Path integration via Hamilton-Jacobi coordinates and applications to potential barriers

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The path integral for the propagator is reduced to an ordinary integral in terms of the generators of a canonical transformation, and is evaluated exactly for square potential barriers in one dimension and for the radial square-well potential in two dimensions.

I. INTRODUCTION

The set of dynamical systems for which one can perform the path-integral quantization and obtain the exact propagator is gradually growing. We wish to add to this list the tunneling through square potential barriers. Because tunneling is, from a particle point of view, a nonclassical phenomenon, it is interesting to see how the process looks from the path-integral point of view where one sums over all possible trajectories. No exact solution of this problem by path integration is known to us. Such problems have previously been discussed in the semiclassical approximation of path integrals only, and compared with the WKB approximation of quantum mechanics.[1,2]

It is remarkable that although the solution of the Schrödinger equation for square potentials is most elementary, their path-integral treatment is by no means trivial. The source of the difficulty is the following. For finite-range potential barriers or wells, the range of the Gaussian coordinate integrations, in the time-graded formulation of the path integrals, is finite. For infinite potential-well problems, or for a particle confined to a half space, this difficulty can be overcome by the method of images.[3,4] This method, however, does not help for potentials of finite height.

In this paper we solve this problem by transforming it into the Hamilton-Jacobi coordinates. In Sec. II we describe the general method and then present the solution for the one-dimensional square-well solution in Sec. III. In Sec. IV we apply the method to the radial hard-core potential in two dimensions, which have also some relevance to the much discussed path-integral problems in polar coordinates.[5]

II. GENERAL THEORY

The propagator for a one-dimensional potential $V(x)$ in the phase-space formulation is given by the functional integral

$$K(x_b,x_a;t_b,t_a) = \int \mathcal{D}p\,\mathcal{D}x \exp\left[\pm\int_{t_a}^{t_b} dt[p\dot{x}-p^2/2m-V(x)]\right] , \quad (1)$$

which is explicitly *defined* by

$$K(x_b,x_a;t_b,t_a)= \lim_{\substack{n\to\infty\\ \epsilon\to 0}} \int \prod_{j=1}^{n} dx_j \prod_{j=1}^{n+1} \frac{dp_j}{2\pi}\exp\{i[p_j(x_j-x_{j-1})-\epsilon(p_j^2/2m)-\epsilon V(x_j)]\} . \quad (2)$$

We shall use the method of canonical transformations to the Hamilton-Jacobi coordinates. This method was earlier applied to linear and quadratic potentials.[6] But for most of the other potentials the new coordinates become elliptic functions of the old coordinates and the method appears to be not tractable. However, in the present problems of tunneling through barriers, it turns out to be very useful, as we shall show. The method of summation over the eigenvalues to obtain the propagator is difficult for the same problem.

The idea here is to convert the Hamiltonian into a null Hamiltonian by absorbing the potential in a new generalized momentum P (or in a new generalized coordinate Q) whose square is the old Hamiltonian. For example, we may set

$$P^2=p^2/2m+V(x) \quad \text{or} \quad P=[p^2/2m+V(x)]^{1/2} . \quad (3)$$

The generating function for this transformation is

$$F_2(x,P,t)=\int^x dx\{2m[P^2-V(x)]\}^{1/2}-P^2t . \quad (4)$$

The new Hamiltonian thus vanishes identically,

$$K\equiv H+\partial F_2/\partial t=0 , \quad (5)$$

and we have the following relations:

$$P=\partial F_2/\partial x=\{2m[P^2-V(x)]\}^{1/2} , \quad (6)$$

$$Q=\partial F_2/\partial P=\int^x \frac{4mPdx}{\{2m[P^2-V(x)]\}^{1/2}}-2Pt . \quad (7)$$

In terms of the new pair of conjugate variables P and Q the action becomes

$$\int dt(p\dot{x}-H)=\int dt(-Q\dot{P}-K+\partial F_2/\partial t) = \int dt(-Q\dot{P}+\partial F_2/\partial t) . \quad (8)$$

