PHYSICAL REVIEW D VOLUME 22, NUMBER 12 15 DECEMBER 1980

Quantum mechanics on the half-line using path integrals

T. E. Clark,* R. Menikoff, and D. H. Sharp
Theoretical Division, Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico 87545
(Received 8 August 1980)

We study the Feynman path-integral formalism for the constrained problem of a free particle moving on the half-line. It is shown that the effect of the boundary condition at the origin can be incorporated into the path integral by a simple modification of the action. The small-time behavior of the Green's function can be obtained from the stationary-phase evaluation of our expression for the path integral, which in this case includes contributions from both the direct and reflected classical paths.

I. INTRODUCTION

Constrained quantum-mechanical problems are sometimes of interest. One of the simplest to consider is one in which a dynamical degree of freedom is restricted to be positive. In this paper we consider the example of a free particle restricted to move on the positive half-line. The constraint that the coordinate be positive results in a boundary condition at the origin, which can be taken account of in a well-known manner in the operator formulation of quantum mechanics. Here we show how this can be done using the path-integral formulation.[1]

In the usual Feynman path integral for the Green's function, the paths are weighted by $\exp[(i/\hbar)S]$, where S is the classical action. Our principal result is that in the constrained problem the boundary condition at the origin can be incorporated into the path integral by a simple modification of the action. This is established by showing that the sum over paths is the continuum limit of a (discrete) random walk, with the continuum boundary conditions accounted for by an elastic barrier at the origin. We also show that a stationary-phase evaluation of our expression for the path integral results in the correct small-time behavior of the exact Green's function for a free particle on the half-line. To obtain this result, it is necessary to include in the evaluation of the integral the contribution of each of the two classical paths (direct and reflected) which connect a given pair of points.

Our approach relies heavily on concepts and techniques familiar in the probability theory of diffusion processes (Brownian motion). In fact, many of our results are already known in this context.[2,3] Here, we are mainly emphasizing their application in quantum-mechanical problems.

II. OPERATOR FORMALISM

In this section we review the standard quantum-mechanical solution for the behavior of a free particle on the half-line. Since the mathematical framework is well known,[4] we simply state without proof the needed results.

The Hamiltonian $H=-(\hbar^2/2m)d^2/dx^2$, regarded as defined on infinitely differentiable functions vanishing outside a closed interval of $(0,\infty)$, is not essentially self-adjoint in $L^2([0,\infty),dx)$. However, it has a continuous one-parameter family of self-adjoint extensions. Physically, the different self-adjoint extensions correspond to the different ways that a wave packet can reflect off the boundary at $x=0$, while conserving probability.[5] Mathematically, the domains of self-adjointness are characterized by the boundary condition at the origin. Specifically, for each $\beta\in(-\infty,\infty]$ there is an extension of the domain of H such that the wave functions in the respective domains satisfy

$$\psi(0)=\beta\psi'(0)\,. \tag{2.1}$$

The Hamiltonian has a continuous spectrum with eigenvalues $0\leqslant\hbar^2p^2/2m\leqslant\infty$ and associated eigenfunctions

$$\psi_p(x)=\left(\frac{2}{\pi}\right)^{1/2}\cos(px+\phi_p)\,, \tag{2.2}$$

where

$$\tan\phi_p=-(1/p\beta)\,. \tag{2.3}$$

For each β the eigenfunctions are normalized

$$\int_0^\infty dx\,\psi_p^*(x)\psi_q(x)=\delta(p-q) \tag{2.4a}$$

and complete

$$\int_0^\infty dp\,\psi_p^*(x)\psi_p(y)=\delta(x-y)\,. \tag{2.4b}$$

Finally, the Green's function is given by

$$G(x,y,t)=\int_0^\infty dp\, e^{-i(\hbar^2/2m)tp^2}\psi_p^*(x)\psi_p(y)$$
$$=(m/2\pi\hbar i t)^{1/2}\left\{\exp\left[\frac{im}{2\hbar}\frac{(x-y)^2}{t}\right]+\exp\left[\frac{im}{2\hbar}\frac{(x+y)^2}{t}\right]\right\}$$
$$-\beta^{-1}\exp\left[\frac{i\hbar}{2m\beta^2}t+\frac{(x+y)}{\beta}\right]\operatorname{erfc}\left[\left(\frac{i\hbar t}{2m\beta^2}\right)^{1/2}+\left(\frac{x+y}{2\beta}\right)\left(\frac{i\hbar t}{2m\beta^2}\right)^{-1/2}\right], \tag{2.5}$$

