Quantum-mechanical results for a free particle inside a box with general boundary conditions

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The wave functions with the most general boundary conditions consistent with the conservation of probability for a free particle inside a box [Phys. Rev. D **42**, 1194 (1990)] are calculated. The exact Green's functions and propagators for some special cases are obtained and a semiclassical approach for the propagators is considered. Finally, the influence of the boundary conditions over the path integral's formalism is briefly discussed.

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I. INTRODUCTION

Quantum-mechanical systems with general boundary conditions exhibit some interesting features concerning bound states, the semiclassical approximation, scattering, the functional integral approach, etc. Recently, these problems have been considered in the literature [2–4]. One of the simplest problems in quantum mechanics, a free particle inside a one-dimensional box, the wave functions of which are considered to have the most general boundary conditions consistent with the conservation of probability, was presented in Ref. [1]. Here, we discuss this system.

In Sec. II, we calculate the Schrödinger equation, finding the eigenfunctions and a general transcendental equation for the eigenvalues that, for some special cases, can be solved explicitly. Then, the exact propagators for these special cases are obtained by the spectral resolution method in Sec. III. In Sec. IV, we propose a modified Van Vleck formula in order to evaluate semiclassically the propagators of the system. For the case of no possibility of current flowing from one wall to the other, we obtain the exact Green's function in Sec. V. Finally, in Sec. VI, we discuss our results and present some remarks.

II. WAVE FUNCTIONS

For the free particle confined inside a one-dimensional box with fixed walls at $x = 0$ and $x = L$, the Schrödinger equation is of the form

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t) \ ,$$
$$\psi(x,t) = 0 \ \text{ if } x < 0 \quad \text{or} \quad x > L \ . \qquad (1)$$

Instead of forcing the wave functions to vanish at the walls, we now study the most general boundary conditions consistent with the conservation of probability [1]

$$\begin{pmatrix} -\psi'(L,t) \\ \psi'(0,t) \end{pmatrix} = \begin{pmatrix} \rho+\beta_L & -\rho\exp(i\theta) \\ -\rho\exp(-i\theta) & \rho+\beta_0 \end{pmatrix} \begin{pmatrix} \psi(L,t) \\ \psi(0,t) \end{pmatrix} \ , \qquad (2)$$

where the 2×2 matrix must be Hermitian. In fact, there is a four-parameter family of boundary conditions each of which leads to unitary time evolution.

Substituting the following wave function satisfying (1) ($k^2 = 2mE/\hbar^2$):

$$\psi_k(x,t) = [A\exp(ikx) + B\exp(-ikx)] \times \exp\left(-\frac{i\hbar k^2}{2m}t\right) , \qquad 0 \le x \le L \ , \qquad (3)$$

into (2), we obtain

$$\{\rho\exp(i\theta) - [ik+\rho+\beta_L]\exp(ikL)\}A + \{\rho\exp(i\theta) + [ik-\rho-\beta_L]\exp(-ikL)\}B = 0 \qquad (4)$$

and

$$\{\rho\exp[i(kL-\theta)] + [ik-\rho-\beta_0]\}A + \{\rho\exp[-i(kL+\theta)] - [ik+\rho+\beta_0]\}B = 0 \ , \qquad (5)$$

which give the transcendental equation

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$$[k^2 - \rho(\beta_0 + \beta_L) - \beta_0\beta_L]\sin(kL)$$
$$-k(2\rho + \beta_0 + \beta_L)\cos(kL) + 2k\rho\cos(\theta) = 0 \quad (6)$$

for the quantized energies. After lengthy but straightforward calculations we find the normalized wave function

$$\psi_k(x,t) = \frac{1}{\sqrt{a}}[\exp(ikx) + c\exp(-ikx)] \times \exp\left(-\frac{i\hbar k^2}{2m}t\right) \quad (7)$$

with

$$c = \frac{i[k + \rho\,\sin(kL-\theta)] + [\rho\,\cos(kL-\theta) - \rho - \beta_0]}{i[k + \rho\,\sin(kL+\theta)] - [\rho\,\cos(kL+\theta) - \rho - \beta_0]} \quad (8)$$

and

$$a = (1+|c|^2)L + \frac{2\sin(kL)}{k}\,\mathrm{Re}[c\exp(-ikL)] \quad (9)$$

for k a real number, or

$$a = 2L\mathrm{Re}[c] + \frac{\sin(kL)}{k}[\exp(ikL) + |c|^2\exp(-ikL)] \quad (10)$$

for k an imaginary number (in this case the energy takes negative values).

Therefore this quantum-mechanical problem has an analytical solution once the quantized energies have been obtained numerically from (6). However, for some special cases this transcendental equation can be solved exactly. Now, we investigate these cases in more detail.