In the time-sliced path integrals, Eq. (2), we introduce the new variables except in the last integral, $\int dp_{n+1}$, which we keep and denote simply by $\int dp$, so that Eq. (2) becomes, using Eq. (8) for each j and the invariance of phase-space volume under canonical transformations,

$$K(x_b,x_a;t_b,t_a) = \int \frac{dp}{2\pi} \prod_{j=1}^{n} \left[dQ_j \frac{dP_j}{2\pi} \right] e^{-iQ_j(P_j-P_{j+1})} e^{iF_2|_a^b} , \quad (9)$$

as can be seen by explicit calculation. As usual the Q_j integrations give $\delta(P_j-P_{j+1})$. The P_j integrations thereafter give $P_1=P_2=\cdots=P_n$. Hence we are left with a simple and general formula

$$K(x_b,x_a;t_b,t_a)=\int \frac{dp}{2\pi} e^{i[F_2(b)-F_2(a)]} , \quad (10)$$

where dp has to be obtained from Eq. (6) in terms of dP, x being constant at end points b and a. Thus the path integration is reduced to an ordinary integration and the whole dynamics is in F_2, more precisely, in the increase of F_2 between the points x_a and x_b.

The propagator (10) satisfies the Schrödinger equation in each variable separately. This is proved easily by inserting K in (10) into the Schrödinger equation and using $\partial F_2/\partial t = P$ and Eq. (6). Furthermore, K is continuous if F_2 is, and the reproducing kernel property of K can be obtained:

$$\psi(x_b,t_b)=\int_{-\infty}^{+\infty} dx_a K(x_b,x_a;t_b,t_a)\psi(x_a,t_a) . \quad (11)$$

Alternatively, if one chooses to define the new coordinate Q as a function of the original Hamiltonian, one has to use the generating function $F_1(x,Q,t)$. In that case the action transforms as

$$\int dt(p\dot{x}-H)=\int dt(P\dot{Q}-\partial F_1/\partial t) , \quad (12)$$

and then, instead of Eq. (10), we obtain the new formula

$$K(x_b,x_a;t_b,t_a)=\int \frac{dp}{2\pi} e^{iP(Q_b-Q_a)+i[F_1(b)-F_1(a)]} , \quad (13)$$

where P stands for $P_1=P_2=\cdots=P_{n+1}\equiv P$. In Sec. IV we shall also use a mixed transformation involving both F_1 and F_2.

III. TUNNELING THROUGH A SQUARE BARRIER

For a collection of potential barriers, Eq. (4) can easily be integrated. For example, for a single barrier

$$V=V_0[\Theta(x+a)-\Theta(x)]\equiv V_0\tilde{\Theta}_1(x) , \quad (14)$$

we obtain

$$F_2(x,P,t)= -P^2t+\sqrt{2m}\,Px\tilde{\Theta}_2(x) + \sqrt{2m}\,(P^2-V_0)^{1/2}x\tilde{\Theta}_1(x)+C , \quad (15)$$

where

$$\tilde{\Theta}_2(x)=\Theta(-x-a)+\Theta(x) \quad (16)$$

and C is an integration constant which may depend on p but which will drop out in the propagator.

From (6) we have, further,

$$dp=\sqrt{2m}\,\tilde{\Theta}_2(x)dP+\frac{2mPdP}{[2m(P^2-V_0)]^{1/2}}\tilde{\Theta}_1(x) . \quad (17)$$

