On the conditions for the classicality of a quantum particle

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Abstract

Conditions under which a quantum particle is described using classical quantities are studied. The one-dimensional (1D) and three-dimensional (3D) problems are considered. It is shown that the sum of the contributions from all quantum corrections (in the WKB sense) strictly vanishes, when a quantum particle interacts with some specific medium. The indices of refraction of such media are found. In this case, the smallness of the Planck constant is not assumed. The momenta of quantum particles in these media and the wave functions of stationary states are determined. It is found that, for the 1D case, there is a localization of the wave in the region of the order of a few de Broglie wavelengths for any finite energy of a quantum particle. For the 3D case with central symmetry, a stationary state, describing a quantum particle with a classical momentum, is defined by the wave function, which takes almost constant values in the region of small values of the index of refraction. The oscillations are damped smoothly with the increase of the index of refraction, so that, the wave packet is formed.

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1 Introduction

Despite the fact that, by now, the mathematical apparatuses of nonrelativistic and relativistic (field) quantum theories have been sufficiently developed with regard to their practical application to explain different physical phenomena, some fundamental questions about the relationship between quantum theory and classical physics still attract intense attention of physicists and mathematicians. In this context, let us mention here the important studies of recent decades, carried out by Nathan Rosen [1] and Gerard ’t Hooft [2].

In the present paper, the conditions under which a quantum particle has a classical momentum, while retaining its wave properties, are studied. By quantum particle, we mean a particle in a given force (potential) field, which is described by the Schrödinger equation. This equation can be reduced to the generalized Hamilton-Jacobi equation for the phase of the wave function [3]. The latter equation differs from the Hamilton-Jacobi equation of classical mechanics in that it contains a term nonlinear with respect to the phase and proportional to $\hbar^2$, which takes into account quantum effects. The WKB method, as is known, consists in expanding a nonlinear part of the generalized Hamilton-Jacobi equation in a series in powers of the Planck constant $\hbar$, followed by equating the terms of the series with the same powers of
The practical application of this method of solving the Schrödinger equation is limited by the conditions imposed on the behavior of the potential (or the reduced wavelength as a function of distance) and its derivatives, which provide a criterion for the validity of the method by evaluating the first of the discarded terms of the WKB asymptotic series [3,4].

However, instead of equating the terms of the asymptotic series with the same powers of $\hbar$ to each other, it is of interest to study the case, when the contributions from all terms of this infinite series are mutually compensated, so that the nonlinear part of the generalized Hamilton-Jacobi equation proportional to $\hbar^2$ strictly vanishes without the assumption of smallness of $\hbar^2$. Then the phase of the wave function is the classical action, whose gradient is the classical momentum of a particle. The wave properties of this particle in such a compensating (in above mentioned sense) medium are described by the second order partial differential equation. Introducing the index of refraction of this medium, created by the specific potential field, one can write the Sturm-Liouville equation equivalent to the Schrödinger equation which contains the de Broglie wavelength $\lambda = (\hbar^2 / 2mE)^{1/2}$ of a particle with the mass $m$ and the energy $E$. The Sturm-Liouville equation has an analytical solution for both one-dimensional (1D) and three-dimensional (3D) problems. Comparison of these solutions with each other allows one to see the difference in wave properties of a particle in 1D and 3D spaces.

In Sect. 2, the conditions for the classicality of a quantum particle in 1D space are studied. The one-dimensional Schrödinger equation is reduced to the one-dimensional nonlinear Hamilton-Jacobi equation for the phase of the wave function. An explicit form of the index of refraction of the medium created by the potential field, in which all quantum effects compensate each other, so that a quantum particle has a classical momentum, is obtained. The field creating such a compensating medium depends not only on the coordinate, but also on the energy of the particle and its mass. The properties of a particle are described by the wave localized in space on scales of the order of a few de Broglie wavelengths for given energy and mass of a particle. In Sect. 3, the conditions for the classicality of a quantum particle in 3D space are investigated. The three-dimensional Schrödinger equation is reduced to the three-dimensional nonlinear Hamilton-Jacobi equation for the phase of the wave function. For the three-dimensional case, an explicit form of the index of refraction of the medium, in which quantum effects are compensated, and the form of the potential field creating such a compensating medium in the case of central symmetry are found. The solutions of the corresponding Sturm-Liouville equation for the wave describing a particle in 3D space are obtained. Section 4 discusses the differences in behavior of particles in compensating media in 1D and 3D spaces.

