quantum reports

Article

A Normalization Condition for the Probability Current in Some Remarkable Cases

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Abstract: Starting from the dynamics of a bouncing ball in classical and quantum regime, we have suggested in a previous paper to add an arbitrary function of time to the standard expression of the probability current in quantum mechanics. In this paper, we suggest a way to determine this function: imposing a suitable normalization condition. The application of our proposal to the case of the harmonic oscillator is discussed.

Keywords: Bohmian mechanics; probability current; quantum velocity

Citation: Feoli, A.; Benedetto, E.; Iannella, A.L. A Normalization Condition for the Probability Current in Some Remarkable Cases. *Quantum Rep.* **2024**, *6*, 147–155. https://doi.org/10.3390/quantum6020012

Academic Editor: Margarita A. Man'ko

Received: 16 March 2024
Revised: 12 April 2024
Accepted: 14 April 2024
Published: 23 April 2024

1. Introduction

The description of the trajectory of a quantum particle is still possible by adopting the de Broglie–Bohm interpretation of quantum mechanics. In a paper of 1953 [1], Einstein underlined a problem in the predictions of the theory regarding the motion of a particle in a box with perfectly reflecting walls. In that case, the solution of Schrödinger equation for stationary states is a real wave function, and the corresponding momentum predicted by the Bohmian mechanics is vanishing. Einstein, on the contrary, believes that if a classical macroscopic body must oscillate between the two walls, a quantum particle, at least for high values of quantum numbers, must also have the same behavior, and he considers the prediction $p = 0$ highly unsatisfying. In order to give an answer to Einstein's objection, it can be very useful to study the particular case of a bouncing ball and to follow the evolution of its velocity in spacetime. In the paper [2], we have already deepened some aspects of the quantum dynamics of a bouncing ball, starting from the analysis contained in a previous article [3], where we had described from a classical and a quantum point of view the behavior of a body of mass m in the potential $V(x) = mgx$, where g is the acceleration of gravity. The ball moves up and down between the points $x = 0$ and $x = h$ with a classical period $\tau = \sqrt{8h/g}$ (bounce period). Summarizing the main results of the previous paper [2], we start from the consideration that in classical physics, the probability that the ball can be found in the region between x and $x + dx$ is proportional to the time the body spends in that region

$$Q(x)dx = Q(x)vdt = \frac{2dt}{\tau}. \tag{1}$$

Hence, the classical probability density $Q(x)$ is related to the magnitude of the classical velocity field $v_c(x) = \sqrt{2(E - V(x))/m}$ of the particle (where $E = mgh$) by the formula

$$Q(x) = \frac{2}{\tau v_c(x)}. \tag{2}$$

In the previous paper [2], we have preserved Equation (2) in the transition from the classical to the quantum regime, supposing that

$$|\psi|^2 = \frac{2}{\tau v_q} \tag{3}$$

This choice was supported by the fact that we recover the classical Formula (2) when we perform a sort of averaging of the quantum probability density in Equation (3). For the bouncing ball, if we start from the result obtained for $|\psi|^2$ in the stationary phase approximation [2]

$$|\psi|^2 \approx 2Q(x)\cos^2\left(\frac{2}{3}|k(h-x)|^{3/2} - \frac{\pi}{4}\right), \tag{4}$$

we observe that $I(x) = 2Q(x)$ represents the upper envelope of the oscillating function reaching all its maximal values. If we take, for each x, half of $I(x)$, we obtain a new function going through all the points at half height of the original solution (4). In general, we can define on a generic oscillating function $f(x)$, an operation $<< f^2 >>$ that calculates this half height function (HHF) that we will call the "HHF average".

$$HHF = << [f(x)]^2 >> = \frac{I(x)}{2}. \tag{5}$$

that in our particular case gives

$$<< |\psi|^2 >> = Q(x). \tag{6}$$

This result can be used to define the quantum velocity v_q of a bouncing ball this way

$$v_q(x) = \frac{2}{\tau|\psi(x)|^2} \tag{7}$$

and it represents only that the quantum velocity field that, using (6), corresponds to the classical field $v_c(x) = \sqrt{2(E - V(x))/m}$ of Equation (2).