where

$$\operatorname{erfc}(z)=\frac{2}{\sqrt{\pi}}\int_0^\infty dx\, e^{-(x+z)^2}.$$

It is easily verified that G satisfies the Schrödinger equation

$$\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)G(x,y,t)=0\,,\quad t\geqslant 0$$

and the boundary conditions

$$G(x,y,0)=\delta(x-y)\,,$$
$$G(0,y,t)=\beta\left(\frac{\partial G}{\partial x}\right)(0,y,t)\,.$$

It will prove useful in later sections to analytically continue this quantum-mechanical problem into a diffusion problem. This is done by letting $t\to -it$. Furthermore, in order to compare the above results with those to be obtained in the next section by summing over paths, it is convenient to have the Laplace transform of $G(x,y,-it)$ with respect to t. This is

$$\tilde{G}(x,y,s)\equiv\int_0^\infty dt\, G(x,y,-it)e^{-st}$$
$$=(m/2\hbar s)^{1/2}\{\exp[-(x-y)(2ms/\hbar)^{1/2}]+\exp[-(x+y)(2ms/\hbar)^{1/2}]\}$$
$$-2(m/2\hbar s)^{1/2}[1+\beta(2ms/\hbar)^{1/2}]^{-1}\exp[-(x+y)(2ms/\hbar)^{1/2}]\,. \tag{2.6}$$

III. EVALUATION OF THE GREEN'S FUNCTION AS A SUM OVER PATHS

In the Feynman formulation of quantum mechanics, the Green's function is expressed as a sum over paths, each path having an appropriate weight. In this section we evaluate the Green's function for a free particle on the half-line as a sum over paths and show that a different result is associated with each distinct self-adjoint extension of the Hamiltonian. To establish these results, we consider the paths as a continuum limit of an appropriate random walk, in which an elastic barrier at the origin accounts for the boundary conditions.

We begin by using a random walk to derive the Green's function for a free particle on the whole line. Consider a random walk in which a particle has an equal probability to move a distance Δx to the left or right in a time interval Δt. Summing over all the ways to go from one point to another gives the total probability for the particle to go from x to y in time t:

$$g(x,y,t)=\left(\frac{1}{2}\right)^n\frac{n!}{\left(\frac{n+m}{2}\right)!\left(\frac{n-m}{2}\right)!}\,,\quad \text{for } n+m \text{ even} \tag{3.1}$$

where n is the number of time steps, $[t/\Delta t]$, m is the number of steps between x and y, $[(x-y)/\Delta x]$, and $[x]$ stands for the largest integer smaller than x.

The generating function for $g(x,y,t)$ is defined by

$$\tilde{g}(x,y,\sigma)=\sum_{n=0}^\infty g(x,y,n\Delta t)\sigma^n\,. \tag{3.2}$$

It satisfies the inhomogeneous difference equation

$$\tilde{g}(x,y,\sigma)=\delta_{x,y}+\tfrac{1}{2}\sigma[\tilde{g}(x+\Delta x,y,\sigma)+\tilde{g}(x-\Delta x,y,\sigma)]\,, \tag{3.3}$$

with the boundary condition $\tilde{g}(x,y,\sigma)\to 0$ as $|x-y|\to\infty$, Eq. (3.3) has the solution

$$\tilde{g}(x,y,\sigma)=(1-\sigma^2)^{-1/2}\lambda^{[|x-y|/\Delta t]}\,, \tag{3.4}$$

where $\lambda=[1-(1-\sigma^2)^{1/2}]/\sigma$.