A. $2\rho + \beta_0 + \beta_L = 0$ and $\theta = (s+\frac{1}{2})\pi, \quad s = 0,1,2,\ldots$

The transcendental Eq. (6) reduces to

$$(2k^2 + \beta_0^2 + \beta_L^2)\sin(kL) = 0\ , \quad (11)$$

which leads to the following quantized energies:

$$E_n^{(A)} = \frac{\hbar^2}{2m}k_n^2 = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2}, \qquad n = 1,2,3,\ldots\ , \quad (12)$$

and

$$E_{\text{bound}}^{(A)} = -\frac{\hbar^2}{2m}\gamma^2 \quad \text{with} \quad \gamma^2 = \frac{\beta_0^2 + \beta_L^2}{2}\ . \quad (13)$$

The corresponding energy eigenfunctions are of the form

$$\psi_n^{(A)}(x,t) = \frac{1}{\sqrt{(1+|c_n|^2)L}} \times [\exp(ik_nx) + c_n\exp(-ik_nx)] \times \exp\left(-\frac{i\hbar\pi^2n^2}{2mL^2}t\right) \quad (14)$$

with

$$c_n = \frac{i[k_n + (-1)^{n+s}\,\frac{\beta_0+\beta_L}{2}] - \frac{\beta_0-\beta_L}{2}}{i[k_n - (-1)^{n+s}\,\frac{\beta_0+\beta_L}{2}] + \frac{\beta_0-\beta_L}{2}} \quad (15)$$

for positive energies and

$$\psi_{\text{bound}}^{(A)}(x,t) = \frac{1}{\sqrt{a_b}}[\exp(-\gamma x) + c_b\exp(\gamma x)] \times \exp\left(i\frac{\hbar}{m}\frac{\beta_0^2+\beta_L^2}{4}t\right) \quad (16)$$

with

$$c_b = \frac{\gamma - i(-1)^s\exp(-\gamma L)\frac{\beta_0+\beta_L}{2} + \frac{\beta_0-\beta_L}{2}}{\gamma + i(-1)^s\exp(\gamma L)\frac{\beta_0+\beta_L}{2} - \frac{\beta_0-\beta_L}{2}} \quad (17)$$

and

$$a_b = 2L\mathrm{Re}[c_b] + \frac{\sinh(\gamma L)}{\gamma}[\exp(-\gamma L) + |c_b|^2\exp(\gamma L)] \quad (18)$$

for negative energies.

B. $\rho = 0$

In this case, the boundary condition (2) decouples and reads $\psi'(0,t) = \beta_0\psi(0,t)$ and $\psi'(L,t) = -\beta_L\psi(L,t)$. In other words, there exists no possibility of current flowing from one wall to the other.

The transcendental Eq. (6) becomes

$$(k^2 - \beta_0\beta_L)\tan(kL) = k(\beta_0 + \beta_L)\ . \quad (19)$$

With the help of (7)–(10) we obtain the energy eigenfunctions

$$\psi_k^{(B)}(x,t) = \frac{1}{\sqrt{a_{(\rho=0)}}} \times \left[\exp(ikx) + \frac{ik-\beta_0}{ik+\beta_0}\exp(-ikx)\right] \times \exp\left(-\frac{i\hbar k^2}{2m}t\right)\ , \quad (20)$$

where

$$a_{(\rho=0)} = 2L + 2\,\frac{(\beta_0+\beta_L)(k^2+\beta_0\beta_L)}{(\beta_0^2+k^2)(\beta_L^2+k^2)} \quad (21)$$

for k real, or

$$a_{(\rho=0)} = 2L\left(\frac{ik-\beta_0}{ik+\beta_0}\right) + \frac{\sin(kL)}{k}\left[\exp(ikL) + \left(\frac{ik-\beta_0}{ik+\beta_0}\right)^2\exp(-ikL)\right] \quad (22)$$

for k imaginary.

We now consider the following special cases: (a) $\beta_0 + \beta_L = 0$, (b) $\beta_0 = \infty$ and $\beta_L = 0$, and (c) $\beta_0 = 0$ and $\beta_L = \infty$.

For the case (a), we have from (19)–(22)

$$E_{n;(a)}^{(B)} = \frac{\hbar^2}{2m}k_n^2 = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2}, \qquad n = 1,2,3,\ldots\ , \quad (23)$$

for positive energy, with the eigenfunctions

$$\psi^{(B)}_{n;(a)}(x,t) = \frac{1}{\sqrt{2L}}\left[\exp(ik_n x) + \frac{\frac{n\pi}{L}+i\beta_0}{\frac{n\pi}{L}-i\beta_0}\exp(-ik_n x)\right] \times \exp\left(-\frac{i\hbar k_n^2}{2m}t\right) , \quad (24)$$

which are more general than the two well known solutions for $\beta_0 = 0$ and $\beta_0 = \infty$ [for $\beta_0 = \infty$, Eqs. (23) and (24) are still valid but with β_L being $+\infty$], and

$$E^{(B)}_{\rm bound} = -\frac{\hbar^2}{2m}\beta_0^2 \quad (25)$$

for negative energy, with the eigenfunction

$$\psi^{(B)}_{\rm bound}(x,t) = \sqrt{\frac{\beta_0}{\sinh(\beta_0 L)}}\exp\left[\beta_0\left(x-\frac{L}{2}\right)\right] \times \exp\left(\frac{i\hbar\beta_0^2}{2m}t\right) . \quad (26)$$

If $\beta_0 < 0\,(\beta_0 > 0)$, (26) is a state bounded to the wall in $x = 0\,(x = L)$. Equations (14) and (16) with $\rho = 0$ reduce respectively to (24) and (26), as they should.