Inserting (17) and (15) into (10) we get with $t_{\hat{a}}=T$, $t_{\hat{b}}=0$,

$$\begin{aligned} K(x_b,x_a;T)= {} & [\tilde{\Theta}_2(x_b)\tilde{\Theta}_2(x_a)+\tilde{\Theta}_1(x_b)\tilde{\Theta}_1(x_a)e^{-iV_0T}](\sqrt{2m}/2\pi)\int dP \exp[i\sqrt{2m}(x_b-x_a)P-iTP^2] \\ & +\tilde{\Theta}_2(x_b)\tilde{\Theta}_1(x_a)(\sqrt{2m}/2\pi)\int dP \exp\{i\sqrt{2m}\,x_bP-ix_a[2m(P^2-V_0)]^{1/2}-iTP^2\} \\ & +\tilde{\Theta}_1(x_b)\tilde{\Theta}_2(x_a)(\sqrt{2m}/2\pi)e^{-iV_0T}\int dP \exp\{i\sqrt{2m}\,x_bP-ix_a[2m(P^2+V_0)]^{1/2}-iTP^2\} . \end{aligned} \quad (18)$$

This result looks simple but could not have been written directly in an easy way. For the simpler case of a potential step at $x=0$, i.e.,

$$V(x)=V_0\Theta(x) , \quad (19)$$

we find

$$\begin{aligned} K(x_b,x_a;T)= {} & \Theta(-x_b)\Theta(-x_a)(\sqrt{2m}/2\pi)\int dP \exp[i\sqrt{2m}(x_b-x_a)P-iTP^2] \\ & +\Theta(-x_b)\Theta(-x_a)(\sqrt{2m}/2\pi)\int dP \exp\{i\sqrt{2m}\,x_bP-ix_a[2m(P^2-V_0)]^{1/2}-iTP^2\} \\ & +\Theta(x_b)\Theta(-x_a)(\sqrt{2m}/2\pi)e^{-iV_0T}\int dP \exp\{i\sqrt{2m}\,x_bP-ix_a[2m(P^2+V_0)]^{1/2}-iTP^2\} \\ & +\Theta(x_b)\Theta(x_a)(\sqrt{2m}/2\pi)e^{-iV_0T}\int dP \exp[i\sqrt{2m}(x_b-x_a)P-iTP^2] . \end{aligned} \quad (20)$$

The verification of (11) is performed by contour integration.

IV. RADIAL POTENTIAL BARRIER IN TWO DIMENSIONS

In this section we will study the two-dimensional radial potential

$$V=V_0\Theta(R-r) . \quad (21)$$

In order to transform the Hamiltonian

$$H=\frac{1}{2m}[P_r^2+(1/r^2)P_\phi^2]+V_0\Theta(R-r) \tag{22}$$

into a null one we employ a "mixed" generating function which is F_2 type in radial coordinates and F_1 type in the angular coordinates:

$$\begin{aligned}F(r,P_r;\phi,Q_\phi)&=-(P_r^2/2m)t+Q_\phi\phi+\int dr[P_r^2-2mV_0\Theta(R-r)-(Q_\phi^2/r^2)]^{1/2}\\&=-(P_r^2/2m)t+Q_\phi\phi+\Theta(R-r)\{[(P_r^2-2mV_0)r^2-Q_\phi^2]^{1/2}-Q_\phi\arccos[Q_\phi/r(P_r^2-2mV_0)^{1/2}]\}\\&\quad+\Theta(r-R)[(P_r^2r^2-Q_\phi^2)^{1/2}-Q_\phi\arccos(Q_\phi/rP_r)]\ ,\end{aligned} \tag{23}$$

whence the momenta and coordinates in terms of the old ones are given by

$$\begin{aligned}P_\phi&=-\phi+\arccos[p_\phi/(p_r^2r^2+p_\phi^2)^{1/2}]\ ,\\P_r&=\Theta(R-r)[(p_r^2+2mV_0)+p_\phi^2/r^2]^{1/2}\\&\quad+\Theta(r-R)[p_r^2-p_\phi^2/r^2]^{1/2}\ ,\\Q_r&=-(P_r/m)r\\&\quad+\Theta(R-r)\frac{r}{p_r^2r^2+p_\phi^2}[(p_r^2+2mV_0)r^2+p_\phi^2]^{1/2}\\&\quad+\Theta(r-R)\frac{r^2p_r}{(p_r^2r^2+p_\phi^2)^{1/2}}\ ,\\Q_\phi&=p_\phi\ .\end{aligned} \tag{24}$$