2 1D problem

Let us consider one-dimensional motion (along the $x$-axis on the interval $x \in (-\infty, \infty)$) of a quantum particle with the mass $m$ and the energy $E$ in the field of the potential $V(x)$. In the case of stationary states, as is well known, the problem reduces to solving the Schrödinger equation, which can be conveniently rewritten in the form

$$\psi''(x) + \frac{1}{\lambda^2} n^2(x) \psi(x) = 0, \quad (1)$$
where $\tilde{\lambda} = \hbar p_0 = (h^2/2mE)^{1/2}$ is the de Broglie wavelength for a freely moving particle with the momentum $p_0$ and the energy $E = p_0^2/2m$, the primes denote differentiation with respect to the variable $x$, and the function

$$n(x) = \sqrt{\frac{E - V(x)}{E}}$$

has a meaning of the index of refraction of the medium, created by the potential $V(x)$.

We will look for a solution to the equation (1) in the form

$$\psi(x) = A(x) \exp \left( \frac{i}{\hbar} S(x) \right), \quad (3)$$

where the amplitude $A$ and the phase $S$ are real functions of $x$. Substituting Eq. (3) into Eq. (1) leads to the set of two differential equations \[4\],

$$\left( S' \right)^2 - \left( \frac{\hbar}{\tilde{\lambda}} \right)^2 n^2 = \frac{\hbar^2}{2} A'' / A, \quad 2A'S' + AS'' = 0.$$  \( (4) \)

The solution to the second equation is trivial: $A = C/\sqrt{S'}$, where $C = const$. As a result, we obtain the equation for a momentum $p \equiv S'$,

$$p^2 - \left( \frac{\hbar}{\tilde{\lambda}} \right)^2 n^2 = \frac{\hbar^2}{2} \left[ \frac{3}{2} \left( \frac{p'}{p} \right)^2 - \frac{p''}{p} \right],$$  \( (5) \)

in which all quantum effects are contained in the nonlinear right-hand side. The equation (5) is the generalized Hamilton-Jacobi equation. It is exact and equivalent to Eq. (1). Since $(\hbar/\tilde{\lambda})^2 = 2mE$, then, in a formal limit $\hbar \to 0$, Eq. (5) describes a motion of a classical particle with a momentum $p(x)$, expressed as a function of the coordinate $x$.

Expanding the right-hand side of Eq. (5) in a series in powers of $\hbar$, we get the asymptotic series (WKB method). Restricting to a finite number of terms in a series requires careful analysis of the value of the first discarded term (for details, see, for example, Refs. [3, 4]).

In this regard, we consider the exact solution of Eq. (5), which describes a quantum particle in the medium with the index of refraction (2). We shall assume that, when a particle is interacting with such a medium, the sum of contributions from all quantum corrections (in the WKB sense) strictly vanishes. In other words, these contributions mutually compensate when summing the whole infinite series in powers of $\hbar$. At the same time, the “smallness” of $\hbar^2$ is not supposed.

For further analysis, it is convenient to pass to dimensionless variables $\tilde{x} = x/\tilde{\lambda}$ and $\tilde{p} = \hbar \lambda p$. Omitting tildes in the notation of dimensionless quantities in what follows, and introducing a new unknown function $Q(x)$, such that

$$p = \exp Q, \quad (6)$$

we rewrite Eq. (5) in the form

$$\exp(2Q) - n^2 = \frac{1}{2} \left[ \frac{1}{2} (Q')^2 - Q'' \right], \quad (7)$$
where the primes denote differentiation with respect to the dimensionless variable $x$. From Eqs. (6) and (7), it follows that the momentum (6) will be the classical momentum of a particle for the function $Q$ satisfying the equation

$$Q'' - \frac{1}{2}(Q')^2 = 0.$$  

(8)

For the boundary condition $Q(1) = 0$, its solution is given by

$$Q = \ln \frac{1}{x^2}.$$  

(9)

It follows from here that the classical momentum is

$$p = \frac{1}{x^2} \quad \text{(or} \quad p = \frac{\hbar \chi}{x^2} \text{for dimensional quantities)},$$  