On the other hand, the usual formula defining the velocity in the de Broglie–Bohm interpretation of quantum mechanics [4–9] is

$$\vec{v} = \frac{\vec{J}}{\rho} = \frac{\hbar}{2im}\frac{\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*}{\psi\psi^*} \tag{8}$$

that can be derived from the continuity equation

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0 \tag{9}$$

It is well known [10] that the integral form of this equation is

$$\frac{d}{dt}\int_V \rho dV + \int_S \vec{J}\cdot\hat{n}dS = 0 \tag{10}$$

where V is the volume contained in the closed surface S.

In electromagnetism, the continuity equation is interpreted in light of the conservation of the charge, and it can be concluded that if in a volume surrounded by a closed surface there is a decrease in the charge in an interval of time, this charge must have passed through the surface as a flux of current density. By analogy with this point of view, in quantum mechanics, there is a conservation of probability. Hence, if in a volume of space the probability of finding a particle decreases, then the probability that this particle has crossed the surface, which is the boundary of that volume, increases.

Of course, the standard approach of Equation (8) leads to a vanishing current density in the case of the stationary states of the bouncing ball that are real wave functions ($\psi = \psi^*$) and do not allow to recover the velocity (7). However, in the paper of 1953 [1], regarding the similar case of a particle in a box of perfectly reflecting walls, Einstein felt that the prediction of a vanishing momentum "violated physical intuition which, for him, required the particle move back and forth" [11]. The answer of Bohm and Hiley [11] to Einstein's objection started from the consideration that "even when the quantum number is high, the wave function has a distribution of nodes, where there is zero probability of finding the particle". The prediction of the theory that "p = 0 is clearly a possibility that is consistent with nodes. Certainly, equiprobability of opposing velocities is not". Is it possible to conciliate the existence of nodes with an oscillatory motion of the particle? On this question, a more detailed discussion can be found in ref. [12].

In order to solve this problem, in the previous paper [2], we have proposed a correction in the expression of the probability current that, in three dimensions, we can write as follows

$$\overrightarrow{J} = \frac{\hbar}{2im}\left[\psi^*\overrightarrow{\nabla}\psi - \psi\overrightarrow{\nabla}\psi^* + \overrightarrow{F}\right] \tag{11}$$

because in the demonstration of the continuity equation in quantum mechanics, there is the freedom to add an arbitrary vector $\overrightarrow{F}(t) = (F_x, F_y, F_z)$ to the standard expression of $\vec{J}$. The consequence is that, even in the case of real wave functions, the probability current is no longer vanishing. A similar result can also be obtained either generalizing the momentum operator Appendixs A and B) or applying a suitable transformation to the wave function (Appendix C).

In particular, for the bouncing ball

$$\vec{v}_q = \frac{\hbar\vec{F}}{2im|\psi|^2} = \frac{\hbar F_x}{2im|\psi|^2}\hat{x} = \pm\frac{2}{\tau|\psi|^2}\hat{x}. \tag{12}$$

and we have

$$F_x = f(t)\frac{4im}{\hbar\tau} \tag{13}$$

where $f(t) = 1$ for $0 < t < \tau/2$ and $f(t) = -1$ for $\tau/2 < t < \tau$ so that $f(t)$ is a square wave that alternates between +1 and -1 with period τ.

From Equation (12), when there is a node in the wave function, the quantum velocity $v_q \to \infty$. Hence, in a node, the probability of finding the particle is zero because the ball acquires at that point an infinite velocity that forbids the ball from remaining long enough to be detected. In this way, our correction of the formula of quantum velocity allows an oscillating motion of the particle even in the quantum regime.

Of course, the quantum velocity tends to infinity in the non-relativistic approximation. A relativistic extension of our model is far beyond the aim of this paper, and in a relativistic framework the probability current is defined in four-dimensional spacetime $J^\mu = \rho u^\mu$ in terms of the four-velocity $u^\mu = \frac{dx^\mu}{d\tau}$ where $d\tau$ is the interval of proper time. In this case, u^μ tends to infinity when $v = \frac{dx}{dt}$ tends to the speed of light. Furthermore, the de Broglie–Bohm interpretation of quantum mechanics has some unsolved problems in its relativistic version that are briefly summarized in [13]. On the other hand, the problem of uniqueness of probability current also in the relativistic domain has been faced by Holland in a very interesting paper [14] and by several authors in other previous publications [15–17].