The kernel can then be obtained from (10) and (13) as

$$\begin{aligned}K(\mathbf{r}_b,r_a;T)&=\int\frac{dp_rdp_\phi}{(2\pi)^2r_b}e^{iP_\phi(Q_b-Q_a)+i[F(b)-F(a)]}\\&\equiv\int\frac{dp_rdp_\phi}{(2\pi)^2r_b}e^{iA_{ba}}\ ,\end{aligned} \tag{25}$$

where we have again set $t_a=0$, $t_b=T$. This kernel can be expressed as the sum of four pieces depending on the values of r_a,r_b.

(i) $r_a<R$, $r_b<R$. We have to evaluate $P_\phi Q_\phi+F$ at the point $\mathbf{r}_a$ and $\mathbf{r}_b$:

$$\begin{aligned}&P_\phi Q_\phi+F\\&\quad=P_\phi Q_\phi+\{rp_r-Q_\phi\arccos[Q_\phi/r(p_r^2+p_\phi^2/r^2)^{1/2}]\\&\qquad+Q_\phi\phi-(P_r^2/2m)t\}\ .\end{aligned}$$

From (24) we observe that the third term cancels with the first and fourth terms. Then we have

$$P_\phi Q_\phi+F=rp_r-(P_r^2/2m)t \tag{26}$$

or

$$A_{ab}=r_bp_r-r_ap_{r_1}-(1/2m)[(p_r^2+2mV_0)+(p_\phi^2/r_b^2]T\ , \tag{27}$$

where we dropped the subscript $(n+1)$ from the momentum at point $\mathbf{r}_b$. In (27) we have to express p_r, which is the radial momentum at the point $\mathbf{r}$, in terms of the momentum at the point $\mathbf{r}_b$. For this purpose we first observe that

$$\begin{aligned}p_r&=[(P_r^2-2mV_0)-Q_\phi^2/r^2]^{1/2}\\&=[(P_r^2-2mV_0)]^{1/2}[(1-\cos^2(P_\phi+\phi)]^{1/2}\\&=[(P_r^2-2mV_0)]^{1/2}\sin(P_\phi+\phi)\ ,\end{aligned} \tag{28}$$

which is valid for every point $\mathbf{r}$. Then, using $P_{r_1}=P_{r_{n+1}}\equiv P_r$, $P_{\phi_1}=P_{\phi_{n+1}}\equiv P_\phi$, we can write p_{r_1} as

$$\begin{aligned}p_{r_1}&=(P_r^2-2mV_0)^{1/2}\sin(P_\phi+\phi_a)\\&=(P_r^2-2mV_0)^{1/2}\sin[P_\phi+\phi_b-(\phi_b-\phi_a)]\\&=(P_r^2-2mV_0)^{1/2}[\sin(P_\phi+\phi_b)\cos(\phi_b-\phi_a)\\&\qquad-\cos(P_\phi+\phi_b)\sin(\phi_b-\phi_a)]\\&=p_r\cos(\phi_b-\phi_a)\\&\quad-(P_r^2-2mV_0)^{1/2}[1-\sin^2(P_\phi+\phi_b)]^{1/2}\sin(\phi_b-\phi_a)\\&=p_r\cos(\phi_b-\phi_a)-\frac{p_\phi}{r_b}\sin(\phi_b-\phi_a)\ .\end{aligned} \tag{29}$$

