of motion for the probability fluid. While Schrödinger's equation is linear, this equation of motion is nonlinear. Mathematically, this is due to the fact that this equation is derived from Schrödinger's equation through the polar transformation (Eq. (14)). In the rest of this paper, we will apply Eq. (39) to various quantum systems, using

the continuity equation as the subsidiary condition. Despite the somewhat involved appearance of Eq. (39), it reduces to simple, integrable nonlinear differential equations when it is applied to the concrete systems that we consider, thanks to the continuity equation. We will see that the dispersive velocity $\vec{\xi}$ plays a significant role in each of these cases.

III. ONE-DIMENSIONAL STATIONARY STATES

For a stationary state, the probability density does not depend on time

$$\frac{\partial \rho}{\partial t} = 0. \tag{40}$$

Thus, according to the continuity equation (Eq. (31)), $\partial J/\partial x = 0$. This means that J is constant along the x-axis. Furthermore, when a particle is confined, J = 0. Hence $\eta = 0$. Though the probability current does not exist, the dispersive process of the probability fluid does take place. Since J = 0, for a particle confined in a one-dimensional potential, the equation of motion for the probability fluid (Eq. (39)) simplifies to

$$\xi \frac{d\xi}{dx} - \beta^2 \frac{d^2 \xi}{dx^2} - \frac{1}{m} \frac{dV}{dx} = 0. \tag{41}$$

This is our basic dynamical equation for one-dimensional stationary states.

From Eqs. (9) and (17), it follows that

$$\frac{1}{\rho}d\rho = -\frac{1}{\beta^2}\xi dx. \tag{42}$$

Integrating Eq. (42), we have

$$\rho = Nexp \left[-\frac{1}{\beta^2} \int \xi dx \right],\tag{43}$$

where N is the normalization constant. This is our basic equation that relates the dispersive velocity to the probability density.

As the first example of application of Eq. (41), let us take the case of the stationary state of a particle in the one-dimensional infinite square potential well. Suppose a particle of mass m is confined in the potential

$$V(x) = \begin{cases} 0, & 0 \le x \le a, \\ \infty, & \text{otherwise.} \end{cases}$$
 (44)

The particle in this potential is free, and Eq. (41) reduces to

$$\beta^2 \frac{d^2 \xi}{dx^2} = \xi \frac{d\xi}{dx}.\tag{45}$$

This simple nonlinear differential equation can be solved in the following way. First, rewrite Eq. (45) as

$$\frac{d^2\xi}{dx^2} = \frac{1}{2\beta^2} \frac{d}{dx} \left(\xi^2\right). \tag{46}$$

Integrating Eq. (46), we have

$$\frac{d\xi}{dx} = \frac{1}{2\beta^2} \xi^2 + c_0, \tag{47}$$

where c_0 is an arbitrary integration constant. Next rewrite Eq. (47) as

$$\frac{d\xi}{c_0 + \xi^2 / 2\beta^2} = dx, (48)$$

and integrate once more, we have

$$\xi = c_1 \beta \tan\left(\frac{c_1}{2\beta}x + c_2\right),\tag{49}$$

where $c_1 = \sqrt{2c_0}$ and c_2 is another arbitrary constant. Substituting Eq. (49) into Eq. (43), we have

$$\rho = N\cos^2\left(\frac{c_1}{2\beta}x + c_2\right). \tag{50}$$

We next impose the boundary conditions: $\rho = 0$ at x = 0 and x = a. These give us

$$c_1 = \frac{2\beta}{a}n\pi$$
 and $c_2 = \frac{\pi}{2}$, (51)

and we obtain

$$\rho_n = -\frac{2}{a}\sin^2\left(\frac{n\pi x}{a}\right). \tag{52}$$

This is the familiar result found in any textbook of quantum mechanics.

One can say, that this is a complicated way to obtain this simple result. We certainly do not need a nonlinear differential equation to solve this quantum system. But the point here is that the physical picture has been changed. When we teach this particular example, we usually remind students of the analogy of the standing waves of a string of length a, reflecting the wave-particle duality in the framework of the standard quantum mechanics. In the view presented here, however, an analogy would be a one-dimensional box filled with this fictitious probability fluid. The fluid particles, that have nothing to do with the particle confined in the box, are moving randomly without changing the density distribution, satisfying Eq. (20)

Using our fluid modeling, how the system gains energy can be easily explained. If we look at Eq. (21), the kinetic energy density of the system is given by $\varepsilon_k = m\rho \xi^2/2$. It is as if, at position x, an infinitesimal volume of fluid having mass $m\rho dx$ moves with velocity ξ , possessing the kinetic energy of $(m\rho \xi^2/2)dx$. The energy of the system is found by summing all of these kinetic energies in the box.