Furthermore, from the result (13), we can deduce a more general property of the vector $\overrightarrow{F}(t)$. Even if it could be, in principle, an arbitrary function of time, the constraint (6) that allows the classical velocity (2) to be recovered from the quantum velocity (7) requires that

$$\overrightarrow{F}(t) = g(t)(B, C, D) \tag{14}$$

where $g(t)$ can have alternatively only the values +1 and -1 (just as the square wave $f(t)$) and B, C and D are constants and the dependence on time regards only the direction of the vector but not its magnitude. This result is confirmed by a demonstration (reported in the Appendix A) obtained by one of us following a different approach [18]. Now, the problem is which way the constants can be determined. Knowing that there will be other possible approaches to the problem of velocity in de Broglie–Bohm quantum mechanics (see, for example, the recent papers of refs. [19,20]), our proposal is to consider a suitable normalization of the probability current.

2. Determination of the Arbitrary Function

In the previous paper [2], we did not derive the Formula (13) from the typical equations of quantum mechanics but from the comparison of the Equation (12) with the expression (7) and the correspondence with its classical analogue (2). Our aim is to justify the solution (13) regarding the bouncing ball, in light of the modified probability current (11), and to suggest also a way to determine the new function F(t) in similar cases. Of course, it would be useful to find a procedure which is valid in general, for all possible physical contexts, but this is beyond the scope of this paper. We know that the arbitrary constant that represents the amplitude of the wave function (derived solving the Schrödinger equation) can be determined case by case, only recurring to an extra condition that is to the constraint

$$\int_V |\psi|^2 dV = 1 \tag{15}$$

In the same way, we can propose a suitable normalization condition that can fix the arbitrary function $F(t)$ in the expression of probability current.

The intuitive interpretation [10] of

$$\vec{J} \cdot \hat{n} dS dt \tag{16}$$

as the probability that a particle crosses the surface element dS in the time dt does not always work because this expression may be negative [21]. Hence, only if the relation (16) is non negative, it can represent a probability, and only in that case can we define the probability that a particle has crossed the surface S in the direction $\hat{n}$ during an interval of time $\Delta t = t_2 - t_1$, the integral of (16) over that surface and that time interval [10]

$$P(S, \hat{n}) = \int_S \int_{t_1}^{t_2} \vec{J} \cdot \hat{n} dS dt \tag{17}$$

In one spatial dimension, the wave function $\psi(x,t)$ has the dimension of $[length]^{-1/2}$, and the probability current has the dimension of $[time]^{-1}$. So, we can propose as the one dimensional expression of (17)

$$P(a, \hat{n}) = \int_{t_1}^{t_2} \vec{J}(a,t) \cdot \hat{n} dt \tag{18}$$

that can be interpreted as the probability that the particle crosses the point $x = a$ in the direction $\hat{n}$. On the x-axis, the normal $\hat{n}$ can have only two possible directions; hence, if the result of the integral is negative, it is enough to invert the direction of the normal to make it positive and suitable to be interpreted as a probability.

We can apply this interpretation to the case of the bouncing ball. From the classical point of view, there are limits for the ball dynamics both in space (from $x = 0$ to $x = h$ and vice versa) and in time (from $t = 0$ and $t = \tau/2$ for the first part of the path and from $\tau/2$ to τ for the descending part). In the transition from classical to quantum regime, it means that there is an equation of normalization of probability density

$$\int_0^\infty |\psi|^2 dx = 1 \tag{19}$$

but also that the probability that the particle crosses a given point a belonging to the interval $[0, h]$ in a time $\tau/2$ is $P(a, \hat{n}) = 1$. From Equation (18), we obtain the normalization condition