(10)

while the medium, in which such a particle is located, is characterized by the index of refraction

$$n = \frac{1}{x^2} \quad \text{(or} \quad n = \left(\frac{\chi}{x}\right)^2 \text{for dimensional quantities}).$$  

(11)

From Eq. (2), it follows that the potential $V(x)$ generating such a medium,

$$V(x) = E \left[1 - \left(\frac{\hbar^2}{2mE}\right)^2 \frac{1}{x^4}\right],$$  

(12)

is a function of not only the coordinate $x$, but also the energy $E$. For the values $\frac{\chi}{x} < 1$, we have $V(x) < 0$, while for $\frac{\chi}{x} > 1$, the potential is $V(x) > 0$, and $V(x = \chi) = 0$. Near $x \sim 0$, the potential $V(x) \sim \frac{E}{x^4}$. It tends to $E$ at $x \to \infty$.

The action of a particle with a classical momentum (10) is

$$S = -\frac{1}{x} = -px \quad \text{(or} \quad S = -\frac{\hbar \chi}{x} = -px \text{for dimensional quantities}).$$  

(13)

The solution of Eq. (1) with the boundary condition $\psi(0) = 0$ has a form

$$\psi(x) = D \left(\frac{x}{\chi}\right) \sin \left(\frac{\chi}{x}\right),$$  

(14)

where the constant $D = \psi(\infty)$.

The function (14) describes stationary states of a quantum particle with a given energy $E$ in the medium with the index of refraction (11). This function has a form of a wave localized on scales of the order of a few $\chi$ near $x = 0$. It is shown in Fig. 1.

Fig. 2 displays the function (14) in the variables $\zeta = \sqrt{\frac{2mE}{\hbar^2}}x$ and $\sqrt{E}$ having the dimensions $[\text{Energy}]^{-1/2}$ and $[\text{Energy}]^{1/2}$, respectively,

$$\psi(x) = \psi(\zeta, \sqrt{E}) = D\sqrt{E}\zeta \sin \left(\frac{1}{\sqrt{E}\zeta}\right).$$  

(15)

With increasing energy $E$, the localization region decreases for a given mass of a particle $m$. The wave shown in Fig. 1 gives a cross section of the function $\psi(\zeta, \sqrt{E})$ corresponding to a single value of $E$. 

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Figure 1: The wave (14) as a function of $x$ in units of the de Broglie wavelength $\lambda$ and for $D = 1$.

Figure 2: The wave (15) as a function of $\zeta = \sqrt{\frac{2m}{\hbar^2}}x$ and $\sqrt{E}$ for $D = 1$. 


3 3D problem

Let’s now turn to a quantum particle with the mass $m$ and the energy $E$ being
under the action of the potential $V(r)$, where $r$ is the radius vector drawn from
the origin to a particle, which is supposed to be point-like. The stationary Schrödinger
equation has a form

$$\nabla^2 \psi(r) + \frac{1}{\lambda^2} n^2(r) \psi(r) = 0,$$

where

$$n(r) = \sqrt{\frac{E - V(r)}{E}}$$

is the index of refraction of the medium created by the potential $V(r)$. We will seek
the solution of Eq. (16) in the form similar to (3),

$$\psi(r) = A(r) \exp \left( \frac{i}{\hbar} S(r) \right),$$

where the amplitude $A$ and the phase $S$ are real functions of $r$. Substituting Eq. (18)
into Eq. (16) and separating the real and imaginary parts, we obtain the set of two
equations for $A$ and $S$ (see Ref. [3]),

$$(\nabla S)^2 + \left( \frac{\hbar}{\lambda} \right)^2 n^2 = \frac{\hbar^2}{A} \nabla^2 A, \quad \nabla (A^2 \nabla S) = 0.$$  (19)

From the second equation, it follows that there exists such a vector function

$$F = A^2 \nabla S,$$  (20)

whose divergence vanishes,

$$\nabla F = 0.$$  (21)