We next find the energy of the system. From Eqs. (49) and (51), we have

$$\xi_n = -\frac{2n\pi\beta^2}{a}\cot\left(\frac{n\pi x}{a}\right). \tag{53}$$

Thus

$$E_n = \frac{1}{2}m \int_0^a \rho_n \xi_n^2 dx = \frac{2n^2 \pi^2 m \beta^4}{a^2},$$
 (54)

which is equal to $n^2\pi^2\hbar^2/2ma^2$, as it should be.

Our method can be applied to the stationary states of a particle in the harmonic potential well. As we expect, the mathematics of this case get more demanding than the case of the rigid box. But this is also true in the standard way to solve Schrödinger's equation. However, in our method, unlike the standard analysis, there is no need to separate out the asymptotic part of the solution thanks to Eq. (43). This equation gives the complete probability density of the harmonic oscillator, including the asymptotic part.

In our method, the physics of a particle in the onedimensional harmonic potential well is very similar to that of a particle in the rigid box. There is no probability current. But the probability fluid possesses a dispersive momentum and a kinetic energy, as well as a potential energy in this case. We can thus calculate the total energy of this fictitious fluid.

We present this case as a problem with a hint: Substituting the harmonic potential into Eq. (41), we obtain a nonlinear differential equation, called the Riccati equation. A nonlinear Riccati equation can always be reduced to a second order linear differential equation. Using some appropriate parametric substitutions, we then obtain the differential equation of which Hermite polynomials are solutions.

IV. GAUSSIAN PROBABILITY DENSITIES: QUASI-CLASSICAL STATES

Next, we examine time-dependent quantum states of a one-dimensional particle, taking the Gaussian probability densities. Let us assume the probability density of the form ¹²

$$\rho(x,t) = \frac{1}{\sqrt{2\pi}\sigma(t)} \exp\left[-\frac{1}{2} \left(\frac{x-\mu(t)}{\sigma(t)}\right)^2\right]. \tag{55}$$

This probability density contains two time-dependent parameters $\mu(t)$ and $\sigma(t)$. The meaning of these two parameters can be seen in the following way. First, we find the expectation value of the position of the particle

$$\langle x \rangle = \int_{-\infty}^{\infty} \rho x dx = \mu(t).$$
 (56)

We may regard $\mu(t)$ as the trajectory of the corresponding classical particle. The classical trajectories, of course, do not have any position ambiguities. But at a given time, the probability density distribution in Eq. (55) has the uncertainty of

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sigma(t), \tag{57}$$

which specifies the dispersive properties of this probability density. Thus, as the corresponding classical particle moves along the trajectory $\mu(t)$, the probability density is spread around this trajectory according to the Gaussian form. Let us call quantum systems corresponding to such probability density the quasi-classical states. ¹³

Equation (42) still holds valid and using Eq. (55), we have

$$\xi(x,t) = \frac{\beta^2}{\sigma^2(t)} [x - \mu(t)]. \tag{58}$$

Equation (58) indicates that the dispersion of the probability density stems from the location of the corresponding classical particle at a given time t.

From the continuity equation (Eq. (31)), it follows that

$$J = -\int \rho_t dx,\tag{59}$$

where the subscript t implies the partial derivative with respect t. We will use the subscript notation in the rest of this article. Substituting Eq. (55) into Eq. (59) and using Eqs. (17) and (58), we obtain

$$J = \rho \mu_t + \frac{\sigma \sigma_t}{\beta^2} D. \tag{60}$$

In Sec. III, we mentioned that the dispersive density D is not a current for one-dimensional stationary states. Looking at Eq. (60) though, this quantity appears as a part of the probability current J, which satisfies the continuity equation. This means that D contributes to a transport of probability fluid. Thus, for quasi-classical states, D can be recognized as a diffusion current. From Eq. (60), it immediately follows that

$$\eta = \mu_t + \frac{\sigma \sigma_t}{\beta^2} \xi. \tag{61}$$

From Eqs. (21), (58), and (61), the kinetic energy density of the system is given by

$$\varepsilon_k = \frac{1}{2} m \rho \mu_t^2 + \frac{1}{2} m \rho \left(1 + \frac{\sigma^2 \sigma_t^2}{\beta^4} \right) \xi^2 + m \rho \frac{\sigma \sigma_t}{\beta^2} \mu_t \xi, \quad (62)$$

and integrating ε_k over the entire space, we obtain the kinetic energy

$$E_k = \frac{1}{2}m\mu_t^2 + \frac{1}{2}m\left(\sigma_t^2 + \frac{\beta^4}{\sigma^2}\right),\tag{63}$$

where Eq. (20) is used. Note that the first term in the right-hand side of Eq. (63) is the kinetic energy of the corresponding classical particle. The second term is due to the dispersive process of the probability fluid, and its origin is purely quantum mechanical (or due to "quantum fluctuations").

