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David W. McLaughlin

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David W. McLaughlin

Department of Mathematics, University Heights Campus and *Courant Institute of Mathematical Science and Research, New York University, New York, New York*

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By developing an analogy between the Feynman path integral and contour integral representations of the special functions, we obtain WKB formulas for barrier penetration from a path integral. We first show that there exists for the path integral a notion of contour independence in the time parameter. We then select an appropriate contour to describe the physical situation of barrier penetration and obtain asymptotic formulas from the function space integral. The method is interpreted as a path integral derivation of the complex ray description of barrier penetration. In the last three sections we investigate several canonical problems of the theory of complex rays with these path integral techniques.

1. INTRODUCTION

Many asymptotic formulas of quantum mechanics have been derived from the Feynman path integral (Refs. 1–6). However, formulas associated with barrier penetration have not been obtained in this manner. Here we obtain these "nonclassical" effects from a path integral representation. Our method may be viewed as an analogue in function space of contour representations of the special functions. That is, we perform an analytic continuation of the function space integral with respect to the time parameter and develop a notion of contour independence in this parameter. Then, by selecting an appropriate contour, we extract the asymptotic behavior of the function space integral.

Consider the Green's function G for the one-dimensional time independent Schrödinger equation

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}G(x,x'|E) + (E - V(x))\,G(x,x'|E) = \hbar\delta(x-x'). \tag{1.1}$$

G may be represented as a Fourier transform,

$$G(x,x'|E+i\epsilon) = -i\int_0^\infty dt\,\exp[(i/\hbar) \times (E+i\epsilon)t]K(x,t|x',0), \qquad \epsilon > 0, \tag{1.2}$$

where K, the kernel of the time-dependent Schrödinger equation, is represented as a path integral,[7]

$$K(x,t|x',0) = \int \mathfrak{D}x(\cdot)\,\exp\{(i/\hbar)S\,[x(\cdot),t]\}, \qquad x(\cdot) \in P(x,t|x',0). \tag{1.3}$$

Here $P(x,t|x',0)$ is the set of paths connecting the space–time points $(x',0)$ and (x,t). $S[x(\cdot),t]$ is the action functional of classical mechanics.

When x and x' lie in the same classically allowed region of space, one may extract the asymptotic behavior of G (as $\hbar$ vanishes) directly from representation (1.2) and (1.3). In this case the method of stationary phase in function space is applicable. However, when x and x' do not lie in the same allowed region, the method fails since no real, critical path at energy E connects x and x'.

To treat this case we introduce an equivalent function space integral representation of G. This equivalent representation is based upon an explicit analytic continuation of $K(x,t|x',0)$ into the lower half t plane by means of a function space integral. As will be discussed in more detail later, existing path integrals, valid in the lower half t plane, are not directly applicable. In Sec. 2, in order to obtain a useful representation, we introduce a notion of the path integral being independent of contour in the t plane, and we show that the representations in question possess this property. In Sec. 3, we utilize this contour independence by selecting a particular contour which is appropriate to the problem at hand. From the function space integral along this contour, we extract the asymptotic behavior of G.

Usually barrier penetration is not considered a semiclassical phenomena. Certainly it cannot be described in terms of real classical paths at fixed energy, which is the primary reason that the effect has not been obtained in previous asymptotic evaluations of path integrals.[8] However, it is known[9,10] that complex valued solutions of Newton's equations do penetrate forbidden regions. Further, if these complex rays are used to construct semiclassical wavefunctions, agreement with WKB calculations is obtained. It is this complex ray description of barrier penetration which we obtain from the path integral, as may be seen from the final formula specialized to one barrier, Eq. (3.9). In fact the path integral provides the most direct derivation of the complex ray formulas, in that both the equation defining the dominant path and the approximate Green's function are obtained directly from an exact representation of G.

Complex ray methods, while useful in many specific problems,[11] have been plagued with mathematical difficulties. For one, in the general case, no rule exists which provides a rationale to select the parameter with respect to which the analytic continuation is to be made. For quantum mechanics the path integral provides the rule. Our calculations show that the time t is the natural parameter.[12] Secondly, the global validity of complex ray methods is difficult to establish. It is very unlikely that path integral methods will soon answer the questions of global existence by providing error estimates accurate "in the large." Nevertheless, the path integral provides an alternative view of the complex rays, a view based upon extremely direct calculations. As such, it should provide insight into these difficult problems. For this reason we use our methods to study several "canonical problems" in the theory of complex rays; the linear potential (Sec. 4), the parabolic barrier (Sec. 5), and the repulsive coulomb potential for the radial Schrödinger equation (Sec. 6). The last example is included primarily to extend the theory to include the radial Schrödinger equation.

