

# Classical mechanics and the propagation of the discontinuities of the quantum wave function

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Geometrical optics can be regarded both as the short-wavelength approximation of the propagation of electromagnetic waves, and as the exact way in which propagate the surfaces of discontinuity of the classical electromagnetic field. In this work we translate this last idea to quantum mechanics (both relativistic and nonrelativistic). We find that the surfaces of discontinuity of the wave function propagate exactly following the classical trajectories determined by the Hamilton-Jacobi equation. As an example, we consider the lack of diffraction of abrupt wave fronts.

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In physics, as in many other areas of science, partially contradicting theories can coexist, such as quantum versus classical mechanics and geometrical versus electromagnetic optics as two paradigmatic examples. The question of their mutual relationship is a basic and critical issue imposed by the consistency of science. This question is specially vivid concerning the relation between classical and quantum mechanics, which has been a subject of active research and controversy from the very beginning of the quantum theory till the present day. It is generally accepted that both classical mechanics and geometrical optics are approximations valid for short wavelengths [1,2]. However, in optics another radically different approach is possible: geometrical optics is the *exact* way in which the surfaces of field discontinuity propagate, irrespective of the magnitude of the wavelength [3]. In this paper we translate this approach from optics to mechanics showing that classical mechanics is the exact way in which the discontinuities of the quantum wave function propagate.

First we recall the basic tools required to address the propagation of discontinuities in optics as well as in quantum mechanics. For both situations, we will consider that the evolution is given by the solution of a system of linear partial differential equations:

$$\sum_{\mu,\nu} \frac{\partial}{\partial x^\mu} (M_j^{\mu,\nu} \psi_\nu) = 0, \quad (1)$$

where  $x^\mu = x, y, z, t$  are the space-time coordinates,  $M_j^{\mu,\nu}$  are functions of  $x^\eta$ , and  $\psi_\nu(x^\mu)$  are the Cartesian components either of a spinorial quantum wave function or of a classical electromagnetic field.

As discussed in Ref. [3], Eqs. (1) are conditions for the components  $\psi_\nu$  at every point where they are continuous, but they cannot establish conditions for the boundary values of  $\psi_\nu$  on a surface of discontinuity. Therefore, in order to deal with discontinuities, it is advantageous to replace Eqs. (1) by integral counterparts. To this end we consider volume integrals of Eq. (1) which can be then suitably converted into surface integrals with the use of the divergence theorem, as carried out in Ref. [3]:

$$\int_\Gamma d\Gamma \sum_{\mu,\nu} \frac{\partial}{\partial x^\mu} (M_j^{\mu,\nu} \psi_\nu) = \sum_{\mu,\nu} \int_\sigma d\sigma_\mu M_j^{\mu,\nu} \psi_\nu = 0, \quad (2)$$

where  $d\Gamma = dx dy dz dt$  is the differential of four-dimensional volume and  $d\sigma_\mu$  are the Cartesian components of the surface element normal to the three-dimensional surface  $\sigma$  enclosing  $\Gamma$ . The last equality in Eq. (2) is fully equivalent to Eq. (1) when  $\psi_\nu$  are continuous. On the other hand Eq. (2) is more general since it can be applied without difficulties when  $\psi_\nu$  are discontinuous.

The objective is to derive conditions for the discontinuities of  $\psi_\nu$  by imposing Eq. (2). Denoting by  $S(x,t)=0$  the surface of discontinuity, we apply Eq. (2) to two volumes  $\Gamma_1, \Gamma_2$  connected by  $S$ , as well as to the whole volume  $\Gamma_1 + \Gamma_2$  (see Fig. 1). This leads to

$$\sum_{\mu,\nu} [\psi_\nu] \frac{\partial S}{\partial x^\mu} M_j^{\mu,\nu} = 0, \quad (3)$$

where  $[\psi_\nu]$  denotes the difference between the boundary values of  $\psi_\nu$  at the two sides of  $S$ . For the sake of definiteness, we have assumed that  $M_j^{\mu,\nu}$  are continuous at  $S$ . These are the conditions we were looking for.