Next, we evaluate the momentum uncertainty for the Gaussian probability densities and see the significance that this kinetic energy has for the uncertainty principle, due to the dispersive process. The momentum uncertainty is given by

$$\Delta P = \sqrt{\langle P^2 \rangle - \langle P \rangle^2}. (64)$$

From Eqs. (19) and (61), we have

$$\langle P \rangle = \int_{-\infty}^{\infty} m \rho \eta dx = m \mu_t \int_{-\infty}^{\infty} \rho dx + \frac{\sigma \sigma_t}{\beta^2} \int_{-\infty}^{\infty} m \rho \xi dx = m \mu_t,$$
(65)

since ρ is normalized and the second integral vanishes according to Eq. (20). To evaluate $\langle P^2 \rangle$, we note that

$$\langle P^2 \rangle = 2mE_k = m^2 \mu_t^2 + m^2 \left(\sigma_t^2 + \frac{\beta^4}{\sigma^2} \right), \tag{66}$$

where E_k is given in Eq. (63). Thus substituting Eqs. (65) and (66) into Eq. (64), we obtain

$$\Delta P = m\sqrt{\sigma_t^2 + \frac{\beta^4}{\sigma^2}}. (67)$$

If the second term in Eq. (63) did not exist, ΔP would have been zero and this would violate the uncertainty principle. Therefore, we see that the kinetic energy due to the dispersive process is an essential feature of quantum mechanics. In Secs. IV A and IV B, we will use Eq. (67) to evaluate ΔP for concrete quantum systems.

Let us next rewrite the equation of motion (Eq. (39)) in one-dimension as

$$\eta_t + \eta \eta_x = \xi \xi_x - \beta^2 \xi_{xx} - \frac{1}{m} V_x.$$
(68)

Substituting Eqs. (58) and (61) into Eq. (68), we then obtain

$$\left(\frac{\sigma_{tt}}{\sigma} - \frac{\beta^4}{\sigma^4}\right)(x - \mu) = -\frac{1}{m}V_x - \mu_{tt}.$$
 (69)

The parameter $\mu(t)$ is the trajectory of the corresponding classical particle to be specified. Equation (69) is a differential equation for the dispersion parameter $\sigma(t)$. We now examine the possible potentials that Eq. (69) allows.

Case 1: Vanishing right-hand side of Eq. (69)

- (a) V = 0 and $\mu = v_0 t$: Corresponding to a free classical particle of velocity v_0 .
- (b) $V = -\alpha x$ and $\mu = \alpha t^2/2m$: Corresponding to an accelerating classical particle of acceleration α .

In both cases, Eq. (69) reduces to

$$\sigma^3 \sigma_{tt} - \beta^4 = 0, \tag{70}$$

because $x - \mu$ cannot be zero for all x. This is the differential equation for the position uncertainty $\sigma(t)$ for case 1.

Case 2: The right-hand side of Eq. (69) is proportional to $x - \mu$

This is the case if

$$V(x) = \frac{1}{2}m\omega^2 x^2,\tag{71}$$

with

$$\mu(t) = A\cos(\omega t - \delta),\tag{72}$$

where ω and δ are real constants. Equations (71) and (72) represent the classical harmonic oscillator. Substituting Eqs. (71) and (72) into Eq. (69), we obtain the differential equation for the dispersive process in this case as

$$\sigma^3 \sigma_{tt} + \omega^2 \sigma^4 - \beta^4 = 0. \tag{73}$$

We will examine the quasi-classical particles for all these cases in the following. We will see that, depending on the potential under which the particle is subject, the probability fluid displays various dispersive behaviors.

A. Free particle

As mentioned in Sec. I, in quantum mechanics, to describe a free particle with a sense of localization, we construct a linear superposition of plane waves to form a wave packet, usually in the Gaussian form.¹⁴ We now show how we can present a free particle in the context of our probability fluid view.