To pass from the random walk to the Brownian-motion description[6] needed in the path-integral formulation, we let $\Delta x \to 0$ and $\Delta t \to 0$ in such a way that $(\Delta x)^2/\Delta t \to (\hbar/m)$. With the identifications $\sigma \to \exp(-s\Delta t)$ and $\sum_n \to (\Delta t)^{-1}\int dt$, the generating function converges to the Laplace transform of the usual Green's function

$$\tilde{g}(x,y,\sigma)(\Delta t/\Delta x) \to \tilde{G}(x,y,s) = (m/2\hbar s)^{1/2}\exp[-(x-y)(2ms/\hbar)^{1/2}]. \quad (3.5)$$

To solve the problem on the half-line requires that the previous discussion be modified to account for the boundary conditions at the origin. In the random-walk description, the appropriate boundary condition is that the particle has a probability γ to be reflected from the origin and a probability $1-\gamma$ to be absorbed. This is called an "elastic barrier" in probability theory.

Let $g_+(x,y,t)$ be the probability to go from x to y $(x,y \in [0,\infty))$ in time t. This transition probability satisfies a simple recursion relation based on the probability for the particle to reach the origin for the first time. In terms of the auxiliary quantities

$g_0(x,y,t)$ = the probability to go from x to y in time t without reaching the origin [$=g_+(x,y,t)$ when $\gamma=0$],

$u(x,t)$ = the probability that the first passage from $x>0$ to 0 occurs at time t,

$v(t)$ = the probability that the first passage from 0 to 0 occurs at time t,

the recursion relations for $g_+(x,y,t)$ can be written as

$$g_+(x,y,n\Delta t) = g_0(x,y,n\Delta t) + \sum_m u(x,m\Delta t)g_+(0,y,(n-m)\Delta t) \quad \text{for } x,\ y>0 \quad (3.6)$$

and

$$g_+(0,y,n\Delta t) = 2\gamma u(y,n\Delta t) + \sum_m v(m\Delta t)g_+(0,y,(n-m)\Delta t) \text{ for } y>0. \quad (3.7)$$

Iterating these recursion relations would express $g_+(x,y,t)$ as a sum over classes of paths, each term corresponding to paths reflected off the origin a definite number of times, n, with an additional weight γ^n. However, since these equations are of convolution type they can be more readily solved by introducing generating functions $\tilde{g}_+$, $\tilde{g}_0$, $\tilde{u}$, and $\tilde{v}$ for g_+, g_0, u, and v, respectively. Then Eqs. (3.6) and (3.7) take the form

$$\tilde{g}_+(x,y,\sigma) = \tilde{g}_0(x,y,\sigma) + \tilde{u}(x,\sigma)\tilde{g}_+(0,y,\sigma) \quad (3.8)$$

and

$$\tilde{g}_+(0,y,\sigma) = 2\gamma\tilde{u}(y,\sigma) + \tilde{v}(\sigma)\tilde{g}_+(0,y,\sigma), \quad (3.9)$$

which have the solution

$$\tilde{g}_+(x,y,\sigma) = \tilde{g}_0(x,y,\sigma) + \frac{2\gamma\tilde{u}(x,\sigma)\tilde{u}(y,\sigma)}{1-\tilde{v}(\sigma)}. \quad (3.10)$$

To complete the solution we must determine $\tilde{g}_0$, $\tilde{u}$, and $\tilde{v}$. The probability $\tilde{g}_0$ corresponds to the case of a totally absorbing barrier. It can be found from the transition probability for a free particle on the whole line as follows. The paths from x to y on the whole line can be divided into two classes: those never reaching the origin and those reaching or passing through the origin. The second class is in one-to-one correspondence with paths from x to $-y$. By subtracting the contribution from this second class of paths we find

$$\tilde{g}_0(x,y,\sigma) = \tilde{g}(x,y,\sigma) - \tilde{g}(x,-y,\sigma),$$

where $\tilde{g}(x,y,\sigma)$ is given by Eq. (3.4).

