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LETTER TO THE EDITOR

Exact propagators for moving hard-wall potentials

M G E da Luz†‡ and Bin Kang Cheng†

† Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19.081, 81531 Curitiba, Brazil
‡ Departamento de Estado Solido, Institute de Física, Unicamp, Caixa Postal 6165, 13081 Campinas, Brazil

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Abstract. The semiclassical approximation has been used to evaluate the exact propagators for two one-dimensional quantum systems: (a) a free particle interacting with one hard-wall potential moving with constant velocity, and (b) a free particle inside a rigid box with one wall moving uniformly in time. The results derived from our propagators are in agreement with those of the corresponding Schrödinger equations.

The propagator can be represented by the sum over paths in the study of quantum mechanics through the Feynman path integral [1, 2]. It is well known that the Feynman approach to quantum mechanics is easy to formulate but results are difficult to evaluate. However, in the semiclassical approximation, only the classical paths contribute to the propagator and calculation of the propagator becomes much simpler. It is also interesting to note that semiclassical propagators are exact in most quantum dynamical systems such as the time-dependent quadratic Lagrangians [3, 4], a free particle [5–7] or an harmonic oscillator [8–10] interacting with a wedge and a free particle in a rigid box with fixed walls [11]. In this letter we discover two more such quantum systems: (a) a free particle interacting with one hard-wall potential moving with constant velocity, and (b) a free particle inside a rigid box with one wall moving uniformly in time.

Hard-wall potential moving with constant velocity. We assume that the hard-wall potential is located at $L(t) = ut$, where u is positive (negative) when it moves to the right (left) along the x-axis. The free particle has only two classical paths, one direct and the other indirect, which start from $x_a > L_a = L(t_a)$ at time t_a and arrive at $x_b > L_b = L(t_b)$ at time t_b.

For the direct path, the classical action is given by

$$S_d = m(x_b - x_a)^2/2T \qquad (T = t_b - t_a) \tag{1}$$

where m is the mass of the free particle. For convenience we consider that $u > 0$ and the initial velocity v is positive when the particle moves to the right along the x-axis, otherwise negative. For the indirect classical path the particle spends the time

$$t' = (x_a - L_a)/(u + v) \tag{2}$$

before hitting the wall and the time

$$t'' = [u(x_b - x_a) + v(x_b - L_a)]/(v + 2u)(v + u) \tag{3}$$

between colliding with the wall and arriving at x_b at time t_b. Here v and $v + 2u$ are, respectively, the speeds of the particle before and after collision with the wall. With the help of equations (2) and (3), we find that the initial speed of the particle must be

$$v = (2L_b - x_a - x_b)/T \tag{4}$$

for the indirect classical path. The corresponding classical action can then be shown to be

$$S_i = \frac{m}{2}\left(\int_0^{t'} v^2\,\mathrm{d}t + \int_0^{t''} (v+2u)^2\,\mathrm{d}t\right)$$

$$= \frac{m}{2T}[(x_b+x_a)^2 - 4u(x_a t_b + x_b t_a - u t_a t_b)]. \tag{5}$$

Using the well known formula of Van Vleck [12], we obtain the semiclassical propagator in the form

$$K_W(x_b, t_b; x_a, t_a)$$

$$= \left(\frac{m}{2\pi\mathrm{i}\hbar t}\right)^{1/2}\left[\exp\left(\frac{\mathrm{i}m}{2\hbar t}(x_b - x_a)^2\right)\right.$$

$$\left. - \exp\left(\frac{\mathrm{i}m}{2\hbar t}[(x_b+x_a)^2 - 4u(x_a t_b + x_b t_a - u t_a t_b)]\right)\right] \tag{6}$$

which reduces to the well known result [13] as expected. In (6) a relative phase of π has been included for the reflected classical path.

The corresponding Schrödinger equation is of the form

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = \mathrm{i}\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{7}$$

with the time-dependent boundary condition

$$\psi[L(t), t] = 0. \tag{8}$$

Substituting the wavefunction

$$\psi_k(x,t) = A\sin[k(x - L(t))]\exp[\mathrm{i}\varphi_k(x,t)] \tag{9}$$

into (7), we obtain

$$\psi_k(x,t) = \left(\frac{2}{\pi}\right)^{1/2}\sin[k(x - L(t))]\exp\left[\frac{\mathrm{i}mux}{\hbar} - \frac{\mathrm{i}\hbar}{2m}\left(\frac{m^2u^2}{\hbar^2} + k^2\right)t\right] \tag{10}$$