We saw that the dispersion of the Gaussian probability density for a free particle is given in Eq. (70). In order to solve this nonlinear differential equation, let

$$\sigma_t = q, \tag{74}$$

then

$$\sigma_{tt} = qq_{\sigma},\tag{75}$$

and Eq. (70) becomes

$$qdq = \beta^4 \frac{d\sigma}{\sigma^3}. (76)$$

Integrating Eq. (76), we have

$$q^2 = c_1 - \frac{\beta^4}{\sigma^2},\tag{77}$$

where c_1 is an integration constant. Since $\sigma = \Delta x$ is the position uncertainty of the particle, σ and q are positive. Then

$$q = \sqrt{c_1 - \frac{\beta^4}{\sigma^2}}. (78)$$

Integrating q with respect to t,

$$\int \frac{d\sigma}{\sqrt{c_1 - \beta^4/\sigma^2}} = t + c_2,\tag{79}$$

where c_2 is another integration constant. Let us specify that the time starts at t = 0, then $c_2 = 0$ and we denote $\sigma(0) = \sigma_0$, the initial position uncertainty. Then after the integration in Eq. (79), we obtain

$$\sigma = \sigma_0 \sqrt{1 + \left(\frac{t}{T}\right)^2},\tag{80}$$

where

$$T = \left(\frac{\sigma_0}{\beta}\right)^2. \tag{81}$$

Thus, according to Eq. (55), the probability density for the free particle is given by

$$\rho(x,t) = \frac{1}{\sqrt{2\pi}\sigma(t)} \exp\left[-\frac{1}{2} \left(\frac{x - v_0 t}{\sigma(t)}\right)^2\right],\tag{82}$$

where $\sigma(t)$ is given in Eqs. (80) and (81).

Recall that $\beta^2 = \hbar/2m$ is the diffusion coefficient. Let us see the effect of this coefficient on the probability density. Figures 1(a) and 1(b) show the density plots for $\beta = 0.10$ and $\beta = 0.15$, respectively. The horizontal axis specifies the time and the vertical, the position of the particle. The grey level indicates the density, brighter white being higher density. The classical trajectory would be a white straight line. As time elapses, the probability density disperses in both

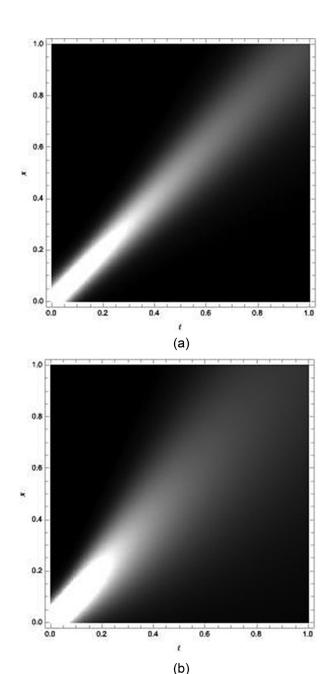


Fig. 1. Plots of one-dimensional Gaussian probability densities: (a) $\beta = 0.10$ and (b) $\beta = 0.15$. Other parameters are chosen as $\sigma_0 = 0.05$ and $v_0 = 1.0$ for both cases.

Figs. 1(a) and 1(b). But the dispersion occurs much quicker and over a larger distance when the particle has a larger diffusion coefficient. Note that the higher mass particle has a lower diffusion coefficient. Thus, as the mass of the particle increases, it behaves more like a classical particle displaying less dispersion. For a free particle, the dispersion of the probability density continues indefinitely.

Next, we consider the kinetic energy for the free particle. The velocity of the corresponding classical particle is $\mu_t = v_0$, and the dispersion $\sigma(t)$ is given in Eqs. (80) and (81). Substituting these into Eq. (63), we obtain

$$E_k = \frac{1}{2}mv_0^2 + \frac{1}{2}m\frac{\beta^4}{\sigma_0^2}.$$
 (83)

The first term is the classical kinetic energy of a free particle. The second term depends on the initial position uncertainty σ_0 . Thus, we may call this kinetic energy the localization energy, or the zero-point energy of the free particle. When the particle is very well localized, σ_0 is small and the zeropoint energy may become very large.

From Eqs. (67), (80), and (81), we have

$$\Delta P = m\beta^2/\sigma_0,\tag{84}$$

and the minimum uncertainty product is

$$\Delta x \Delta P = m\beta^2 = \frac{\hbar}{2},\tag{85}$$

occurring at t = 0. The uncertainty principle is satisfied.

For a particle under a constant acceleration, the differential equation for the dispersion $\sigma(t)$ is the same as for a free particle, as discussed at the beginning of this section. Thus, the same discussion holds valid for this case as for the free particle, except for the classical path, which is parabolic in this case.