For the cases (b) and (c), a careful analysis of the Schrödinger equation shows that in (19) we can assume $\beta_0\beta_L = 0$. Thus we find the quantized energies $(n = 0, 1, 2, \ldots)$

$$E^{(B)}_{n;(b)} = E^{(B)}_{n;(c)} = \frac{\hbar^2}{2m}\frac{(n+\frac{1}{2})^2\pi^2}{L^2} \quad (27)$$

and the energy eigenfunctions

$$\psi^{(B)}_{n;(\pm)}(x,t) = \frac{1}{\sqrt{2L}}\left[\exp\left(i\frac{(n+\frac{1}{2})\pi}{L}x\right) \pm \exp\left(-i\frac{(n+\frac{1}{2})\pi}{L}x\right)\right] \times \exp\left[-\frac{i\hbar(n+\frac{1}{2})^2\pi^2}{2mL^2}t\right] , \quad (28)$$

where the plus sign stands for the case (c) and the minus sign for the case (b). There are no negative values to the energy in these two cases.

We should remark that the special cases considered above are all the possible cases having an analytical solution for Eq. (6). Any other condition for the parameters ρ, β_0, β_L, and θ can be solved only numerically.

III. EXACT PROPAGATORS

The exact propagators can be evaluated by summing over the energy eigenfunctions. For the parameter conditions (A), we obtain the exact propagator from (14) and (16) by $(T = t_b - t_a)$

$$\begin{aligned} K^{(A)}(x_b,x_a;T) &= \psi^{(A)}_{\rm bound}(x_b,t_b)\psi^{(A)*}_{\rm bound}(x_a,t_a) + \sum_{n=1}^{\infty}\psi^{(A)}_n(x_b,t_b)\,\psi^{(A)*}_n(x_a,t_a) \\ &= K^{(A)}_{\rm bound}(x_b,x_a;T) + \frac{1}{2L}\sum_{n=-\infty}^{\infty}\frac{1}{\gamma^2+(\frac{n\pi}{L})^2} \\ &\quad\times\left\{\left[\left(\frac{n\pi}{L}\right)^2+\gamma^2-2(-1)^{n+s}\frac{n\pi}{L}\beta_+\right]\exp\left[\frac{in\pi}{L}(x_b-x_a)\right] \right.\\ &\quad\left.+\left[\left(\frac{n\pi}{L}\right)^2-\gamma^2-2i\frac{n\pi}{L}\beta_-\right]\exp\left[\frac{in\pi}{L}(x_b+x_a)\right]\right\} \\ &\quad\times\exp\left(-\frac{i\hbar\pi^2n^2}{2mL^2}T\right) , \end{aligned} \quad (29)$$

where $\beta_\pm = (\beta_0 \pm \beta_L)/2$. Considering $\rho = -\beta_+ = 0$, (29) gives the correct propagator for the case (a) in the parameter conditions (B), or

$$\begin{aligned} K^{(B)}_{(a)}(x_b,x_a;T) &= K^{(B)}_{\rm bound}(x_b,x_a;T) \\ &\quad+\frac{1}{2L}\sum_{n=-\infty}^{\infty}\left[\exp\left(\frac{in\pi}{L}(x_b-x_a)\right)+\frac{\frac{n\pi}{L}-i\beta_0}{\frac{n\pi}{L}+i\beta_0}\exp\left(\frac{in\pi}{L}(x_b+x_a)\right)\right] \\ &\quad\times\exp\left(-\frac{i\hbar\pi^2n^2}{2mL^2}T\right) , \end{aligned} \quad (30)$$

where

$$K^{(B)}_{\rm bound}(x_b,x_a;T) = \frac{\beta_0}{\sinh(\beta_0 L)}\exp[\beta_0(x_b+x_a-L)]\exp\left(\frac{i\hbar\beta_0^2}{2m}T\right) . \quad (31)$$

For $\beta_0 = 0$ and $\beta_0 = \infty$, the propagator (30) reduces to the well known propagators [5]

$$K^{(B)}_{\pm;(a)}(x_b,x_a;T)=\frac{1}{2L}\left[\theta_3\left(\frac{\pi(x_b-x_a)}{2L},-\frac{\pi\hbar T}{2mL^2}\right)\pm\theta_3\left(\frac{\pi(x_b+x_a)}{2L},-\frac{\pi\hbar T}{2mL^2}\right)\right]\ , \tag{32}$$

where the plus sign stands for $\beta_0=0$ and the minus sign for $\beta_0=\infty$. Hereafter, $\theta_j(z,\tau)$ will represent one of the Jacobi theta functions (see the Appendix).

Finally, for the cases (b) and (c) in (B), we have

$$\begin{aligned}K^{(B)}_{(\pm)}(x_b,x_a;T)&=\sum_{n=0}^{\infty}\psi^{(B)}_{n;(\pm)}(x_b,t_b)\,\psi^{(B)*}_{n;(\pm)}(x_a,t_a)\\&=\frac{1}{2L}\sum_{n=-\infty}^{\infty}\left[\exp\left(\frac{i(n+\frac{1}{2})\pi}{L}(x_b-x_a)\right)\pm\exp\left(\frac{i(n+\frac{1}{2})\pi}{L}(x_b+x_a)\right)\right]\\&\quad\times\exp\left(-\frac{i\hbar\pi^2(n+\frac{1}{2})^2}{2mL^2}T\right)\\&=\frac{1}{2L}\left[\theta_2\left(\frac{\pi(x_b-x_a)}{2L},-\frac{\pi\hbar T}{2mL^2}\right)\pm\theta_2\left(\frac{\pi(x_b+x_a)}{2L},-\frac{\pi\hbar T}{2mL^2}\right)\right]\ .\end{aligned}\tag{33}$$