In the first two examples there is a feature of particular interest, namely, integrands possessing critical points which coalesce. In the linear case, when both x and x' lie in the classically forbidden region, a pair of such points produces the relative factor of $\frac{1}{2}\exp(\frac{1}{2}i\pi)$ between the "direct" and "reflected" terms, Eq. (4.14). In the quadratic case, as E approaches the top of the barrier, an infinite number of critical points coalesce at infinity (Fig. 7), preventing the approximation from being uniform.

The idea of an analytic continuation of the path integral with respect to time is not new. Our starting point, Eq. (2.1), was used by Babbitt[13] and by Feldman[14] in early proofs of the existence of the path integral. However, to our knowledge, we are the first to formulate this notion of the contour independence of the Feynman path integral and to utilize this property for calculational purposes. The present work may be viewed as the first application of the "existence formulas" of Babbitt and Feldman.

While the general analogy between this work and contour representations is striking, it does not cover the specific details of the actual continuation procedure. In fact, no natural analogue of this procedure exists for classical, N-dimensional integrals. Such an analogue would be the continuation of an integral such as $\int \cdots \int dx_1 \cdots dx_N f(x_1, \ldots, x_N)$ with respect to the labeling indices $(1, 2, \ldots, N)$. In function space this labeling is continuous, making the entire procedure possible.

2. PATH INDEPENDENCE OF THE REPRESENTATIONS

In this section we define the basic representations and develop the notion of contour independence for these representations. Consider any point t_0 in the lower half complex t plane. To define $K(x, t_0 | x', 0)$, it seems natural to partition into N subdivisions the ray connecting the origin with t_0 (Fig. 1), and to construct the path integral as a limit of N-fold integrals

$$K(x, t_0 | x', 0) = \lim_{N \to \infty} \left(\frac{mN}{2\pi i \hbar t_0}\right)^{N/2} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 \cdots dx_{N-1} \times \exp\left[\frac{i}{\hbar} \sum_{j=1}^{N} \left(\frac{mN}{2t_0}(x_j - x_{j-1})^2 - V(x_j)\frac{t_0}{N}\right)\right],$$
$$x_0 \equiv x', \quad x_N \equiv x. \tag{2.1}$$

Certainly if $V(\cdot)$ is (real) continuous and bounded below, the N-fold integral exists—convergence being guaranteed by the Gaussian term. In fact for such potentials Babbitt has proven that (2.1) is a valid representation of K in the lower half t plane, and Feldman has extended this class to include all potentials which are Riemann approximable and bounded below.[15] He also established that the limit is independent of the partition of the ray. In this paper we consider the N-fold averaging together with the limit on N as the definition of a function space integral and denote it by

$$K(x, t_0 | x', 0) = \int_{x(\cdot) \in P(x, t_0 | x', 0)} \mathfrak{D}x(\cdot) \times \exp\{(i/\hbar) S[x(\cdot), t_0]\} \tag{2.2}$$

In definition (2.1) the variables of integration $\{x_j\}$ are real. This forces the class of paths $P(x, t_0 | x', 0)$ to be composed of real-valued functions along the ray, that is

$$P(x, t_0 | x', 0) \equiv \{x(\cdot): \text{ray} \to R \mid x(0) = x', x(t_0) = x\}. \tag{2.3}$$

However, this representation is not particularly suitable for asymptotic evaluation. The saddle point method (in function space) indicates that, as $\hbar$ vanishes, certain critical paths should dominate the behavior of the integral. These critical paths are defined by the variational problem,

$$\delta S[x(\cdot), t_0] = 0, \quad x(0) = x', \quad x(t_0) = x, \tag{2.4}$$

or equivalently by the two point boundary value problem,

$$m \frac{d^2 x(\tau)}{d\tau^2} = -\frac{dV}{dx}, \quad x(0) = x', \quad x(t_0) = x. \tag{2.5}$$

In general the solution $\bar{x}(\cdot)$ of (2.5) will not be real valued along the ray connecting the origin with t_0. [This may be easily seen by solving (2.5) in a simple case such as the linear potential.] Thus, the critical path $\bar{x}(\cdot)$ will not be a member of the class P.

One's first thought is to modify representation (2.2) by enlarging the class P to include complex valued paths. We are hesitant to do this, however, because of the extreme convergence difficulties which would result.[16] We prefer to replace the ray connecting the origin and t_0 with a general rectifiable contour $\Gamma: \tau = \tau(s), s \in [0,1], \tau(0) = 0, \tau(1) = t_0$. This replacement is permissible because, as we will now show, there exists a notion of contour independence. In Sec. 3 we show that the replacement is useful for asymptotic evaluations.