B. Quasi-classical states of the harmonic oscillator

For the harmonic oscillator, the differential equation for $\sigma(t)$ is given in Equation (73). Looking at this equation, we see that there are two possible cases. First, if σ is constant, $\sigma_{tt} = 0$, and we have

$$\sigma_c = \frac{\beta}{\sqrt{\omega}},\tag{86}$$

where the subscript "c" refers to the coherent state. In this case, the probability density is

$$\rho_c(x,t) = \frac{1}{\sqrt{2\pi}\sigma_c} \exp\left[-\frac{1}{2} \left(\frac{x - \mu(t)}{\sigma_c}\right)^2\right],\tag{87}$$

where the classical trajectory $\mu(t)$ is given in Eq. (72). This is the coherent state of the harmonic oscillator. 15 Figures 2(a) and 2(b) show two cycles of density plots of the coherent states for $\beta = 0.3$ and $\beta = 0.7$, respectively. In each of these density plots, the degree of dispersion from the classical trajectory does not fluctuate as time elapses since σ_c is constant. But in Fig. 2(b), the oscillating strip is thicker because the diffusion coefficient is higher.

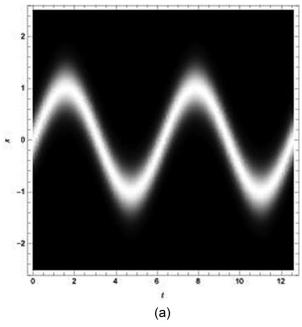
The other possibility is that the degree of dispersion fluctuates as time elapses and σ is a function of time t. The resulting quantum states are the squeezed-states of the harmonic oscillator.¹⁶ In this case, if $\sigma_t = q$, then Eq. (73)

$$\frac{1}{2}\frac{d}{d\sigma}q^2 = \frac{\beta^4}{\sigma^3} - \omega^2\sigma. \tag{88}$$

Integrating Eq. (88) with respect to σ , we have

$$q^2 = c - \frac{\beta^4}{\sigma^2} - \omega^2 \sigma^2,\tag{89}$$

where c is an integration constant. Thus



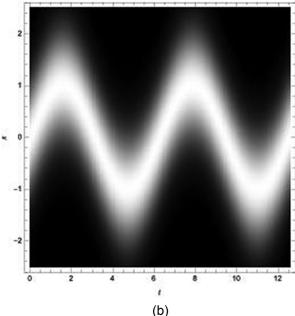


Fig. 2. Coherent states of the harmonic oscillator: (a) $\beta=0.3$ and (b) $\beta=0.7$. Other parameters are set as $\omega=1$, $\delta=\pi/2$, and A=1.

$$\sigma_t = \pm \sqrt{c - \frac{\beta^4}{\sigma^2} - \omega^2 \sigma^2},\tag{90}$$

and

$$\int \frac{d\sigma}{\sqrt{c - \beta^4/\sigma^2 - \omega^2 \sigma^2}} = \pm (t - t_0), \tag{91}$$

where t_0 is an arbitrary constant with the unit of time. After carrying out the integration in Eq. (91), we obtain

$$2\sqrt{c\sigma^2 - \omega^2\sigma^4 - \beta^4} + i\left(\frac{c}{\omega} - 2\omega\sigma^2\right)$$
$$= \exp[\pm i2\omega(t - t_0)]. \tag{92}$$

The imaginary part of Eq. (92) is

$$\frac{c}{\omega} - 2\omega\sigma^2 = \pm \sin[2(\omega t - \theta_0)],\tag{93}$$

where $\theta_0 = \omega t_0$. Because *c* is an arbitrary constant, Eq. (93) gives the dispersion $\sigma(t)$ of the form

$$\sigma_s(t) = \sigma_{s0} \sqrt{1 + \gamma \sin[2(\omega t - \theta_0)]}, \tag{94}$$

where the subscript s refers to the squeezed state and $0 \le \gamma < 1$, so that σ is a real and positive constant. The constant σ_{s0} can be determined by substituting Eq. (94) into Eq. (73). The result is

$$\sigma_{s0} = \frac{\beta}{\sqrt{\omega^2 (1 - \gamma^2)4}}.\tag{95}$$

The constant γ specifies the degree of squeezing. When $\gamma = 0$, $\sigma_s \to \sigma_c$, and the squeezed state reduces to the coherent state. As γ approaches 1, the squeezing becomes distinct. The squeezing occurs when

$$\sin[2(\omega t - \theta_0)] = -1,\tag{96}$$

at which times $\sigma(t)$ becomes minimum.