Since the vectors $F$ and $\nabla S$ are collinear, then from Eq. (20) it follows the condition

$$A^2 (\nabla S)^2 = F|\nabla S|,$$  (22)

where $F = |F|$. From here, the amplitude is obtained,

$$A = \sqrt{\frac{F}{|\nabla S|}},$$  (23)

and Eq. (19) reduces to the nonlinear Hamilton-Jacobi equation for the momentum

$$p = \nabla S,$$

$$\left( \frac{p}{\hbar} \right)^2 - \frac{1}{\lambda^2} n^2 = \sqrt{\frac{p}{E}} \sqrt{\nabla^2 F} \sqrt{\frac{F}{p}},$$  (24)

where $p = |p|$. The right-hand side of this equation, which describes quantum
effects, is equal to

$$- \frac{1}{2} \left[ \frac{\nabla^2 p}{p} - \frac{3}{2} \left( \frac{\nabla p}{p} \right)^2 \right] + \frac{1}{\sqrt{F}} \nabla^2 \sqrt{F} + 2 \sqrt{\frac{p}{F}} \nabla \frac{1}{\sqrt{p}} \nabla \sqrt{F}.$$  (25)
The modulus of the vector $F$ in Eq. (24) is a function of the coordinate $r$. Under the assumption that $\sqrt{F}$ is a slowly varying function of $r$, such that $\nabla \sqrt{F} \approx 0$ and $\nabla^2 \sqrt{F} \approx 0$, Eq. (24) turns out to be independent of $F$,

$$p^2 - \left( \frac{\hbar}{\lambda} \right)^2 n^2 = \hbar^2 \sqrt{p} \nabla^2 \sqrt{1 \over p}. \quad (26)$$

Similarly to a one-dimensional problem, we define a momentum $p$ as

$$p(r) = \sqrt{2mE} \exp Q(r). \quad (27)$$

Then Eq. (26) will take the form more simple for further analysis

$$\exp(2Q) - n^2 = \frac{1}{2} \left[ \frac{1}{2} (\nabla Q)^2 - \nabla^2 Q \right]. \quad (28)$$

Here we have passed to dimensionless quantities $\tilde{r} = {r \over \lambda}$ and $\tilde{p} = \hbar \lambda p$ (below we omit tildes). Quantum effects do not affect a particle with a momentum $p$, if the unknown function $Q(r)$ satisfies the equation

$$\nabla^2 Q - \frac{1}{2} (\nabla Q)^2 = 0. \quad (29)$$

In the case of central symmetry, $Q = Q(r)$, Eq. (29) takes the form

$$\frac{\partial^2 Q}{\partial r^2} + 2 \frac{\partial Q}{r \partial r} - \frac{1}{2} \left( \frac{\partial Q}{\partial r} \right)^2 = 0. \quad (30)$$

Its partial solution with the boundary condition $Q(1) = 0$ is following

$$Q = \ln r^2. \quad (31)$$

The classical momentum of a quantum particle is

$$p = r^2, \quad (32)$$

and the action equals to

$$S = \frac{1}{3} r^3 = \frac{1}{3} pr. \quad (33)$$

They satisfy the boundary conditions: $p(0) = 0$ and $S(0) = 0$.

The index of refraction is

$$n = r^2 \quad (34)$$

(cp. with Eq. (11) for the 1D problem). In the case of central symmetry, Eq. (16) with the index of refraction (34) simplifies

$$\frac{\partial^2 \psi}{\partial r^2} + 2 \frac{\partial \psi}{r \partial r} + r^4 \psi = 0. \quad (35)$$

Its solution has a form

$$\psi(r) = \frac{1}{\sqrt{6} \sqrt{\gamma}} \left\{ C_1 \Gamma \left( \frac{5}{6} \right) J_{-1/6} \left( \frac{r^3}{3} \right) + C_2 \Gamma \left( \frac{7}{6} \right) J_{1/6} \left( \frac{r^3}{3} \right) \right\}, \quad (36)$$

1Here we restrict ourselves to considering only the $s$ state.
where $C_1$ and $C_2$ are constants of integration, $\Gamma$ is the Gamma function, $J_\alpha$ is the Bessel function of fractional order $\alpha = \pm 1/6$.

