

BOUNDARY CONDITIONS IN TUNNELING VIA QUANTUM HYDRODYNAMICS

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Abstract

Via the hydrodynamical formulation of quantum mechanics, a novel approach to the problem of tunneling through sharp-edged potential barriers is developed. Above all, it is shown how more general boundary conditions follow from the continuity of mass, momentum, and energy.

1 Introduction

A commonly used assumption in quantum mechanics [1,2,3,4] is that the boundary conditions on a surface σ where the potential undergoes a finite jump reduce to the requirement that both the wave function (ψ) and its derivative ($\partial\psi/\partial x$) be continuous on σ . We show below through the hydrodynamical formulation of quantum mechanics how more general boundary conditions follow from the continuity of mass, momentum, and energy densities. With these new boundary conditions, a novel approach to tunneling through sharp-edged potential barriers is presented.

2 Formulation

Let us consider the dynamics of a quantum particle described by the coupled hydrodynamical equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v)}{\partial x} = 0, \quad (1)$$

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} + \frac{1}{m} \frac{\partial(V + V_{qu})}{\partial x} = 0, \quad (2)$$

where Equation (1) represents the mass conservation law with mass density $\rho = \phi^2$ and Equation (2) describes trajectories of a particle with velocity $v = (\hbar/m)(\partial S/\partial x)$, subject to an external potential V and the quantum potential $V_{qu} = -(\hbar^2/2m\phi)(\partial^2\phi/\partial x^2)$, which accounts

for quantum-wave features, such as interference and diffraction [5,6]. The wave function has been expressed in the polar form $\psi = \phi \exp(iS)$. Equations (1) and (2) yield

$$\hbar \frac{\partial S}{\partial t} + \left(\frac{mv^2}{2} + V_{qu} + V \right) = 0, \quad (3)$$

and the corresponding Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi. \quad (4)$$

From Equations (1) and (2), we obtain the conservation laws for the momentum and energy densities as follows:

$$\frac{\partial J}{\partial t} + \frac{\partial P}{\partial x} + \frac{\rho}{m} \frac{\partial V}{\partial x} = 0, \quad (5)$$

$$\frac{\partial U}{\partial t} + \frac{\partial Q}{\partial x} = 0, \quad (6)$$

where

$$J = \rho v, \quad (7)$$

$$P = \rho v^2 - \frac{\hbar^2}{4m^2} \left[\frac{\partial^2 \rho}{\partial x^2} - \frac{1}{\rho} \left(\frac{\partial \rho}{\partial x} \right)^2 \right], \quad (8)$$

$$U = \rho \left(\frac{mv^2}{2} + V_{qu} + V \right), \quad (9)$$

$$Q = vU + \frac{\hbar^2}{2m^2} \left(\phi \frac{\partial^2 \phi}{\partial x \partial t} - \frac{\partial \phi}{\partial t} \frac{\partial \phi}{\partial x} \right) \quad (10)$$

are the momentum, momentum flux, energy, and energy flux densities, respectively. The momentum density ρv appearing in the hydrodynamical equations can be shown to be the real part of a more general quantum mechanical local momentum field \mathcal{P} defined from the momentum-density operator

$$\mathcal{P} = \frac{\hbar}{i} \psi^* \frac{\partial \psi}{\partial x} = m\rho(v + iu), \quad (11)$$

where $v = (\hbar/m)(\partial S/\partial x)$ and $u = -(\hbar/2m\rho)(\partial \rho/\partial x)$.

It follows now that the boundary conditions for the continuity of mass, momentum, and energy are:

$$\rho, \rho v, \rho u, \text{ and } \rho \left(\frac{mv^2}{2} + V_{qu} + V \right). \quad (12)$$

In terms of the wave function and from Equation (3) the above conditions are equivalent to: $\psi^* \psi$, $\psi^*(\partial \psi/\partial x)$, and $(\partial S/\partial t)$.