Figures 3(a)-3(c) show the probability densities of the squeezed-states, for $\theta_0=0$, $\theta_0=\pi/4$, and $\theta_0=3\pi/4$. The squeezing appears as bright white spots, satisfying the condition given in Eq. (96). By changing the parameter θ_0 , we can obtain the entire spectrum of the squeezing phenomena.¹⁷

The words "coherent state" and "squeezed state" are used in quantum mechanics and quantum optics, and they stem from the concept of waves. Since our "modeling" is not of waves, but rather of fluid and diffusion, the words lose their original meaning.

Before closing this section, we evaluate the uncertainty product $\Delta x \Delta P$ for the squeezed states. Substituting Eqs. (94) and (95) into Eq. (67), we obtain

$$\Delta P = m\omega\sigma_s\sqrt{1 - \gamma\sin[2(\omega t - \theta_0)]}.$$
 (97)

Since $\Delta x = \sigma(t)$, we have

$$\Delta x \Delta P = m\omega \sigma_s^2 \sqrt{1 - \gamma^2 \sin^2[2(\omega t - \theta_0)]}.$$
 (98)

When squeezing occurs, we have

$$(\Delta x \Delta P)_{min} = m\beta^2 = \frac{\hbar}{2},\tag{99}$$

according to Eq. (96). This is the minimum uncertainty product, and the uncertainty principle is satisfied.

V. FREE PARTICLE SOLITONS

In Secs. III–IV, we have examined dispersive properties of the probability densities of various one-particle quantum systems, applying our dynamic equation and the continuity equation to these systems. Unlike Schrödinger's equation, Eq. (39) is nonlinear. It is well known that, when effects of nonlinearity are balanced by dispersion, solitons result. ^{18,19} It might happen that the cancellation of nonlinearity and dispersion takes place in our probability fluid

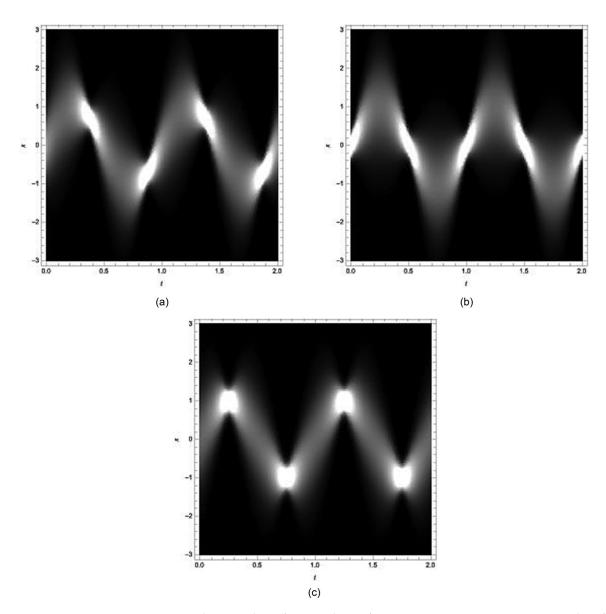


Fig. 3. Squeezed-states of the harmonic oscillator: (a) $\theta_0=0$, (b) $\theta_0=\pi/4$, and (c) $\theta_0=3\pi/4$. Other parameters are set as A=1, $\omega=2\pi$, $\delta=\pi/2$, $\beta=1$, and $\gamma=0.9$.

method and the soliton emerges as a solution of our dynamical equation. In this section, we show that this is in fact the case.

The soliton would be the ultimate quasi-classical representation of a free particle, in that its dispersion remains constant, as in the coherent state of the harmonic oscillator, and the particle remains more like a classical particle maintaining its initial localization. However, this localization is never point-like.

In Sec. IV, we examined the Gaussian representation of a free particle. We saw that, in the absence of a potential, the probability density disperses indefinitely. We need some kind of "confining potential" to prevent an indefinite dispersion. But this potential cannot be stationary. Otherwise, the particle is not free. Thus, such a potential must be a function of space and time. The question is whether or not such a potential exists.

To find the potential that will give rise to the soliton, let us assume a probability density

$$\rho(x,t) = \frac{1}{2\sigma_0} \operatorname{sech}^2\left(\frac{x - v_0 t}{\sigma_0}\right),\tag{100}$$

where v_0 is the velocity of the corresponding classical free particle and σ_0 , a constant with the unit of length. Figure 4 shows the density plot of Eq. (100). Comparing Fig. 4 with Figs. 1(a) and 1(b), we see that, unlike the Gaussian probability density, there is no change in dispersion as time elapses for the soliton probability density.