$$P(a, \hat{n}) = \int_0^{\tau/2} \vec{J}(a, t) \cdot \hat{n} dt = 1 \tag{20}$$

If we use the standard formula for the probability current, the result of the integral is vanishing, leading to a paradox of a bouncing ball that does not move but that can be found at rest in a given position $x = a$ belonging to the interval $[0, h]$. On the contrary, if we adopt our modified Formula (11), we obtain

$$P(a, \hat{n}) = \frac{\hbar}{2im} \int_0^{\tau/2} \vec{F}(t) \cdot \hat{n} dt = 1 \tag{21}$$

that holds for each position $x = a$ in the interval $[0, h]$. At this point, remembering the discussion at the end of the previous section, we consider from Equation (18) that F(t) is a constant B during this interval of time; hence, in the present case, it is easy to calculate

$$B = \frac{4im}{\hbar\tau}. \tag{22}$$

Of course, in the interval of time $[\tau/2, \tau]$ the particle reverses direction, but the magnitude of the function $F(t)$ remains the same because it derives from

$$P(a, \hat{n}_1) = \frac{\hbar}{2im} \int_{\tau/2}^{\tau} \vec{F}(t) \cdot \hat{n}_1 dt = 1 \tag{23}$$

where $\hat{n}_1 = -\hat{n} = -\hat{x}$. Putting together those results, we finally obtain the expression of the function $F(t) = f(t)B$ written in Equation (13) using the probabilistic approach of quantum mechanics by imposing a suitable normalization condition on the probability current.

Of course, the procedure followed for the bouncing ball can be applied in other similar cases, such as the harmonic oscillator.

3. Harmonic Oscillator

It is very easy to apply our model to the case of the harmonic oscillator. The classical potential is

$$V = \frac{1}{2} k x^2, \tag{24}$$

and the classical total energy is

$$E_{cl} = \frac{1}{2} k A^2, \tag{25}$$

where A is the maximal amplitude of oscillation in

$$x_{cl}(t) = A \cos(\omega t + \varphi) \tag{26}$$

and the period is

$$\tau = \frac{2\pi}{\omega} = 2\pi \sqrt{\frac{m}{k}}. \tag{27}$$

The corresponding classical probability density is

$$Q(x) = \frac{1}{\pi\sqrt{A^2 - x^2}} \tag{28}$$

such that the relation

$$Q(x) = \frac{2}{\tau v_c(x)} \tag{29}$$

holds and

$$v_c(x) = \sqrt{\frac{2(E-V)}{m}}. \tag{30}$$

In the quantum regime, the solution of the Schrödinger equation using WKB approximation is

$$\psi(x) = \frac{D}{\sqrt{K(x)}} \cos\left[\int_{-A}^{x} dz K(z) + \varphi\right] \tag{31}$$

where

$$K(x) = \frac{\sqrt{2m(E-V(x))}}{\hbar} = \frac{\sqrt{km(A^2-x^2)}}{\hbar}. \tag{32}$$

We underline that the WKB approximation fails at the classical turning points $x = A$ and $x = -A$ and that there are two different WKB solutions: one for the classical region $-A < x < A$ and another one for the classically forbidden region. Since our aim is only to show a simple application of our model, we restrict our study only to the classical region.

Hence,

$$\psi(x) = \frac{D}{\sqrt[4]{\frac{km}{\hbar^2}(A^2-x^2)}} \cos\left[\int_{-A}^{x} dz \left(\frac{\sqrt{km}}{\hbar}\right)\sqrt{A^2-z^2} + \varphi\right] \tag{33}$$

and the wave function satisfying the Langer boundary condition at the turning point in $x = -A$ is [22]

$$\psi(x) = \frac{D}{\sqrt[4]{\frac{km}{\hbar^2}(A^2-x^2)}} \cos\left[\frac{1}{2}\frac{\sqrt{km}}{\hbar}\left(x\sqrt{A^2-x^2} + A^2 \arctan\left(\frac{x}{\sqrt{A^2-x^2}}\right) + \frac{\pi}{2}\right) - \frac{\pi}{4}\right] \tag{34}$$