The propagator (29) can be written as the following forms ($x_\pm=x_b\pm x_a$):

$$\begin{aligned}K^{(A)}(x_b,x_a;T)&=K^{(B)}_{+;(a)}(x_b,x_a;T)+K^{(A)}_{\text{bound}}(x_b,x_a;T)\\&\quad-\frac{1}{L}\sum_{n=-\infty}^{\infty}\frac{1}{\gamma^2+(\frac{n\pi}{L})^2}\left[(-1)^{n+s}\frac{n\pi}{L}\beta_+\exp\left(\frac{in\pi}{L}x_-\right)\right.\\&\quad\left.+\left(\gamma^2+i\frac{n\pi}{L}\beta_-\right)\exp\left(\frac{in\pi}{L}x_+\right)\right]\exp\left(-\frac{i\hbar\pi^2n^2}{2mL^2}T\right)\ ,\end{aligned}\tag{34}$$

which is useful for γ being small ($\gamma\to 0$), or

$$\begin{aligned}K^{(A)}(x_b,x_a;T)&=K^{(B)}_{-;(a)}(x_b,x_a;T)+K^{(A)}_{\text{bound}}(x_b,x_a;T)\\&\quad-\frac{1}{L}\sum_{n=-\infty}^{\infty}\frac{1}{\gamma^2+(\frac{n\pi}{L})^2}\left\{(-1)^{n+s}\frac{n\pi}{L}\beta_+\exp\left(\frac{in\pi}{L}x_-\right)\right.\\&\quad\left.+\left[i\frac{n\pi}{L}\beta_--\left(\frac{n\pi}{L}\right)^2\right]\exp\left(\frac{in\pi}{L}x_+\right)\right\}\exp\left(-\frac{i\hbar\pi^2n^2}{2mL^2}T\right)\ ,\end{aligned}\tag{35}$$

which is useful for γ being large ($\gamma\to\infty$). Unfortunately, the sums in the above equations cannot be evaluated exactly.

For sufficient small γ, namely, $\gamma<\pi/L$, we can ensure the convergence of the series

$$\frac{\frac{n\pi}{L}}{\gamma^2+(\frac{n\pi}{L})^2}=\frac{i}{2}\sum_{j=0}^{\infty}\frac{1}{(\frac{in\pi}{L})^j}[\gamma^{(j-1)}+(-\gamma)^{(j-1)}] \tag{36}$$

and

$$\frac{\gamma^2}{\gamma^2+(\frac{n\pi}{L})^2}=-\frac{1}{2}\sum_{j=0}^{\infty}\frac{1}{(\frac{in\pi}{L})^{j+1}}[\gamma^{(j+1)}+(-\gamma)^{(j+1)}]\ . \tag{37}$$

Thus Eq. (34) can be expanded as

$$\begin{aligned}K^{(A)}(x_b,x_a;T)&=K^{(A)}_{\text{bound}}(x_b,x_a;T)+K^{(B)}_{+;(a)}(x_b,x_a;T)\\&\quad+\frac{1}{2L}\sum_{j=0}^{\infty}\left\{\frac{(-1)^s}{i}\beta_+[\gamma^{(j-1)}+(-\gamma)^{(j-1)}]\sum_{n=-\infty}^{\infty}(-1)^n\frac{1}{(\frac{in\pi}{L})^j}\right.\\&\quad\times\exp\left(\frac{in\pi}{L}x_-\right)\exp\left(-\frac{i\hbar\pi^2n^2}{2mL^2}T\right)+[\gamma^{(j+1)}+(-\gamma)^{(j+1)}]\\&\quad\times\sum_{n=-\infty}^{\infty}\frac{1}{(\frac{in\pi}{L})^{j+1}}\exp\left(\frac{in\pi}{L}x_+\right)\exp\left(-\frac{i\hbar\pi^2n^2}{2mL^2}T\right)+\beta_-\\&\quad\left.\times[\gamma^{(j-1)}+(-\gamma)^{(j-1)}]\sum_{n=-\infty}^{\infty}\frac{1}{(\frac{in\pi}{L})^j}\exp\left(\frac{in\pi}{L}x_+\right)\exp\left(-\frac{i\hbar\pi^2n^2}{2mL^2}T\right)\right\}\ .\end{aligned}\tag{38}$$

Now, integrating in (38) the identity

$$\frac{d^j}{dz^j}\left(\frac{1}{\alpha^j}\exp[\alpha z]\right)=\exp[\alpha z]\ , \tag{39}$$

we have

$$\begin{aligned}K^{(A)}(x_b,x_a;T)&=K^{(A)}_{\mathrm{bound}}(x_b,x_a;T)+K^{(B)}_{+;(a)}(x_b,x_a;T)\\&+\frac{1}{2L}\sum_{j=0}^{\infty}\left\{\frac{(-1)^s}{i}\beta_+[\gamma^{(j-1)}+(-\gamma)^{(j-1)}]\int_{\alpha_j(T)}^{x_-}dz_j\right.\\&\times\int_{\alpha_{j-1}(T)}^{z_j}dz_{j-1}\cdots\int_{\alpha_1(T)}^{z_2}dz_1\,\theta_4\left(\frac{\pi z_1}{2L},-\frac{\pi\hbar T}{2mL^2}\right)+[\gamma^{(j+1)}+(-\gamma)^{(j+1)}]\\&\times\int_{\alpha_{j+1}(T)}^{x_+}dz_{j+1}\cdots\int_{\alpha_1(T)}^{z_2}dz_1\,\theta_3\left(\frac{\pi z_1}{2L},-\frac{\pi\hbar T}{2mL^2}\right)+\beta_-[\gamma^{(j-1)}+(-\gamma)^{(j-1)}]\\&\left.\times\int_{\alpha_j(T)}^{x_+}dz_j\ldots\int_{\alpha_1(T)}^{z_2}dz_1\,\theta_3\left(\frac{\pi z_1}{2L},-\frac{\pi\hbar T}{2mL^2}\right)\right\}\ ,\end{aligned}\tag{40}$$

where each $\alpha_j(T)$ is any one of the roots for the equation

$$\sum_{n=-\infty}^{\infty}\frac{1}{(\frac{in\pi}{L})^j}\exp\left(\frac{in\pi}{L}\alpha_j(T)\right)\exp\left(-\frac{i\hbar\pi^2n^2}{2mL^2}T\right)=0\ . \tag{41}$$