From the continuity equation (Eq. (31)), it follows that

$$J = -\int \rho_t dx = \rho v_0, \tag{101}$$

and thus

$$\eta = v_0. \tag{102}$$

The dynamic equation (Eq. (39)) in one-dimension is

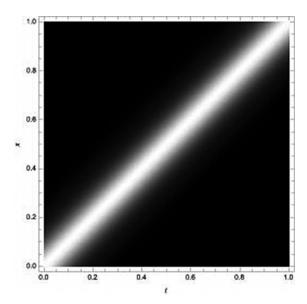


Fig. 4. Free particle soliton. $v_0 = 1$ and $\sigma_0 = 0.09$.

$$\eta_t + \eta \eta_x = \xi \xi_x - \beta^2 \xi_{xx} - \frac{1}{m} V_x.$$
 (103)

Due to Eq. (102), Eq. (103) reduces to

$$\xi \xi_x - \beta^2 \xi_{xx} - \frac{1}{m} V_x = 0. \tag{104}$$

Note Eq. (104) is identical to Eq. (41), which appeared in the discussion of the one-dimensional stationary states in Sec. III. From Eq. (104), it follows that

$$V(x,t) = \int m(\xi \xi_x - \beta^2 \xi_{xx}) dx.$$
 (105)

Next, we find the dispersive velocity ξ . Substituting Eq. (100) into Eq. (42), we have

$$\xi(x,t) = \frac{2\beta^2}{\sigma_0} \tanh\left(\frac{x - v_0 t}{\sigma_0}\right). \tag{106}$$

Substituting Eq. (106) into Eq. (105), we obtain the desired potential for the soliton

$$V(x,t) = -\frac{8m\beta^4}{\sigma_0}\rho(x,t). \tag{107}$$

The potential given in Eq. (107) is proportional to the negative of the probability density of the soliton. The appearance of a potential proportional to the probability density is not unique to our discussion here. In the analysis of Bose-Einstein condensates, the interaction between particles is represented as a potential proportional to the probability density of the atoms in the nonlinear Schrödinger equation.²⁰

But in our case, we are not assuming any external influence. An external object, whatever it is, cannot move with the soliton. The particle is assumed to be free. A possible interpretation is that the soliton, if it exists in this manner, generates its own potential and the soliton is self-sustaining, just like the solitory waves of water or light. We suspect that

this phenomenon is a manifestation of combined effects of dispersion and nonlinearity. This issue deserves a further examination. Such a study, however, goes beyond the scope of this article.

In order to justify this point, let us look at Eq. (104) again. As mentioned before, this equation is identical to that used in the one-dimensional stationary states. However, the physical system considered here is dynamical, and the process develops as time elapses. Thus, we next rewrite Eq. (104) as a dynamical equation. From the one-dimensional continuity equation, and Eqs. (15) and (102), it follows that

$$\rho_t = -v_0 \rho_x. \tag{108}$$

From Eqs. (104), (107), and (108), we obtain

$$\rho_t = \frac{\sigma_0 v_0}{8\beta^4} \left(\xi \xi_x - \beta^2 \xi_{xx} \right). \tag{109}$$

Equation (109) shows that the time-development of the soliton probability density is due to its own dispersive velocity.

Next, we show that the energy of the soliton can be negative, if it is moving slowly and thus is self-confined. Substituting Eqs. (100), (102), and (106) into Eq. (21), and integrating ε_K over the probability fluid, we obtain the kinetic energy of the soliton

$$\left\langle \frac{P^2}{2m} \right\rangle = \frac{1}{2} m v_0^2 + \frac{2}{3} m \frac{\beta^4}{\sigma_0^2}.$$
 (110)

The potential energy of the soliton can be obtained as

$$\langle V \rangle = \int_{-\infty}^{\infty} \rho V dx = -\frac{8}{3} m \frac{\beta^4}{\sigma_0^2}.$$
 (111)

Thus, the energy of the soliton is

$$E = \left\langle \frac{P^2}{2m} \right\rangle + \left\langle V \right\rangle = \frac{1}{2} m v_0^2 - 2m \frac{\beta^4}{\sigma_0^2}. \tag{112}$$

When E = 0, the velocity of the soliton is

$$v_{0c} = 2\frac{\beta^2}{\sigma_0}.\tag{113}$$

Looking at Eq. (113), we see that, when the velocity of the particle v_0 is below this critical velocity v_{0c} , the energy of the soliton becomes negative, and the "free particle" is self-confined in its own potential. Though this situation appears strange, we have to remember that the confining potential moves with the soliton.