3 Tunneling

Next consider the stationary flow of particles with incident energy E striking a potential barrier of height V and width L : $V(x) = V$ for $0 < x < L$ and zero elsewhere. The wave functions for $x < 0$ (incidence region 1), $0 < x < L$ (tunneling region 2), and $x > L$ (transmission region 3) are given respectively by

$$\begin{aligned}\psi_1(x, t) &= \sqrt{\rho_1} \exp(iS_1) \\ &= \sqrt{1 + a^2 + 2a \cos(2kx - \alpha)} \\ &\times \exp i \left(-\omega t + \frac{\alpha}{2} + \tan^{-1} \left[\frac{1-a}{1+a} \tan(kx - \frac{\alpha}{2}) \right] \right),\end{aligned}\quad (13)$$

$$\begin{aligned}\psi_2(x, t) &= \sqrt{\rho_2} \exp(iS_2) \\ &= \sqrt{[c^2 e^{2\bar{q}x} + d^2 e^{-2\bar{q}x} + 2dc \cos(\gamma - \delta)] / \bar{q}} \\ &\times \exp i \left(-\omega t + \frac{\gamma + \delta}{2} + \tan^{-1} \left[\frac{ce^{\bar{q}x} - de^{-\bar{q}x}}{ce^{\bar{q}x} + de^{-\bar{q}x}} \tan\left(\frac{\gamma - \delta}{2}\right) \right] \right),\end{aligned}\quad (14)$$

$$\psi_3(x, t) = \sqrt{\rho_3} \exp(iS_3) = b \exp i(-\omega t + kx + \beta), \quad (15)$$

where $k^2 = 2mE/\hbar^2$ and $\bar{q}^2 = 2m(V - E)/\hbar^2$.

The boundary conditions from (12) where the potential undergoes a finite jump read:

$$\rho_1(0) = \rho_2(0), \quad (16)$$

$$\rho_2(L) = \rho_3(L), \quad (17)$$

$$\rho_1'(0) = \rho_2'(0), \quad (18)$$

$$\rho_2'(L) = \rho_3'(L), \quad (19)$$

$$\rho_1(0)v_1(0) = \rho_2(0)v_2(0), \quad (20)$$

$$\rho_2(L)v_2(L) = \rho_3(L)v_3(L), \quad (21)$$

$$\left(\frac{\partial S_1}{\partial t} \right)_0^- = \left(\frac{\partial S_2}{\partial t} \right)_0, \quad (22)$$

$$\left(\frac{\partial S_2}{\partial t} \right)_L = \left(\frac{\partial S_3}{\partial t} \right)_L. \quad (23)$$

By applying the above boundary conditions on Equations (13), (14), and (15), we obtain:

$$1 + a^2 + 2a \cos \alpha = \frac{c^2 + d^2 + 2cd \cos(\gamma - \delta)}{\bar{q}}, \quad (24)$$

$$\frac{c^2 e^{2\bar{q}L} + d^2 e^{-2\bar{q}L} + 2cd \cos(\gamma - \delta)}{\bar{q}} = b^2, \quad (25)$$

$$2ak \sin \alpha = (c^2 - d^2), \quad (26)$$

$$c = d e^{-2\bar{q}L}, \quad (27)$$

$$1 - a^2 = \frac{2d^2 e^{-2\bar{q}L} \sin(\gamma - \delta)}{k}, \quad (28)$$

$$\frac{2d^2 e^{-2\bar{q}L} \sin(\gamma - \delta)}{k} = b^2. \quad (29)$$

From Equations (25) and (27), we have

$$b^2 = \frac{2d^2 e^{-2\bar{q}L} [1 + \cos(\gamma - \delta)]}{\bar{q}}, \quad (30)$$