However, for large values of γ, there is no similar expansion in a convergent series for Eq. (35) so that it can be regrouped in terms of Jacobi theta functions.

IV. SEMICLASSICAL PROPAGATORS

In the semiclassical approach, the propagator is given by the well known Van Vleck formula [6–8]

$$K(x_b,x_a;T)=\frac{1}{\sqrt{2\pi i\hbar}}\sum_{\mathrm{cl}}\left|\frac{\partial^2S_{\mathrm{cl}}}{\partial x_b\partial x_a}\right|^{\frac12}\times\exp\left[\frac{i}{\hbar}S_{\mathrm{cl}}(x_b,x_a;T)-i\frac{\pi}{2}\mu\right] \tag{42}$$

with $S_{\mathrm{cl}}(x_b,x_a;T)$ being the classical action and μ the corresponding Morse index.

However, due to the different boundary conditions of our system, we need to consider a more general approximation to the propagator than Eq. (42). Thus we propose a modified Van Vleck formula [9–11]

$$K(x_b,x_a;T)=\frac{1}{\sqrt{2\pi i\hbar}}\sum_{j=0}^{4}\sum_{n_j}\left|\frac{\partial^2S_{n_j}}{\partial x_b\partial x_a}\right|^{\frac12}\times F_j(n_j,\beta_0,\beta_L)\exp\left(\frac{i}{\hbar}S_{n_j}\right)\ , \tag{43}$$

where now we introduce a preexponential factor $F_j(n_j,\beta_0,\beta_L)$. In (43) we have assumed that the general boundary conditions at the walls change the usual amplitudes in the Van Vleck formula but not the phases (given by the classical actions).

In the corresponding classical system, the particle has four classes ($j=1,2,3,4$) of classical paths [5] which start from x_a at time t_a and arrive in x_b at time t_b. We classify these classes by considering which walls (located in $x=0$ or in $x=L$) the particle collides with on the first and last time:

(1) the first collision with the wall in $x=L$ and the last collision with the wall in $x=0$ or no collisions at all;

(2) both the first and the last collision with the wall in $x=0$;

(3) the first collision with the wall in $x=0$ and the last collision with the wall in $x=L$; or

(4) both the first and the last collision with the wall in $x=L$.

Furthermore, each class has an infinite number of classical paths which can be specified by the number of collisions between the particle and the wall in $x=0$ $(n_j+\varepsilon_j)$ or by the number of collisions between the particle and the wall in $x=L$ (n_j). For each class, we have, respectively, $\varepsilon_1=0,\ n_1=0,1,2,\ldots$; $\varepsilon_2=1,\ n_2=0,1,2,\ldots$; $\varepsilon_3=0,\ n_3=1,2,3,\ldots$; $\varepsilon_4=-1,\ n_4=1,2,3,\ldots$.

The classical actions are given by [5]

$$S_{n_j}=\frac{m}{2T}(y+x+2n_jL)^2\ . \tag{44}$$

In the above equation, x and y represent different quantities for different classes of paths, i.e., (1) $y=x_b,x=-x_a$; (2) $y=x_b,x=x_a$; (3) $y=-x_b,x=x_a$; and (4) $y=-x_b,x=-x_a$.

As is well known, each time the particle hits a wall the contribution of the classical path to the propagator suffers a phase change by π (for the wave function vanishing in this wall) or no phase change [for $(\partial\psi/\partial x)/\psi=0$ in this wall]. We are therefore led to write the preexponent factors as

$$F_j(n_j,\beta_0,\beta_L) = f_j(n_j,\beta_0,\beta_L) \times \exp\{i[(n_j+\varepsilon_j)\,\varphi_0(\beta_0) + n_j\,\varphi_L(\beta_L)]\} \tag{45}$$

with $0 \le \varphi_0(\beta_0)$, $\varphi_L(\beta_L) < 2\pi$. The most difficult part of evaluating the semiclassical propagator turns out to be the determination of f_j, φ_0, and φ_L.