where we have chosen $A = (2/\pi)^{1/2}$ in order to satisfy the flux condition in quantum mechanics [14]. Using the spectral relation

$$K_W(x_b, t_b; x_a, t_a) = \int_0^\infty \psi_k^*(x_a, t_a)\psi_k(x_b, t_b)\,\mathrm{d}k \tag{11}$$

and the identity 3.898-1 in [15], we obtain equation (6) after integrating over the variable k. Furthermore, it vanishes at the moving wall or $K_W(x_b, t_b; ut_a, t_a) = K_W(ut_b, t_b; x_a, t_a) = 0$. Therefore, we conclude that the semiclassical propagator (6) is exact.

Rigid box with one wall moving uniformly with time. We assume that the fixed wall is located at $x=0$ and the moving wall at $x=l_0+ut=l(t)$ with $u>0$ and $l_0>0$. The free particle has an infinite number of classical paths which start from x_a at time t_a and arrive at x_b at time t_b. For the case of $x_a<x_b$, we can classify the classical paths by specifying which walls (the fixed or the moving) the particle collides with on the first and last collisions. There are four classes, namely:

(1) the first collision with the moving wall or no collisions at all;
(2) both the first and the last collisions with the fixed wall;
(3) the first collision with the fixed wall and the last collision with the moving wall;
(4) both the first and the last collisions with the moving wall.

Let us first consider the simplest case of $x_a=x_b=0$. In this special case, all the classical paths belong to class (1) as defined above. After careful analysis, we have

$$(v-2ju)t'_j=l_{j+1} \tag{12}$$

$$u(t''_j+t'_j)=l_{j+1}-l_j \qquad (j\geqslant 1) \tag{13}$$

$$(v-2ju)t''_j=l_j \qquad (j\geqslant 1) \tag{14}$$

with the initial condition

$$ut'_0=l_1-l_0-ut_a=l_1-l_a. \tag{15}$$

Hereafter, l_j $(j\geqslant 1)$ is the position of the moving wall when the particle hits it for the jth time and the particle spends t'_j (t''_j) travelling from $x=0$ $(x=l_j)$ to arrive at $x=l_j$ $(x=0)$ before (after) the jth collision with the moving wall. In deriving the above relations, the reduction speed of the particle by $2u$ after each collision with the moving wall has been taken into account.

Solving equations (12)–(15), we obtain

$$l_n=vl_a/[v-(2n-1)u] \qquad (n\geqslant 1) \tag{16}$$

$$t'_j=vl_a/(v-2ju)[v-(2j+1)u] \tag{17}$$

$$t''_j=vl_a/(v-2ju)[v-(2j-1)u] \tag{18}$$

$$t_j=t''_j+t'_j=2vl_a/[v-(2j-1)u][v-(2j+1)u]. \tag{19}$$

With the help of equations (16)–(19), we find

$$T=t_b-t_a=\sum_{j=1}^{n}(t'_{j-1}+t''_j)=\frac{2nl_a}{v-2nu}. \tag{20}$$

Therefore the initial speed of the particle must be

$$v=2nu+2nl_a/T=2nl_b/T \tag{21}$$

for a classical path which hits the moving wall n times. Now the corresponding classical action is given by

$$\begin{aligned} S_n&(0,t_b;0,t_a)\\ &=\frac{m}{2}\left(\int_0^{t'_0}v^2\,\mathrm{d}t+\sum_{j=1}^{n-1}\int_0^{t_j}(v-2ju)^2\,\mathrm{d}t+\int_0^{t''_n}(v-2nu)^2\,\mathrm{d}t\right)\\ &=2mn^2l_al_b/T \qquad (t_j=t'_j+t''_j) \end{aligned} \tag{22}$$

after straightforward evaluations.

For the general case of $x_a<x_b$, equation (12) should be modified as follows:

$$vt'_0=l_1+x \tag{23}$$

and

$$(v-2ju)t'_j=l_{j+1} \tag{24}$$

and equation (14) with $j=n$ should be changed to

$$(v-2nu)t_n' = l_n + y. \tag{25}$$

In equations (23)-(25), x and y respresent different quantities in the different classes of classical paths, ie.

(1) $x=-x_a$, $y=x_b$;
(2) $x=x_a$, $y=x_b$;
(3) $x=x_a$, $y=-x_b$;
(4) $x=-x_a$, $y=-x_b$.