Inserting (29) into (27) and using (25) we have the first term of the kernel:

$$\begin{aligned}K_1&=\Theta(R-r_a)\Theta(R-r_b)\\&\quad\times\int\frac{dp_rdp_\phi}{(2\pi)^2r_b}\exp[-(iT/2m)(p_r^2+2mV_0+p_\phi^2/r_b^2)]\\&\qquad\times\exp[ir_bp_r-ir_ap_r\cos(\phi_b-\phi_a)\\&\qquad\quad+i(p_\phi/r_b)r_a\sin(\phi_b-\phi_a)]\ ,\end{aligned} \tag{30}$$

which after integrations gives

$$\begin{aligned}K_1&=\Theta(R-r_b)\Theta(R-r_a)(m/2\pi iT)e^{-iV_0T}\\&\quad\times\exp\{(im/2T)[r_b^2+r_a^2-2r_ar_b\cos(\phi_b-\phi_a)]\}\ .\end{aligned} \tag{31}$$

(ii) $r_b>R$, $r_a>R$. This part can be worked out in a way similar to the previous case and leads to

$$\begin{aligned}K_2&=\Theta(r_b-R)\Theta(r_a-R)(m/2\pi iT)\\&\quad\times\exp\{i(m/2T)[r_b^2+r_a^2-2r_ar_b\cos(\phi_b-\phi_a)]\}\ .\end{aligned} \tag{32}$$

(iii) $r_b < R$, $r_a > R$. Using

$$p_{r_1} = P_r \sin(P_\phi + \phi_a) \tag{33}$$

we obtain

$$A_{ab} = r_b p_r - P_r \sin(P_\phi + \phi_a) - (T/2m)[p_r^2 + 2mV_0 + (p_\phi^2/r_b)] ,$$

or expressing p_r in terms of the new momenta,

$$A_{ab} = r_b (P_r^2 - 2mV_0)^{1/2} \sin(P_\phi + \phi_b) - r_a P_r \sin(P_\phi + \phi_a) - (T/2m) P_r^2 . \tag{34}$$

Finally, inserting (32) into (25) and transforming these integration variables to the new momenta by

$$dp_r dp_\phi = r_b P_r dP_r dP_\phi ,$$

we get

$$K_3 = \Theta(R - r_b)\Theta(r_a - R) \times \int \frac{P_r dP_r dP_\phi}{(2\pi)^2} \exp[i r_b (P_r^2 - 2mV_0)^{1/2} \sin(P_\phi + \phi_b)] \times \exp[-i r_a P_r \sin(P_\phi + \phi_a) - i(T/2m)P_r^2] . \tag{35}$$

(iv) $r_b > R$, $r_a < R$. This time p_{r_1} is given by

$$p_{r_1} = (P_r^2 - 2mV_0)^{1/2} \sin(P_\phi + \phi_a) , \tag{36}$$

and we have

$$A_{ab} = r_b P_r \sin(P_\phi + \phi_b) - r_a (P_r^2 - 2mV_0)^{1/2} \sin(P_\phi + \phi_a) - (T/2m) P_r^2 . \tag{37}$$

Thus the last term of the kernel is

$$K_4 = \Theta(r_b - R)\Theta(R - r_a) \times \int \frac{P_r dP_r dP_\phi}{(2\pi)^2} \exp[i r_b P_r \sin(P_\phi + \phi_b)] \times \exp[-i r_a (P_r^2 - 2mV_0)^{1/2} \sin(P_\phi + \phi_b) - i(T/2m)P_r^2] . \tag{38}$$

The final form of the kernel is

$$K = K_1 + K_2 + K_3 + K_4 , \tag{39}$$

with four terms given by Eqs. (31), (32), (35), and (38). One can easily check that this kernel satisfies the Schrödinger equation at points $\mathbf{r}_a$ and $\mathbf{r}_b$, and also satisfies the condition $K \rightarrow \delta(\mathbf{r}_a - \mathbf{r}_b)$ as $T \rightarrow 0$. Finally, we would like to emphasize that the calculation we presented in this section may also be suggestive as an explicit presentation of a polar coordinate path integral.

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