From the normalization condition (15) we can determine the constant

$$D = \sqrt{\frac{2km}{\pi\hbar}} \tag{35}$$

so that

$$|\psi|^2 = \frac{2}{\pi\sqrt{A^2-x^2}} cos^2\left[\frac{1}{2}\frac{\sqrt{km}}{\hbar}\left(x\sqrt{A^2-x^2} + A^2 \arcsin\left(\frac{x}{A}\right) + \frac{\pi}{2}\right) - \frac{\pi}{4}\right] \tag{36}$$

where $A^2 = 2E_n/k$ and $E_n = \hbar\omega(n+1/2)$. Applying the correction to the probability current proposed in Equation (11) and the normalization condition (20), we also obtain in the case of the harmonic oscillator the result (22) where τ is given now by Equation (27). The consequence is that the quantum velocity is:

$$|\vec{v}_q| = \frac{\hbar F_x}{2im|\psi|^2} = \frac{\hbar B}{2im|\psi|^2} = \frac{2}{\tau|\psi(x)|^2}. \tag{37}$$

We have also shown that for the harmonic oscillator, in the WKB approximation, the formula of quantum velocity (37) (proposed by us in a previous paper [2]) holds. This formula was developed considering the classical Formula (2) and substituting the classical probability density $Q(x)$ with the quantum one $|\psi|^2$, noting that $<< |\psi|^2 >>= Q(x)$.

4. Conclusions

We have described the problems connected with the definition of velocity in the de Broglie–Bohm interpretation of quantum mechanics, and we have suggested a way to generalize the concept of probability current at least for the bouncing ball and similar cases of one dimensional periodic motions. Our model can conciliate the oscillatory motion with the existence of nodes of the wave function. We explicitly examined the case of the harmonic oscillator.

Author Contributions: Conceptualization, A.F.; methodology, A.F., A.L.I. and E.B.; formal analysis, A.F., A.L.I. and E.B.; investigation, A.F., A.L.I. and E.B.; resources, A.F., A.L.I. and E.B.; writing—original draft preparation, A.F., A.L.I. and E.B.; writing—review and editing, A.F., A.L.I. and E.B.; supervision, A.F.; funding acquisition, A.F. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by research funds of the University of Sannio.

Data Availability Statement: No datasets were generated or analyzed during the current study.

Conflicts of Interest: The authors declare no conflicts of interest.

Appendix A

We briefly summarize in this appendix the demonstration made by one of us [18] to obtain a nonvanishing momentum in the case of real wave functions R as solutions of the time-independent Schrödinger equation. Following Dirac [23], the momentum operator can be written

$$\hat{P}_x = -i\hbar\frac{\partial}{\partial x} + f(x) \tag{A1}$$

where $f(x)$ is an arbitrary real function. The time-independent Schrödinger equation, in one dimension

$$\frac{\hat{p}^2}{2m}\psi + V\psi = E\psi \tag{A2}$$

becomes

$$\frac{1}{2m}\left[-i\hbar\frac{\partial}{\partial x} + f(x)\right]\left[-i\hbar\frac{\partial}{\partial x} + f(x)\right]\psi + V\psi = E\psi \tag{A3}$$

Assuming that $\psi = R(x)$ is a real function, the previous equation splits into a real part:

$$\frac{1}{2m}\left[-\hbar^2\frac{\partial^2 R}{\partial x^2} + f(x)^2 R\right] + VR = ER \tag{A4}$$

and an imaginary part:

$$-\frac{\partial f}{\partial x}R - 2f(x)\frac{\partial R}{\partial x} = 0 \tag{A5}$$