Considering the special cases

$$f_j(n_j,0,0) = f_j(n_j,\infty,\infty) = f_j(n_j,0,\infty) = f_j(n_j,\infty,0) = 1 \tag{46}$$

and

$$\varphi_0(0) = \varphi_L(0) = 0, \varphi_0(\infty) = \varphi_L(\infty) = \pi\ , \tag{47}$$

we have from (43)–(47) (see [5] for derivations)

$$K(x_b,x_a;T;0,0) = \sqrt{\frac{m}{2\pi i\hbar T}}\left[\exp\left(\frac{im(x_b-x_a)^2}{2\hbar T}\right)\theta_3\left(\frac{m(x_b-x_a)L}{\hbar T},\frac{2mL^2}{\pi\hbar T}\right) + \exp\left(\frac{im(x_b+x_a)^2}{2\hbar T}\right)\theta_3\left(\frac{m(x_b+x_a)L}{\hbar T},\frac{2mL^2}{\pi\hbar T}\right)\right] \tag{48}$$

for $\beta_0 = \beta_L = 0$, and

$$K(x_b,x_a;T;\infty,\infty) = \sqrt{\frac{m}{2\pi i\hbar T}}\left[\exp\left(\frac{im(x_b-x_a)^2}{2\hbar T}\right)\theta_3\left(\frac{m(x_b-x_a)L}{\hbar T},\frac{2mL^2}{\pi\hbar T}\right) - \exp\left(\frac{im(x_b+x_a)^2}{2\hbar T}\right)\theta_3\left(\frac{m(x_b+x_a)L}{\hbar T},\frac{2mL^2}{\pi\hbar T}\right)\right] \tag{49}$$

for $\beta_0 = \infty$ and $\beta_L = \infty$. Applying the identity (A4) in the Appendix, the above equations reduce to the exact propagators (32). For the cases of $\beta_0 = 0$, $\beta_L = \infty$ (with the plus sign) and $\beta_0 = \infty$, $\beta_L = 0$ (with the minus sign), we have

$$\begin{aligned} K(x_b,x_a;T;\pm) &= \sqrt{\frac{m}{2\pi i\hbar T}}\left[\sum_{n_1=0}^{\infty}(-1)^{n_1}\exp\left(\frac{mi}{2\hbar T}(x_b-x_a+2n_1L)^2\right)\right.\\ &\quad \pm\sum_{n_2=0}^{\infty}(-1)^{n_2}\exp\left(\frac{mi}{2\hbar T}(x_b+x_a+2n_2L)^2\right)\\ &\quad +\sum_{n_3=1}^{\infty}(-1)^{n_3}\exp\left(\frac{mi}{2\hbar T}(-x_b+x_a+2n_3L)^2\right)\\ &\quad \left.\pm\sum_{n_4=1}^{\infty}(-1)^{n_4}\exp\left(\frac{mi}{2\hbar T}(-x_b-x_a+2n_4L)^2\right)\right]\\ &= \sqrt{\frac{m}{2\pi i\hbar T}}\left[\sum_{n=-\infty}^{\infty}(-1)^{n}\exp\left(\frac{mi}{2\hbar T}(x_b-x_a+2nL)^2\right)\right.\\ &\quad \left.\pm\sum_{n=-\infty}^{\infty}(-1)^{n}\exp\left(\frac{mi}{2\hbar T}(x_b+x_a+2nL)^2\right)\right]\ , \end{aligned} \tag{50}$$

which can be written, in terms of the Jacobi θ functions, as

$$K(x_b,x_a;T;\pm) = \sqrt{\frac{m}{2\pi i\hbar T}}\left[\exp\left(\frac{im(x_b-x_a)^2}{2\hbar T}\right)\theta_4\left(\frac{m(x_b-x_a)L}{\hbar T},\frac{2mL^2}{\pi\hbar T}\right) \pm \exp\left(\frac{im(x_b+x_a)^2}{2\hbar T}\right)\theta_4\left(\frac{m(x_b+x_a)L}{\hbar T},\frac{2mL^2}{\pi\hbar T}\right)\right]\ . \tag{51}$$

Finally, with the help of the identities (A6) and (A7) in the Appendix, we find from (51) the exact propagators (33).

To derive the previous results, identities (A4) and (A6) are essential since the classical actions (44) are quadratic in $x_b \pm x_a$, whereas these terms appear as linear arguments of the Jacobi θ functions in the exact propagators. As far as we know, there are no similar identities for expressions of the more general form $\sum_{n=-\infty}^{\infty} g_n \exp[in^2u + inw]$. Therefore the modified Van

Vleck formula (43), a sum over classical paths but with generalized amplitudes, cannot give the exact propagators (29) and (30). In the particular case of (30), the terms in $x_b - x_a$ can be obtained from the classical paths (we observe that these terms come from the classical paths where the numbers of the collisions with the walls at $x = 0$ and $x = L$ are the same), but the terms in $x_b + x_a$ cannot be obtained from the other classical paths. Finally, for the more general cases, i.e., propagators related to eigenvalues satisfying Eqs. (6) or (19), a semiclassical approach is impracticable since we do not have a "good quantum number" [such as n in $k_n = n\pi/L$ or in $k_n = (n + 1/2)\pi/L$] to associate with the "good classical number" (the number of collisions between the particle and the walls).

V. GREEN'S FUNCTIONS

In this section we only consider the case of decoupled boundary conditions, i.e., $\rho = 0$. The Green's function is given by the differential equation

$$\frac{\hbar^2}{2m}\left(z^2 + \frac{\partial^2}{\partial x_b^2}\right) G(x_b, x_a; z) = \delta(x_b - x_a) \; . \tag{52}$$

Moreover, $G(x_b, x_a; z)$ must satisfy the same boundary conditions imposed on the wave functions; thus we have

$$\frac{\partial}{\partial x_b} G(x_b, x_a; z)\bigg|_{x_b=0} = \beta_0 G(x_b, x_a; z)\bigg|_{x_b=0} \tag{53}$$

and

$$\frac{\partial}{\partial x_b} G(x_b, x_a; z)\bigg|_{x_b=L} = -\beta_L G(x_b, x_a; z)\bigg|_{x_b=L} \; . \tag{54}$$

