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A theorem on boundary functions for quantum shutters

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Abstract

We prove for one-dimensional time-dependent quantum absorbing (and reflecting) slits that for right-moving incident waves, the Laplace transform of the boundary function must have singular points at the complex roots of $\sqrt{s} \pm \mathrm{i}\sqrt{(\mathrm{i}\varepsilon/\hbar)} = 0$. We test our result against the exact case of the Moshinsky absorbing (and reflecting) shutter, and the agreement is perfect. In the same Moshinsky problem, when the approximated Kirchhoff boundary condition is used, the transmitted wave is a superposition of right- and left-moving Moshinsky packets. Neglecting the wrong directed wave components we get the exact solution.

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1. Introduction

Quantum transient currents resulting from the decay of a compound state in nuclear reactions, or the chopping of monoenergetic beams of particles into pulses, are just some of the particular cases that can be described with the theory of transmission of quantum waves passing through slits opening with a finite velocity. The earliest reports by Moshinsky [1] and Gerasimov et al. [2], were for one-dimensional (1D) slits opening with infinite velocities. More recently, theoretical and experimental time-dependent quantum phenomena, given for 3D slits opening with finite velocities, have been extensively reported [3–6].

All quantum time-dependent slits are reduced to the following theory. Consider a continuous beam of free particles, of energy $\varepsilon = p^2/2m$, moving in the direction of the z-axis: $\psi = \exp[\mathrm{i}(pz - \varepsilon t)/\hbar]$. For all negative times, the beam is interrupted by a completely absorbing shutter located at the plane $z = 0$. Suddenly, at time $t = 0$, the shutter begins to open with a velocity v_0 allowing the free evolution of the initially interrupted beam of particles. What is the transmitted wave function at the right of the shutter?

One approach to the shutter problem implies solving, as a boundary-value problem for the semi-infinite region $z \geqslant 0$, the *time-dependent* Schrödinger equation

$$\frac{\partial\psi}{\partial t} = \mathrm{i}\gamma\nabla^2\psi, \quad \gamma \equiv \frac{\hbar}{2m}. \tag{1}$$

Since the absorbing shutter opens at $t = 0$, the initial condition for all $z > 0$ is $\psi(\mathbf{r}, 0) = 0$. The imposed boundary conditions (BC) at the shutter wall, $z = 0$, can be either of Dirichlet or Neumann type. Since our discussion is independent of this choice, for simplicity we take the Dirichlet case.

According with the general theory of partial difference equations [7], given the 1D free propagators, $g_1(x, t; x_0, t_0)$ and $g_2(y, t; y_0, t_0)$, for the infinite (x, y) space,

$$g_1 g_2 = \frac{\theta(t - t_0)}{4\pi\mathrm{i}\gamma(t - t_0)}\exp\left[\frac{\mathrm{i}[(x - x_0)^2 + (y - y_0)^2]}{4\gamma(t - t_0)}\right], \tag{2}$$

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and the free propagator $g_3(z,t;z_0,t_0)$, for $0 \leqslant z < \infty$, which satisfies $g_3 = 0$ at the boundary $z = 0$,

$$g_3 = \frac{\theta(t-t_0)}{\sqrt{4\pi \mathrm{i}\gamma(t-t_0)}}\left\{\exp\left[\frac{\mathrm{i}(z-z_0)^2}{4\gamma(t-t_0)}\right] - \exp\left[\frac{\mathrm{i}(z+z_0)^2}{4\gamma(t-t_0)}\right]\right\}, \tag{3}$$

the general expression for the transmitted wave at the right of the shutter is:

$$\psi(\mathbf{r},t;v_0) = \mathrm{i}\gamma \int_0^t \mathrm{d}t_0 \left.\frac{\partial g_3}{\partial z_0}\right|_{z_0=0} \iint_{-\infty}^{+\infty} \mathrm{d}x_0\,\mathrm{d}y_0\, g_1 g_2 \psi_0(x_0,y_0,t_0;v_0), \tag{4}$$

where ψ_0 is the boundary function at $z = 0$ and

$$\left.\frac{\partial g_3}{\partial z_0}\right|_{z_0=0} = \frac{z\exp[\mathrm{i}z^2/4\gamma(t-t_0)]}{\sqrt{4\pi}[\mathrm{i}\gamma(t-t_0)]^{3/2}}. \tag{5}$$

Eq. (4) is an *exact* integral representation for the transmitted wave function at $z \geqslant 0$. However, it cannot be used because, for each particular shutter, nobody knows what the *exact* expression of the boundary function ψ_0 is. Pauli put a remedy to this complication accepting the scalar Kirchhoff approximation used in Optics [8], where the approximation assumes that the boundary function is given by the product of the incident plane wave in the *absence* of any screen, evaluated at $z = 0$, times a transmission function T. For an absorbing shutter we have:

$$\psi_0(x,y,t;v_0) \equiv \exp(-\mathrm{i}\varepsilon t/\hbar)T(x,y,t;v_0). \tag{6}$$

The function T is just a time-dependent mask, defined by $T = 1$ for the open boundary and $T = 0$ for the closed one.