Considering the last equation, we have

$$-\frac{dln|f|}{dx} = 2\frac{dln|R|}{dx} \tag{A6}$$

Through integration, we obtain the solution:

$$|f| = \frac{A}{|R|^2} \tag{A7}$$

where A is a positive arbitrary constant. Hence, the Equation (A4) becomes

$$\frac{f(x)^2}{2m} = E - V + \frac{\hbar^2}{2m}\frac{1}{R}\frac{\partial^2 R}{\partial x^2} \tag{A8}$$

where the first term can be interpreted as the kinetic energy in which the momentum is

$$p = \pm f(x) = \pm\frac{A}{|R|^2} \tag{A9}$$

Appendix B

In this appendix, we show some properties of the generalized momentum operator (A1) used in the Appendix A. First of all, the operator (A1) is hermitian (self-adjoint):

$$< \psi|\hat{P}_x\phi > = \int_a^b dx\psi^*\left(-i\hbar\frac{\partial\phi}{\partial x}\right) + \int_a^b \psi^* f(x)\phi dx$$
$$= [-i\hbar(\psi^*\phi)]_a^b - \int_a^b dx\left(-i\hbar\frac{\partial\psi^*}{\partial x}\right)\phi + \int_a^b f(x)\psi^*\phi dx. \quad \text{(A10)}$$

Therefore

$$< \psi|\hat{P}_x\phi > = \int_a^b dx\left(-i\hbar\frac{\partial\psi}{\partial x}\right)^*\phi + \int_a^b (f(x)\psi)^*\phi dx =< \hat{P}_x\psi|\phi >. \quad \text{(A11)}$$

The demonstration works if $f(x)$ is a real function and if ψ and ϕ are "wave functions that satisfy suitable boundary conditions. The conditions usually holding in practice are that they vanish at the boundaries" [23].

Finally, we find the relation of the operator (A1) with the corresponding generator of spatial translation that we denote d_x following the Dirac notation [23]. The translation of the position of an infinitesimal quantity δx is given by

$$\widehat{x}_d = \left(1 + \delta x\widehat{d}_x\right)\widehat{x}\left(1 - \delta x\widehat{d}_x\right) = \widehat{x} + \delta x\left[\widehat{d}_x, \widehat{x}\right] = \widehat{x} - \delta x\widehat{1} \quad \text{(A12)}$$

if

$$\left[\widehat{d}_x, \widehat{x}\right] = -\widehat{1}. \quad \text{(A13)}$$

The relation $\hat{P}_x = i\hbar\widehat{d}_x$ can be conserved because $\widehat{d}_x = -\frac{\partial}{\partial x} + \frac{f(x)}{i\hbar}$ satisfies (A13).

Appendix C

The transformation of the probability current

$$\overrightarrow{J} \to \overrightarrow{J}' = \overrightarrow{J} + \overrightarrow{G}(t) \quad \text{(A14)}$$

can also be obtained, avoiding changing the Formula (8) by which we usually calculate the velocity, by using a suitable transformation of the wave function

$$\psi \to \psi' = e^{\frac{i}{\hbar}S'}R = e^{\frac{i}{\hbar}(\alpha+S)}R \quad \text{(A15)}$$

in which

$$\overrightarrow{p} = \vec{\nabla}S' = \vec{\nabla}\alpha + \vec{\nabla}S = \frac{\overrightarrow{G}(t)}{R^2} + \vec{\nabla}S \quad \text{(A16)}$$

because

$$\overrightarrow{J} \to \overrightarrow{J}' = \overrightarrow{G}(t) + R^2\vec{\nabla}S = \overrightarrow{J} + \overrightarrow{G}(t). \quad \text{(A17)}$$

In this framework, all the equations of "the quantum theory of motion" of the "de Broglie–Bohm" interpretation

$$\frac{\partial S}{\partial t} + \frac{\left(\vec{\nabla}S\right)^2}{2m} + V - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} = 0 \quad \text{(A18)}$$

$$\frac{\partial R^2}{\partial t} + \vec{\nabla}\cdot\left(R^2\frac{\vec{\nabla}S}{m}\right) = 0. \quad \text{(A19)}$$

remain the same after substituting S with S'. Furthermore, the probability density R^2 is not affected by this transformation.

However, the really interesting case remains the one in which the time-independent Schrödinger equation has as a solution a real wave function [18]. This case, examined following the approach in the Appendix A, can lead to a modified Hamilton–Jacobi Equation (A8) whose solution R is such that there is no longer the equilibrium between classical and quantum potential invoked by Bohm [5,6] to explain the vanishing in each point of the quantum velocity field.

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