Considering the ideas in Refs. [4] and [12–14], we propose the following expression for the Green's function:

$$\begin{aligned} G(x_b, x_a; z) = \frac{m}{i\hbar^2 z} \Bigg\{ & \left[\exp[iz\,|x_b - x_a|] + \frac{iz + \beta_0}{iz - \beta_0} \exp[iz(x_b + x_a)]\right] \\ & - \frac{1}{F(z)} \left[\exp[-izx_a] + \frac{iz + \beta_0}{iz - \beta_0} \exp[izx_a]\right] \\ & \times \left[\exp[izx_b] + \frac{iz - \beta_0}{iz + \beta_0} \exp[-izx_b]\right] \Bigg\} \end{aligned} \tag{55}$$

that satisfies Eq. (52) (here we recall the relation $\frac{1}{2}(d^2/dx^2)\,|x| = \delta(x)$ [15]). Finally, by choosing

$$F(z) = 1 + \frac{iz(\beta_0 + \beta_L) + (z^2 - \beta_0\beta_L)}{iz(\beta_0 + \beta_L) - (z^2 - \beta_0\beta_L)} \exp[-2izL] \; , \tag{56}$$

Eqs. (53) and (54) are also satisfied.

As is well known, the Green's function has the spectral representation

$$G(x_b, x_a; z) = \sum_n \frac{\varphi_n(x_b)\varphi_n^*(x_a)}{\frac{\hbar^2}{2m}z^2 - E_n} \; . \tag{57}$$

The poles are the eigenvalues of the system and the residues their eigenvectors, which can be obtained by $(\hbar^2/2m\, k_n^2 = E_n)$

$$\varphi_n(x)\,\varphi_n^*(x) = \frac{\hbar^2}{2m} \lim_{z \to k_n} (z^2 - k_n^2)\, G(x, x; z) \; . \tag{58}$$

For our Green's function, the poles are given by the particular values of $z = k$ such that $F(k) = 0$, or

$$(k^2 - \beta_0\beta_L)\tan(kL) = k(\beta_0 + \beta_L) \; , \tag{59}$$

in agreement with the quantization condition, Eq. (19). From Eqs. (55) and (58), we find

$$\begin{aligned} \varphi_k(x)\,\varphi_k^*(x) = \frac{1}{a_R} & \left[\exp(ikx) + \frac{ik - \beta_0}{ik + \beta_0} \exp[-ikx]\right] \\ \times & \left[\exp(-ikx) + \frac{ik + \beta_0}{ik - \beta_0} \exp[ikx]\right] \end{aligned} \tag{60}$$

with

$$a_R = -i \lim_{z \to k} \left(\frac{2k}{z^2 - k^2}\right) F(z) \tag{61}$$

for k a real number, and

$$\begin{aligned} \varphi_k(x)\,\varphi_k(x) = \frac{1}{a_I} & \left[\exp(ikx) + \frac{ik - \beta_0}{ik + \beta_0} \exp[-ikx]\right] \\ \times & \left[\exp(ikx) + \frac{ik - \beta_0}{ik + \beta_0} \exp[-ikx]\right] \end{aligned} \tag{62}$$

with

$$a_I = -i \lim_{z \to k} \left(\frac{ik - \beta_0}{ik + \beta_0}\right) \left(\frac{2k}{z^2 - k^2}\right) F(z) \tag{63}$$

for k an imaginary number. With the help of Eq. (59) we find, after tedious but straightforward manipulations, that Eqs. (61) and (63) lead to the correct normalization constants, Eqs. (21) and (22), respectively. Therefore all the results in Sec. II for the case of $\rho = 0$ are recovered by the Green's function (55), as they should.

VI. CONCLUDING REMARKS

The most general boundary conditions consistent with the conservation of probability for the wave functions of a free particle inside a box lead to a four-parameter family of self-adjoint extensions of the free Hamiltonian. Here, we have discussed the quantum mechanics of this system. First, we investigated the Schrödinger equation, finding the normalized eigenfunctions and a general transcendental equation for the eigenvalues [Eq. (6)], which could be solved explicitly in some special cases. These solutions showed a result already pointed out in the literature, i.e., even for repulsive potentials, general boundary conditions introduce bound states in the system. Second, the exact propagators for the special cases mentioned above were obtained by using the spectral resolution method. They are written in terms of the Jacobi theta functions θ_2, θ_3, and θ_4; in contrast with the exact solution for the usual boundary conditions given in terms of θ_3. Also, semiclassical propagators have been proposed through a modified Van Vleck formula, over the classical paths but summed with generalized preexponential factors. This formula was capable of giving the exact results only for a few cases. The main reasons for this can be understood considering two statements. (a) In the semiclassical approximation, the correct boundary conditions for the propagator must be taken into account by the phases due to the Morse index. However, more general boundary conditions can become too complicated to be given only by the phase factors in the Van Vleck formula. (b) These more general boundary conditions can bring, in a Feynman integral sense, paths without classical analogies, but with important contributions for the propagator. Finally, for the case of no current flowing from one wall to the other, we solved the differential equation for the Green's function with the appropriate boundary conditions, finding the correct eigenvalues and eigenfunctions for the system, as we should.