The probability $\tilde{u}$ is equivalent to the well-known "gambler's ruin" problem on the interval $[0,\infty)$. The solution is[6]

$$\tilde{u}(x,\sigma) = \lambda^{[x/\Delta x]}, \quad (3.11)$$

where as before $\lambda=[1-(1-\sigma^2)^{1/2}]/\sigma$. Finally, the probability v is related to u by

$$v(t) = \gamma u(\Delta x, t-\Delta t)$$

or

$$\tilde{v}(\sigma) = \gamma\sigma\tilde{u}(\Delta x,\sigma). \quad (3.12)$$

Combining these results with Eq. (3.10) we obtain

$$\tilde{g}_+(x,y,\sigma) = [1-\sigma^2]^{-1/2}\left\{\lambda^{[|x-y|/\Delta x]} + \lambda^{[|x+y|/\Delta x]} - \left[1+\left(\frac{\gamma}{1-\gamma}\right)(1-\sigma^2)^{1/2}\right]^{-1}\lambda^{[(x+y)/\Delta x]}\right\}. \quad (3.13)$$

Passing to the continuum limit as before, with the additional condition $\gamma \to 1-\Delta x/\beta$, we recover the Green's function for a free particle on the half-line, Eq. (2.5). Note that for $\beta>0$, $\gamma \nearrow 1$ as $\Delta x \to 0$ and thus γ has a conventional probability interpretation. For $\beta<0$, $\gamma \searrow 1$ as $\Delta x \to 0$. In this case γ can simply be considered as a parameter which has the effect of changing the relative weights of paths such that those which hit the origin are more probable.

IV. EFFECT OF BOUNDARY CONDITIONS ON THE FEYNMAN PATH INTEGRAL

In the previous section we saw that the Green's function (2.5) could be derived by making the problem a discrete random walk on the half-line with an elastic barrier, summing over paths and taking an appropriate continuum limit. However, in continuum language the Feynman "sum-over-paths" is usually, and most conveniently, written as an integral over paths, with each path receiving the weight $\exp[(i/\hbar)$ (classical action)]. In this section we show, by a direct probability theory calculation, that the effect of the boundary at the origin can be included in this prescription by adding a simple term to the action or, equivalently, by modifying the free measure on paths.

Our principal result is that the path integral for the Green's function for a free particle on the half-line is

$$G(x,y,T)=\int \mathfrak{D}_+(x(t))\exp\left[\frac{i}{\hbar}\left(\int_0^T \frac{m}{2}\dot{x}^2(t)dt + \frac{\hbar^2}{m\beta}\int_0^T \delta(x(t))dt\right)\right], \tag{4.1}$$

where $x(t)\geq 0$, $x(0)=x$, and $x(T)=y$. Equation (4.1) is a formal expression, which must be interpreted as an appropriate limit. We will discuss the derivation of each of the three factors in Eq. (4.1).

The first term in the exponential in Eq. (4.1) is the usual action for a free particle. It results by the central limit theorem from the random walk on the whole line in the limit $(\Delta x)^2/\Delta t \to \hbar/m$.

To interpret the second term in the exponential we introduce a quantity called "local time" in probability theory. The local time at $x=0$ for a path ω is defined as

$$t_l(0,\omega)=\tfrac{1}{2}\lim_{\Delta x\to 0}\frac{\mu\{0\leq s\leq t; x(s,\omega)<\Delta x\}}{\Delta x}, \tag{4.2}$$

where μ is Lebesque measure. Note that t_l has dimensions of 1/velocity. For the random walk on the half-line discussed in Sec. III, $t_l(0,\omega)=n\Delta t/\Delta x$, where n is the number of times the path ω hits the origin. Thus, for Δx small,

$$\exp\left[-\frac{\hbar}{m\beta}t_l(0,\omega)\right]=\exp\left(-\frac{n\Delta x}{\beta}\right)\approx\left(1-\frac{\Delta x}{\beta}\right)^n. \tag{4.3}$$

By interpreting $\gamma=1-\Delta x/\beta$ as the probability for a single reflection from the origin, one sees that the exponential of the local time accounts for the probability that a particle on a given path is reflected from the boundary. From Eq. (4.2), we readily see that the local time can be written formally as

$$t_l(0,\omega)=\sum_{\{t<T;\, x(t)=0\}}[1/|dx/dt|]=\int_0^T \delta(x(t))dt. \tag{4.4}$$

Thus, we have accounted for both the exponential weighting factors in Eq. (4.1).