We next evaluate the uncertainty product for this soliton. As shown in Fig. 4, the dispersion of the probability density does not depend on time. Hence, we can evaluate the position uncertainty Δx at any time. It is easiest to do this at time t = 0, and we obtain

$$\Delta x = \frac{\pi \sigma_0}{2\sqrt{3}}.\tag{114}$$

The momentum uncertainty can be evaluated from Eq. (110) and $\langle P \rangle = mv_0$. The result is

$$\Delta P = \frac{2}{\sqrt{3}} m \frac{\beta^2}{\sigma_0}.$$
 (115)

Thus, the desired uncertainty product is

$$\Delta x \Delta P = \frac{\pi \, \hbar}{3 \, 2}.\tag{116}$$

The factor $\pi/3$ is 1.05, and

$$\Delta x \Delta P > \frac{\hbar}{2}.\tag{117}$$

The product is slightly above $\hbar/2$, satisfying the uncertainty principle.

For the Gaussian free particle representation, Eq. (85) gives the minimum uncertainty product of $\hbar/2$, occurring at time t = 0. For t > 0, the product is larger than $\hbar/2$, monotonically increasing. There initially was no guarantee that the above-described solitonic free particle state satisfied the uncertainty principle, so that this should be checked. However, Eq. (117) shows that the uncertainty product is constant and slightly above $\hbar/2$ at all times.

VI. CONCLUSION

Rewriting the wave function in a polar form and transforming Schrödinger's equation into two real equations, we showed that one of them reduces to the continuity equation, and the other, to a nonlinear dynamical equation for the probability fluid. We consider these as if they were the basic equations of quantum mechanics and apply them to several one-dimensional quantum systems, obtaining familiar results using this unfamiliar method. We give physical interpretation to each of these examples employing the language of fluid mechanics and diffusion theory. Also included is a discussion of the free particle soliton as a quantum state.

One might wonder if there is a fluid dynamics analogue of Eq. (39). Indeed there exists such an analogue with some caveats. Let us compare Eq. (39) with a version of Euler's equation of fluid dynamics²

$$\frac{\partial \vec{v}}{\partial t} + \frac{1}{2} \vec{\nabla}(v^2) - \vec{v} \times (\vec{\nabla} \times \vec{v}) = f_{\text{app}} - \frac{1}{\rho} \vec{\nabla} p, \qquad (118)$$

where \vec{v} is the velocity and p is the pressure at each point of the fluid, at time t. If we assume that the fluid is irrotational, then $\vec{\nabla} \times \vec{v} = 0$. The quantity f_{app} denotes the applied force per unit volume. Let us assume this to be zero as well. The term $-\vec{\nabla}p/\rho$ corresponds to $-\vec{\nabla}V/m$ in Eq. (39), since the potential V confines the probability fluid. Then we see that the current velocity $\vec{\eta}$ corresponds to the velocity \vec{v} of the classical fluid. On the other hand, dispersive velocity ξ , as we defined it, is a purely quantum mechanical quantity as we saw throughout this paper. Consequently, the dispersive velocity $\vec{\xi}$ is absent in Eq. (118). Thus, it appears that Eq. (39) is a quantum mechanical version of Euler's equation, containing both fluid dynamics and diffusion process.

Since our method relies on a nonlinear dynamical equation, there may be restrictions as to how much further it can be developed. For example, probability density does not allow simple linear combinations, and the superposition principle does not apply. Also, not having tried ourselves, it is not clear if we can solve problems in dimensions higher than 1. In this context, it will be interesting to see if we can analyze the H-atom in terms of the probability fluid, starting from Eq. (39).

On the other hand, however, if we look at fluid dynamics, its fundamental equation, Euler's equation, is intrinsically nonlinear, even though its dynamics simply reflects Newton's second law. Looking at superb richness of fluid dynamics, we suspect that the future development of our approach may not be so prohibiting.

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⁹E. Nelson, "Derivation of the Schrödinger Equation from Newtonian Mechanics," Phys. Rev. 150, 1079-1085 (1966). In this paper, Nelson used the polar transformation, as we do in Eq. (15). As a consequence, our Eq. (39) is identical to Nelson's Eq. (48b). The physical interpretation, however, is different. Nelson attempted to show that his "stochastic mechanics" yields the basic equations equivalent to the Schrödinger equation. And Eq. (48b) appears as a bridge between the two. Our method, however, is to consider Eq. (39) as if it were the fundamental equation of motion for the probability fluid. Our intention here is to explore the probability density focusing on its dispersive behavior. We do not introduce any physical hypothesis and try to delve further into a deeper layer of quantum mechanics, as Nelson attempted to do.

 10 The quantity D is not a current in this case since it is not a part of J, which satisfies the continuity equation. In other words, D does not contribute to a transport of the probability density in this case. We will see later that, in some cases, D becomes a part of J (see, for example, Eq. (60)). In such case, we recognize D as a current.

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