This formalism can be applied directly to optics provided that the light propagates in the vacuum or in a nondispersive linear media in absence of free charge and currents. For dispersive media, we have to restrict ourselves to time-harmonic waves. In such a case, the Maxwell equations can be recasted in the form (1) being  $M_j^{\mu,\nu}$  proportional to the dielectric constant and the magnetic permeability. Expressing  $S$  on the form  $S(x,t) = L(x) - ct$ , this formalism leads to the eikonal equation (for isotropic media for simplicity) [3]

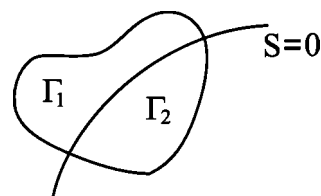


FIG. 1. Diagram illustrating the volumes  $\Gamma_1$  and  $\Gamma_2$  joined by the surface of discontinuity  $S=0$ .

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$$(\nabla L)^2 = n^2, \quad (4)$$

where  $n$  is the index of refraction. This equation implies that the surface of discontinuity propagates along the rays of geometrical optics [2,3].

Next we turn our attention to the quantum case. Since we are dealing with first-order partial differential equations we can begin with relativistic propagation equations:

$$i\hbar \frac{\partial \Psi}{\partial t} = \left( \sum_{j=1}^3 -i\hbar c \alpha_j \frac{\partial}{\partial x^j} + mc^2 \beta + V(\mathbf{x}) \right) \Psi, \quad (5)$$

where  $\Psi(\mathbf{x}, t)$  is a vector wave function, and  $\alpha_j, \beta$  are constant matrices satisfying

$$(c\boldsymbol{\alpha} \cdot \mathbf{p} + mc^2 \beta)^2 = c^2 \mathbf{p}^2 + m^2 c^4, \quad (6)$$

for any real three-dimensional vector  $\mathbf{p}$ , where  $\boldsymbol{\alpha}$  is a vector notation for the three matrices  $\alpha_j$ .

At this stage we cannot apply directly the above formalism because the inhomogeneous term  $(mc^2 \beta + V)\Psi$  impedes to express Eq. (5) on the form (1). As in classical optics we can avoid this difficulty by restricting our analysis to time-harmonic wave functions for which

$$\Psi(\mathbf{x}, t) = \frac{i\hbar}{E} \frac{\partial \Psi(\mathbf{x}, t)}{\partial t}, \quad (7)$$

in some volume  $\Gamma$ , where  $E$  is a constant. Using this condition we can express Eq. (5) as

$$\left[ c \sum_{j=1}^3 \alpha_j \frac{\partial}{\partial x^j} + (E - mc^2 \beta - V) \frac{1}{E} \frac{\partial}{\partial t} \right] \Psi = \mathbf{0}, \quad (8)$$

which is already of the form (1). Then, the application of Eq. (3) leads to

$$\left( Ec\boldsymbol{\alpha} \cdot \nabla S - mc^2 \beta \frac{\partial S}{\partial t} \right) [\Psi] = (V - E) \frac{\partial S}{\partial t} [\Psi]. \quad (9)$$

Squaring the above equation and using Eq. (6) we get

$$E^2 c^2 (\nabla S)^2 + m^2 c^4 \left( \frac{\partial S}{\partial t} \right)^2 = (V - E)^2 \left( \frac{\partial S}{\partial t} \right)^2, \quad (10)$$

whenever  $[\Psi] \neq \mathbf{0}$ . Since the Hamiltonian we are considering is time independent, we can use the method of separation of variables to separate out the time in the form  $S(\mathbf{x}, t) = W(\mathbf{x}) - Et$ . From Eq. (10) we get

$$E = \sqrt{c^2 (\nabla W)^2 + m^2 c^4} + V. \quad (11)$$

In the nonrelativistic limit  $|\nabla W| \ll mc$  so that

$$E - mc^2 \approx \frac{(\nabla W)^2}{2m} + V. \quad (12)$$

Equations (11) and (12) are the main result of this paper. We have found that the surface of discontinuity of harmonic wave functions must satisfy the classical Hamilton-Jacobi

equation for the relativistic Hamiltonian  $H = \sqrt{c^2 \mathbf{p}^2 + m^2 c^4} + V(\mathbf{x})$  or  $H = \mathbf{p}^2 / (2m) + V(\mathbf{x})$  in the nonrelativistic limit. Therefore, the surfaces where the wave function is discontinuous evolve following classical trajectories [4]. The result is exact since no approximation nor limiting procedure whatsoever have been used.