Finally, we discuss the part of the measure which we have denoted by $\mathfrak{D}_+(x(t))$. This is the measure for the case of total reflection ($\beta=\infty$) and is determined as follows. At a totally reflecting barrier the particle, upon reaching the origin, moves to the right with probability 1, whereas in the unconstrained problem the particle could move left or right with probability $\frac{1}{2}$. Thus the measure for the totally reflecting case $[x(t)\geq 0]$ is obtained by simply multiplying the usual measure by a factor of 2 each time the path hits the origin,

$$\mathfrak{D}_+(x(t))=\mathfrak{D}(x(t))\exp\left[\ln 2\int_0^T\left|\frac{dx}{dt}\right|\delta(x(t))dt\right], \tag{4.5}$$

i.e., the measure $\mathfrak{D}_+(x(t))$ is the same as the measure for the quantity $|x'(t)|$, where $x'(t)$ is a path on the whole line, with the usual measure $\mathfrak{D}(x'(t))$.

One important check of Eq. (4.1) results from computing the path integral in the stationary-phase approximation, which should reproduce the small-time behavior of the Green's function (2.5). In the stationary-phase approximation, the dominant contribution to the path integral comes from the classical paths. Owing to the barrier at the origin, there are two classical paths from x to y ($x>0$ and $y>0$): the direct path and the path reflected once at the origin.

The contribution to the path integral from the direct path is as usual

$$I_{\text{direct}}\propto\exp\left[\frac{im}{2\hbar}\frac{(x-y)^2}{T}\right]. \tag{4.6}$$

For the reflected path, both terms in the effective action contribute to the path integral. Since, classically, the particle suffers an elastic reflection, the reflected path corresponds to a path ending at the image point $-y$. Thus the contribution of the reflected path to Eq. (4.1) is

$$I_{\text{reflected}}\propto 2\exp\left[\frac{im}{2\hbar}\frac{(x+y)^2}{T}-\frac{i\hbar}{m\beta}\frac{T}{(x+y)}\right]. \tag{4.7}$$

Aside from a normalization constant $(m/2\pi\hbar T)^{1/2}$, the sum of $I_{\text{direct}}+I_{\text{reflected}}$ is precisely equal to the Green's function (2.5) in the limit T small, with x and y fixed.

Having recovered the small-time behavior of the Green's function from Eq. (4.1), we can infer that this functional integral incorporates the information contained in the Schrödinger equation, together with the appropriate boundary conditions. Furthermore, the Green's function at finite times can be obtained from its small-time behavior using Feynman's prescription for evaluating the functional integral by dividing the time into small intervals and evaluating the limit of the resulting multiple integrals.

An interaction can be included in Eq. (4.1) by adding a potential to the action. This gives the usual Feynman-Kac formula, with an extra term to account for the boundary. Singular potentials may require special treatment since (1) the Hamiltonian may be essentially self-adjoint or (2) the self-adjoint extensions may not be conveniently characterized by the value of the logarithmic derivative of the wave function at the origin.

ACKNOWLEDGMENTS

It is a pleasure for the authors to thank Dr. J. Kiskis and Professor A. S. Wightman for their valued comments on this work. This work was supported by the U.S. Department of Energy.

---

*Permanent address: Department of Physics, Purdue University, West Lafayette, Indiana 47907.

[1]A review of previous work on constrained path integrals can be found in M. S. Marinov, Phys. Rep. 60C, 1 (1980).

[2]W. Feller, *Probability Theory and Its Applications* (Wiley, New York, 1950), Vol. I.

[3]K. Itô and H. P. McKean, Jr., *Diffusion Processes and Their Sample Paths* (Academic, New York, 1965). This reference contains specific results on Brownian motion with elastic barriers.

[4]M. Reed and B. Simon, *Methods of Modern Mathematical Physics: Functional Analysis* (Academic, New York, 1972), Vol. I.

[5]For a discussion of this point see A. S. Wightman, in *High Energy Electromagnetic Interactions and Field Theory*, edited by M. Lévy (Gordon and Breach, New York, 1967), pp. 171–291.

[6]See Feller, Ref. 2., Chap. 14.