Near the origin, we have

$$
\psi(r \sim 0) \sim \frac{C_1}{r} + \frac{C_2}{\sqrt{6}}. \tag{37}
$$

Retaining only a regular solution that corresponds to the choice $C_1 = 0$, we find that the function $\psi$ is constant at the origin,

$$
\psi(r = 0) = \frac{C_2}{\sqrt{6}}. \tag{38}
$$

At $r \to \infty$, the function $\psi$ oscillates and slowly tends to zero in accordance with the exact expression

$$
\psi(r) = \frac{C_2}{\sqrt{6} \sqrt{r}} \frac{1}{\sqrt{r}} \Gamma \left( \frac{7}{6} \right) J_{1/6} \left( \frac{r^3}{3} \right). \tag{39}
$$

It describes the stationary state of a quantum particle with the given energy $E$ in the medium with the index of refraction (34) created by the potential

$$
V(r) = E \left[ 1 - \left( \frac{2mE}{\hbar^2} \right)^2 r^4 \right] \tag{40}
$$

(in physical units). It depends on the energy $E$ and is an alternating function of $r$: $V(r) < 0$ for $\left( \frac{r}{\lambda} \right)^4 > 1$, $V(r) > 0$ for $\left( \frac{r}{\lambda} \right)^4 < 1$, and vanishes at $r = \lambda$.

Fig. 3 shows the function (39), where $r$ is expressed in units of $\lambda$. This function is almost constant in the region $r < 1$, where the index of refraction (34) is small. In the region $r > 1$, the medium damps the oscillations, whose amplitude decreases as $r^{-2}$ for $r \to \infty$. The amplitude of the corresponding wave is largest near $r = 0$ and the function (39) has the form of a wave packet.

The behavior of the wave (39) as a function of energy and distance from the origin is given in Fig. 4. The same variables $\zeta = \sqrt{\frac{2m}{\hbar^2}} r$ and $\sqrt{E}$ are used as for the
\[
\psi(\zeta, \sqrt{E}) = C_2 \frac{1}{\sqrt{6}} \sqrt{\frac{1}{\zeta \sqrt{E}}} \Gamma \left( \frac{7}{6} \right) J_{1/6} \left( \frac{1}{3} (\zeta \sqrt{E})^3 \right). \tag{41}
\]

With increasing $\zeta$ and/or $E$, the amplitude of this oscillating wave decreases as $\zeta^{-2}$ and/or $E^{-1}$, respectively. Fig. 3 is a cross section of the wave $\psi(\zeta, \sqrt{E})$ corresponding to a given energy $E$.

4 Conclusion

In the present paper, we study the behavior of a quantum particle, when all quantum corrections (in the sense of the WKB series) are strictly compensated. This is possible only for potential fields of a special kind (see Eqs. (12) and (40) for the 1D and 3D problems, respectively). The corresponding potentials depend not only on the distance from the origin, but also on the energy of the stationary state of a quantum particle. The Schrödinger equations (11) and (16) are reformulated in terms of the indices of refraction $n$ (111) and (34) of the media created by the potentials $V$ (12) and (40), respectively. In such media, strict compensation of quantum corrections from nonlinear part of the Hamilton-Jacobi equations (5) and (24) occurs. The equations (11) with (111) and (16) with (34) admit exact analytical solutions in the form of Eqs. (14) and (39). These solutions demonstrate differences in the wave properties of a quantum particle in the 1D and 3D cases. The wave (14) is localized on scales of a few de Broglie wavelengths $\lambda$ for any energy $E$ of the stationary state of a quantum particle. In the 3D case, the amplitude of the wave (39) is largest near the origin. The amplitude smoothly decreases in the region
$r \gg 1$, where the index of refraction, given by Eq. (34), increases according to the quadratic law. The function (39) has the form of a wave packet.

The differences in the wave properties of quantum particles in the 1D and 3D spaces can be explained by the different forms of the potentials (12) and (40) which generate the corresponding compensating media. For the 1D problem, the potential energy (12) takes large negative values according to $V(x) \sim -E(\lambda/x)^4$ in the region $x \ll \lambda$ ensuring the attraction of a particle to the origin. This leads to the localization of the wave in the region of the order of a few de Broglie wavelengths. The potential energy (40) of the 3D problem as a function of distance $r$ is constant, $V(r) \sim E$ for $r \ll \lambda$, and tends to negative values in accordance with $V(r) \sim -E(r/\lambda)^4$ for $r \gg \lambda$. As a result, the compensating medium with the index of refraction (34) composes the wave structure (39) in the form of a wave packet.

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