This behavior parallels the optical case. The main difference is that mechanics always includes inhomogeneous source terms that are the origin of the dispersive character of the quantum propagation of massive particles. As it occurs in optics, the dispersion limits the generality of the approach and force us to consider just harmonic waves.

It is important to stress that the condition (7) does not necessarily implies that  $\Psi$  is a stationary state. For instance we can have  $\Psi(\mathbf{x}, t) = A_1(\mathbf{x}) e^{-iEt/\hbar}$  in a given volume  $\Gamma_1$  and  $\Psi(\mathbf{x}, t) = A_2(\mathbf{x}) e^{-iEt/\hbar}$  in a different volume  $\Gamma_2$  being  $A_1, A_2$  two different eigenfunctions of a Hamiltonian with a degenerate eigenvalue  $E$ . Moreover we may have  $A_1 = \mathbf{0}$ .

As a particular example supporting the above results we can invoke the lack of diffraction of a beam of free particles having an abrupt leading edge (the discontinuity) caused by the opening or closing of an absorbing shutter. Such a situation can be addressed following the approach of Ref. [5] where this problem is examined in the optical domain leading to the conclusion that the front of the wave propagates without distortion or diffraction [5,6] (the so-called electromagnetic missiles).

The main difference between matter and light is the different dispersion relation. However, as discussed in Ref. [5], the propagation of the front of the wave is determined by the highest frequencies, and in such a limit the two dispersion relations tend to coincide. In the quantum case this lack of diffraction is a signature of classical propagation. The relativistic character of the beam of particles appears to be essential. The nonrelativistic propagation is so strongly dispersive that the discontinuity would hardly survive the evolution [7].

Incidentally, let us note that the approximate relation (short-wavelength limit) may be regarded as being included in the exact relationship (propagation of discontinuities) as a particular case. When the wavelength tends to zero the wave passes from maximum to minimum in increasingly short space-time distances. Loosely speaking, this might be understood as some kind of effective discontinuity taking place at every point.

Finally, we show that it is possible to arrive directly to the nonrelativistic result (12) from the scalar Schrödinger equation for time-harmonic wave functions after splitting it in two equations

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla \cdot \Phi + V \frac{i\hbar}{E} \frac{\partial \psi}{\partial t}, \quad (13)$$

$$\frac{i\hbar}{E} \frac{\partial \Phi}{\partial t} = \nabla \psi,$$

where the last equation defines  $\Phi$  and we have used the condition (7) for  $\Phi$  and  $\psi$ . The application of Eq. (3) leads to

$$i(E-V)\frac{1}{E}[\psi]\frac{\partial S}{\partial t} = -\frac{\hbar}{2m}[\Phi]\cdot\nabla S, \quad (14)$$

$$\frac{i\hbar}{E}[\Phi]\frac{\partial S}{\partial t} = [\psi]\nabla S.$$

The elimination of the discontinuities  $[\Phi]\neq\mathbf{0}$ ,  $[\psi]\neq 0$  and the separation of the time  $S=W-Et$  leads directly to Eq. (12).

For completeness we quote other approaches looking also for exact coincidence between classical and quantum motions. The evolution of the wave function is governed by classical Hamilton-Jacobi equations with the addition of extra potential terms called quantum potentials. There are particular dynamical systems where the quantum potential is constant so that quantum and classical evolutions coincide [8]. Other investigations concerning the relation between relativistic quantum mechanics and the classical electromagnetic field can be found in Ref. [9].

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