N93-27327

BOUNDARY CONDITIONS IN TUNNELING VIA QUANTUM HYDRODYNAMICS

Antônio B. Nassar

Physics Department
University of California, Los Angeles
Los Angeles, CA 90024
and
Physics Department
Harvard-Westlake School
3700 Coldwater Canyon, North Hollywood, CA 91604

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

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

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

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

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

and the corresponding Schrödinger equation

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

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

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

$$\frac{\partial U}{\partial t} + \frac{\partial Q}{\partial x} = 0, \tag{6}$$

where

$$J = \rho v, \tag{7}$$

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

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

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

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

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

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:

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

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

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

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

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

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

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

$$\rho_1(0) = \rho_2(0), \tag{16}$$

$$\rho_2(L) = \rho_3(L), \tag{17}$$

$$\rho_1'(0) = \rho_2'(0), \tag{18}$$

$$\rho_2'(L) = \rho_3'(L), \tag{19}$$

$$\rho_1(0)v_1(0) = \rho_2(0)v_2(0), \tag{20}$$

$$\rho_2(L)v_2(L) = \rho_3(L)v_3(L), \tag{21}$$

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

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

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

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

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

$$2ak\sin\alpha = (c^2 - d^2), \tag{26}$$

$$c = de^{-2\overline{q}L}, \tag{27}$$

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

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

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

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

which combined with Equation (29) gives

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

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

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

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

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

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

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

Equations (28) and (29) imply that

$$a^2 = 1 - b^2, \tag{36}$$

which inserted into Equation (35) gives

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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.

References

[1] A. S. Davydov, *Quantum Mechanics* (Pergamon Press, 2nd edition, Oxford, 1965).

[2] E. Merzbacher, *Quantum Mechanics* (John Wiley, 2nd edition, New York, 1970).

[3] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, 3rd edition, New York, 1970).

[4] A. P. French and E. F. Taylor, *An Introduction to Quantum Physics* (MIT Series, W. W. Norton, New York, 1978).

[5] D. Bohm, C. Dewdney, and B. J. Hiley, Nature (London) **315**, 294 (1985).

[6] D. Bohm and B. J. Hiley, Phys. Rev. Lett. **55**, 2511 (1985).