In Optics, the Kirchhoff BC works best in the short-wavelength limit, in which the diffracting openings have dimensions large compared to the wavelength. Obviously when the quantum shutter is in the initial process of opening, the Kirchhoff BC cannot give reliable results. We claim that in quantum diffraction the validity of the Kirchhoff approximation is a dubious one, specially at short times and/or fast periodic choppers [9]. The problem is that in every beam chopping experiment reported so far, nothing but the Kirchhoff BC has been used to theoretically explain the experimental outcomes [9–11]. This happens, we believe, because there is no other simple choice for a BC in the quantum literature.

After reviewing a few properties about the 1D quantum shutters, the purpose of the present work is first to make the fundamental assumption that the direction of the transmitted wave is the same as the direction of the incident one. Next, we prove that the Laplace transform of the boundary function must have a particular analytic structure in the complex s-plane, with singular points defined by the complex equation $\sqrt{s} \pm \mathrm{i}\sqrt{\mathrm{i}\varepsilon/\hbar} = 0$. We test our theorem against the Moshinsky shutter, where the *exact* transmitted and boundary functions are well known. The agreement is perfect. Next we show that for the same Moshinsky problem, the Kirchhoff approximation yields a transmitted wave which has components that travel in the wrong direction. By just neglecting the wrong component we get the exact solution to the Moshinsky shutter.

2. One-dimensional case

For simplicity, let us consider in Eq. (4) the 1D case, where the transmitted function ψ depends only on z and t. This happens if the boundary function ψ_0 depends only on time t not on (x, y). In such case, since

$$\iint_{-\infty}^{+\infty} \mathrm{d}x_0\,\mathrm{d}y_0\; g_1 g_2 = 1, \tag{7}$$

the *exact* 1D transmitted function becomes

$$\psi(z,t;v_0) = \mathrm{i}\gamma \int_0^t \mathrm{d}t_0 \left.\frac{\partial g_3}{\partial z_0}\right|_{z_0=0} \psi_0(t_0;v_0). \tag{8}$$

This relation is still a dead end; we cannot get the transmitted wave ψ because we do not know the boundary function ψ_0. However, assuming that we can get some extra information about ψ, we can use the integral equation (8) to derive some properties about ψ_0. To do so, we provide the needed extra information about ψ making the following:

Assumption. For a right-moving monoenergetic beam of particles falling upon an absorbing shutter with a transmission functions T such that $T = 1$ for the open boundary and $T = 0$ for the closed one. The transmitted wave function has to be a right-moving wave packet:

$$\psi(z,t;v_0) = \mathrm{e}^{\mathrm{i}(pz-\varepsilon t)/\hbar}A(z,t;v_0), \tag{9}$$

where $A(z,t;v_0)$ is a transient amplitude such that for long times

$$\lim_{t\to\infty} A(z,t;v_0) = 1. \tag{10}$$

Assumption (9) means that the transmitted wave has the same direction as the incident one. Eq. (10) means that for long times the transient behavior is gone. These assumptions are based on physical insight, no prove is intended.

If the assumptions are accepted, we have enough information to derive some analytic properties of the boundary function ψ_0. Indeed, substituting Eq. (9) into (8) we get

$$\mathrm{e}^{\mathrm{i}(pz-\varepsilon t)/\hbar}A(z,t;v_0) = \mathrm{i}\gamma \int_0^t \mathrm{d}t_0 \left.\frac{\partial g_3(t-t_0)}{\partial z_0}\right|_{z_0=0} \psi_0(t_0;v_0). \tag{11}$$

This is a Volterra integral equation which imposes very restrictive conditions on the analytic structure of ψ_0.

Since the integral in Eq. (11) is a convolution type, a Laplace transform $\mathscr{L}$ gives an algebraic condition for $\mathscr{L}[\psi_0(t)] \equiv \tilde{\psi}_0(s)$. Using Laplace transform tables [12] we