As a final remark, we would like to make a few comments about the "delicate" problem of the measure in the path integral context. To obtain the propagator by using directly the Feynman path integral is very difficult to accomplish. The problem becomes worse if we impose some constraints on the integrals, for example, the presence of infinite barriers. These constraints play an important role in the definition of the correct measure of the path integral and consequently in the "selection" of the paths to be summed. For a free particle on the half line, this was investigated for the usual [16] and more general [2] boundary conditions. In the very interesting work of Carreau, Farhi, and Gutmann [1], a functional integral for the present system was constructed with the correct measure. Unfortunately, the explicit solution of this path integral was not carried out. Here, we have taken a more "pedestrian" approach. We have solved the Schrödinger equation and then, with these solutions, we have obtained the exact propagators. However, it is instructive to discuss our results, in the light of the path integrals, with the help of the following equivalence:

$$\int \mathcal{D}[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right) \equiv \sum_n \psi_n^*(x_a, t_a)\, \psi_n(x_b, t_a)\ , \quad (64)$$

where $\mathcal{D}[x(t)]$ denotes the measure over the paths $x(t)$ and $S[x(t)]$ their actions.

Rewriting Eq. (30) as

$$K^{(B)}_{(a)}(x_b, x_a; T) = K^{(B)}_{+;(a)}(x_b, x_a; T) + K^{(B)}_{\text{bound}}(x_b, x_a; T) - \frac{1}{L} \sum_{n=-\infty}^{\infty} \frac{i\beta_0}{\frac{n\pi}{L} + i\beta_0} \exp\left(\frac{in\pi}{L}(x_b + x_a)\right) \exp\left(-\frac{i\hbar\pi^2 n^2}{2mL^2} T\right) \quad (65)$$

or

$$K^{(B)}_{(a)}(x_b, x_a; T) = K^{(B)}_{-;(a)}(x_b, x_a; T) + K^{(B)}_{\text{bound}}(x_b, x_a; T) + \frac{1}{L} \sum_{n=-\infty}^{\infty} \frac{\frac{n\pi}{L}}{\frac{n\pi}{L} + i\beta_0} \exp\left(\frac{in\pi}{L}(x_b + x_a)\right) \exp\left(-\frac{i\hbar\pi^2 n^2}{2mL^2} T\right)\ , \quad (66)$$

we see that, in principle, Eqs. (34) and (65) can formally be written as

$$K(x_b, x_a; T) = \int \mathcal{D}_0[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right) + \int \mathcal{D}_{**}[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right) \quad (67)$$

and Eqs. (35) and (66) as

$$K(x_b, x_a; T) = \int \mathcal{D}_\infty[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right) + \int \mathcal{D}_*[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right)\ . \quad (68)$$

In the above equations, the path integral with the measure $\mathcal{D}_0[x(t)]$ gives the propagator for the case of $\rho = 0$ and $\beta_0 = \beta_L = 0$, and the path integral with the measure $\mathcal{D}_\infty[x(t)]$ gives the usual propagator ($\rho = 0$ and wave functions vanishing at the walls). Then we can interpret the second term in the right-hand side of Eqs. (67) and (68) as being the contribution of the new paths, "created" by the more general boundary conditions. We also mention that for the cases (b) and (c) in the boundary conditions (B), the propagators (33) are obtained from the propagators (32) by the change $n \to n + \frac{1}{2}$. Thus, instead of creating new paths for the path integrals, these boundary conditions seem to do some kind of rescaling in the measures $\mathcal{D}_\infty[x(t)]$ and $\mathcal{D}_0[x(t)]$.

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APPENDIX A

In this Appendix we list some of the properties of the Jacobi θ functions that we have used to evaluate our main results. Good sources of definitions and properties of the Jacobi θ functions can be found in Refs. [17,18].

The Jacobi θ functions are defined as

$$\theta_2(z,\tau) = \sum_{n=-\infty}^{\infty} \exp\left\{i[\pi(n+\tfrac{1}{2})^2\tau + (2n+1)z]\right\} , \tag{A1}$$

$$\theta_3(z,\tau) = \sum_{n=-\infty}^{\infty} \exp[i(\pi n^2\tau + 2nz)] , \tag{A2}$$

$$\theta_4(z,\tau) = \sum_{n=-\infty}^{\infty} (-1)^n \exp[i(\pi n^2\tau + 2nz)] . \tag{A3}$$

The following relations are essential for our purpose:

$$\theta_3(u,\tau) = (-i\tau)^{-\frac{1}{2}} \exp\left[-\frac{iu^2}{\pi\tau}\right] \theta_3\left(\frac{u}{\tau}, -\frac{1}{\tau}\right) \tag{A4}$$

and

$$\theta_3\left(z + \frac{\pi\tau}{2}, \tau\right) = \exp\left[-i\left(\frac{\pi\tau}{4} + z\right)\right] \theta_2(z,\tau) . \tag{A5}$$

If in (A4) we consider $u = z + \pi\tau/2$, we find from (A5)

$$\theta_2(z,\tau) = (-i\tau)^{-\frac{1}{2}} \exp\left[-\frac{iz^2}{\pi\tau}\right] \theta_3\left(\frac{z}{\tau} + \frac{\pi}{2}, -\frac{1}{\tau}\right) . \tag{A6}$$

Finally, the following simple relations are also useful:

$$\theta_3(-z,\tau) = \theta_3(z,\tau) ,$$
$$\theta_4\left(z + \frac{\pi}{2}, \tau\right) = \theta_3(z,\tau) ,$$
$$\theta_3(z \pm \pi, \tau) = \theta_3(z,\tau) . \tag{A7}$$

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