Now we can repeat all the calculations and obtain

$$T=(x+y+2nl_a)/(v-2nu) \tag{26}$$

so the initial speed of the particle must be

$$v=2nu+(2nl_a+x+y)/T=(2nl_b+x+y)/T \tag{27}$$

for the classical path to have n collisions with the moving wall. The corresponding classical action is given by

$$S_n^{(j)}(x_b, t_b; x_a, t_a) = \frac{m}{2T}\Big((2nl_0+x+y)^2+4nu[(xt_b+yt_a)+nl_0(t_a+t_b)]+4n^2u^2t_at_b\Big) \qquad (j=1,2,3,4). \tag{28}$$

Using the well known formula of Van Vleck, we finally write the semiclassical propagator in the form

$$K_{WW}(x_b, t_b; x_a, t_a) = \left(\frac{m}{2\pi\mathrm{i}\hbar T}\right)^{1/2}\left(\sum_{n=0}^{\infty}\exp[\mathrm{i}S_n^{(1)}/\hbar]-\sum_{n=0}^{\infty}\exp[\mathrm{i}S_n^{(2)}/\hbar] + \sum_{n=1}^{\infty}\exp[\mathrm{i}S_n^{(3)}/\hbar]-\sum_{n=1}^{\infty}\exp[\mathrm{i}S_n^{(4)}/\hbar]\right). \tag{29}$$

Here a relative phase of π for the classical paths of classes (2) and (4) has been included since they have an odd number of collisions with the moving wall. Substituting (28) with different values of j into (29), we obtain the semiclassical propagator as

$$K_{WW}(x_b, t_b; x_a, t_a) = \left(\frac{m}{2\pi\mathrm{i}\hbar T}\right)^{1/2}\left[\exp\left(\frac{\mathrm{i}m(x_b-x_a)^2}{2\hbar T}\right)\theta_3\left(\frac{m(x_bl_a-x_al_b)}{\hbar T}, \frac{2ml_al_b}{\pi\hbar T}\right) - \exp\left(\frac{\mathrm{i}m(x_a+x_b)^2}{2\hbar T}\right)\theta_3\left(\frac{m(x_bl_a+x_al_b)}{\hbar T}, \frac{2ml_al_b}{\pi\hbar T}\right)\right] \tag{30}$$

where $\theta_3(z,\tau)$ is the Jacobi theta function [15]. Applying the following identity:

$$\theta_3(z,\tau)=(-\mathrm{i}\tau)^{-1/2}\exp(-\mathrm{i}z^2/\pi\tau)\theta_3(z/\tau, -1/\tau) \tag{31}$$

to (30), we get the propagator in the form

$$K_{WW}(x_b, t_b; x_a, t_a)$$
$$= \frac{2}{\sqrt{l_a l_b}} \exp\left[\frac{imu}{2\hbar}\left(\frac{x_b^2}{l_b} - \frac{x_a^2}{l_a}\right)\right] \sum_{n=1}^{\infty} \exp\left[\frac{in^2\pi^2\hbar}{2mu}\left(\frac{1}{l_b} - \frac{1}{l_a}\right)\right]$$
$$\times \sin(n\pi x_b/l_b)\sin(n\pi x_a/l_a). \tag{32}$$

In deriving the above equation we also used the definition of the theta function $\theta_3(z, \tau)$.

We derive the time-dependent wavefunctions from the propagator (32) by spectral resolution

$$\psi_n(x, t) = \left(\frac{2}{l(t)}\right)^{1/2} \exp\left(\frac{imux^2}{2\hbar l(t)}\right) \sin[n\pi x/l(t)] \exp\left(\frac{in^2\pi^2\hbar}{2mul(t)}\right). \tag{33}$$

These are in agreement with those of the corresponding Schrödinger equation [16–18]. We should remark that the authors of [16] inserted an extra factor, $\exp(-in^2\pi^2\hbar/2mul_0)$, in the wavefunctions in order to include the fixed-wall case. However, it is apparent that this factor does not appear in the propagator, hence we conclude that the semiclassical propagator (30) is exact [19].

In this letter, we have discovered two more quantum systems in which the entire contribution to the propagator comes from the classical paths alone and the relative phase of each classical path depends on the total number of collisions between the particle and the walls (fixed or moving). With the help of Van Vleck, we evaluated these semiclassical propagators which happen to be exact. A study of the case in which the hard-wall potential moves periodically in time [17, 18] is in progress and will be reported in due course.

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