which combined with Equation (29) gives

$$\tan \left(\frac{\gamma - \delta}{2} \right) = \frac{k}{\bar{q}}, \quad (31)$$

$$\sin(\gamma - \delta) = \frac{2k\bar{q}}{\bar{q}^2 + k^2}, \quad (32)$$

$$\cos(\gamma - \delta) = \frac{\bar{q}^2 - k^2}{\bar{q}^2 + k^2}. \quad (33)$$

Equations (29) and (33) allow us to write Equation (30) as

$$b^2 = \left(\frac{4\bar{q}}{\bar{q}^2 + k^2} \right) d^2 e^{-2\bar{q}L}, \quad (34)$$

which, in turn, combined with Equations (27) and (33), reduces Equation (24)

$$1 + a^2 + 2a \cos \alpha = b^2 \left(\frac{\bar{q}^2 - k^2}{2\bar{q}^2} \right) \left(1 + \frac{\bar{q}^2 + k^2}{\bar{q}^2 - k^2} \cosh 2\bar{q}L \right). \quad (35)$$

Equations (28) and (29) imply that

$$a^2 = 1 - b^2, \quad (36)$$

which inserted into Equation (35) gives

$$a \cos \alpha = b^2 \left(1 + \left[\frac{\bar{q}^2 + k^2}{2\bar{q}^2} \right] \sinh^2 \bar{q}L \right) - 1. \quad (37)$$

By the same procedure above, Equation (26) can be rewritten as

$$a \sin \alpha = - \left(\frac{\bar{q}^2 + k^2}{4k\bar{q}} \right) b^2 \sinh 2\bar{q}L. \quad (38)$$

Combination of Equations (36), (37), and (38) leads to

$$b^{-2} = \frac{\left[1 + \left(\frac{\bar{q}^2 + k^2}{2\bar{q}^2} \right) \sinh^2 \bar{q}L \right]^2 + \left(\frac{\bar{q}^2 + k^2}{4k\bar{q}} \right)^2 \sinh^2 2\bar{q}L}{1 + \left(\frac{\bar{q}^2 + k^2}{2\bar{q}^2} \right) \sinh^2 \bar{q}L}. \quad (39)$$

Using the identity $\sinh^2 2\bar{q}L = 4(\sinh^2 \bar{q}L + \sinh^4 \bar{q}L)$, and after dividing the numerator by the denominator in Equation (39), we arrive at the known result

$$b^{-2} = 1 + \left(\frac{\bar{q}^2 + k^2}{2k\bar{q}} \right)^2 \sinh^2 \bar{q}L. \quad (40)$$

4 Boundary Conditions for Dissipative Systems

Next we show below that the boundary conditions (12) are not only more general but the assumption that “ ψ and $(\partial\psi/\partial x)$ are continuous at σ ” is physically incorrect for dissipative systems. To this end, let us consider the dynamics of a quantum particle in the tunneling region described by Equation (1) and

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} + \frac{1}{m} \frac{\partial (V + V_{qu})}{\partial x} = -\nu v, \quad (41)$$

where ν is the friction coefficient, and the term on the right-hand side of Equation (41) accounts for the dissipation. By expressing the wave function as before [see Equation (3)] we have

$$\hbar \left(\frac{\partial S}{\partial t} + \nu S \right) + \left(\frac{mv^2}{2} + V_{qu} + V \right) = 0. \quad (42)$$

The new boundary conditions now are given by Equations (16) through (21) plus

$$\left(\frac{\partial S_1}{\partial t} \right)_0 = \left(\frac{\partial S_2}{\partial t} + \nu S_2 \right)_0, \quad (43)$$

$$\left(\frac{\partial S_2}{\partial t} + \nu S_2 \right)_L = \left(\frac{\partial S_3}{\partial t} \right)_L, \quad (44)$$

which shows the discontinuity in the phase of the wave function at σ . In an upcoming publication, we will detail the application of the above boundary conditions and show that friction on the tunneling of a particle through a single, sharp-edged rectangular barrier diminishes the transmission coefficient.

5 Acknowledgments

Assistance by A. Boutefnouchet in the preparation of this manuscript is gratefully acknowledged.

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