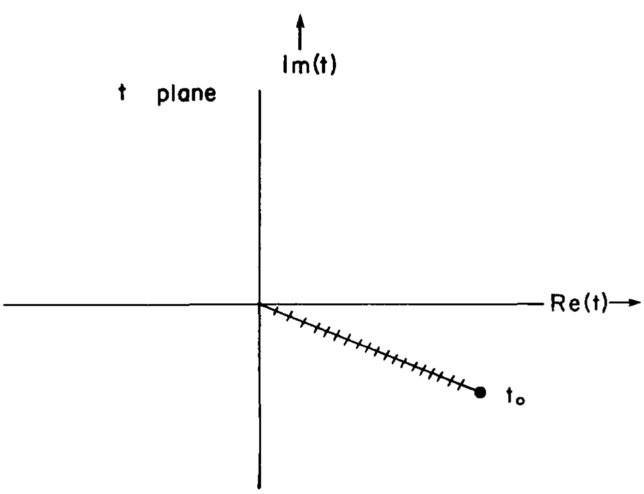

FIG. 1. Partition of ray.

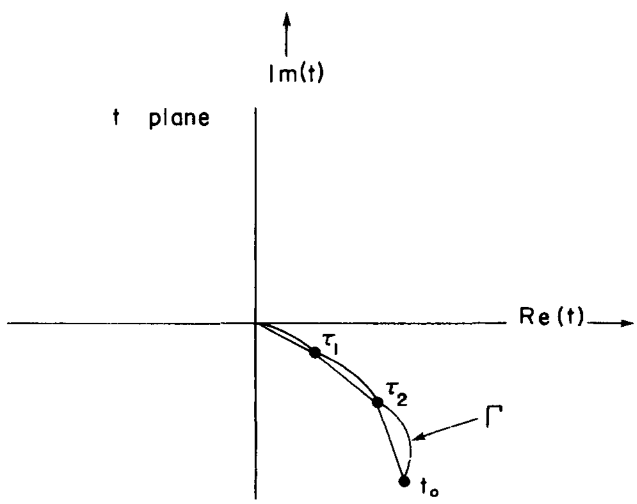

FIG. 2. A typical contour Γ.

If contour Γ has decreasing imaginary part (Fig. 2),

$$\mathrm{Im}(\tau(s_1)) < \mathrm{Im}(\tau(s_2)), \quad s_1 > s_2, \tag{2.6}$$

an N-fold partition of Γ will certainly yield an N fold convergent integral. The following simple lemma makes it clear that the path integral exists along Γ, actually being independent of Γ.

For notational convenience we define the operators K^t as

$$(K^t\psi)(x) \equiv \int_{-\infty}^{\infty} K(x,t\,|\,x',0)\,\psi(x')dx', \qquad \psi \in L^2(R),\ \mathrm{Im}\,t \le 0, \tag{2.7}$$

and K_N^t as

$$(K_N^t\psi)(x) = \left(\frac{mN}{2\pi i\hbar t}\right)^{N/2} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_0 \cdots dx_{N-1} \times \exp\left[\frac{i}{\hbar}\sum_{j=1}^{N}\left(\frac{mN}{2t}(x_j - x_{j-1})^2 - V(x_j)\frac{t}{N}\right)\right]\psi(x_0),$$
$$\psi \in L^2(R), \quad \mathrm{Im}\,t \le 0, \quad x_N = x. \tag{2.8}$$

The operators K^t form a holomorphic semigroup in C^-, the lower half t plane union the real axis, and the operators K_N^t are uniformly bounded (in N) by 1.[17,18]

Lemma: For any τ and τ_1 such that τ, τ_1, and $(\tau - \tau_1)$ all lie in the lower half complex plane,

$$K^\tau\psi = \lim_{N\to\infty} K_N^{\tau_1}K_N^{\tau-\tau_1}\psi \text{ for all } \psi \in L^2(R).$$

Proof: Consider two complex numbers τ and τ_1, satisfying $\mathrm{Im}\,\tau < 0$, $\mathrm{Im}\,\tau_1 < 0$, and $\mathrm{Im}(\tau - \tau_1) < 0$. Since K^τ is a holomorphic semigroup in C^-;

$$K^\tau = K^{\tau_1}K^{(\tau-\tau_1)}. \tag{2.9}$$

Applying representation (2.1), one obtains

$$K^\tau = (\lim_{N\to\infty} K_N^{\tau_1}) \cdot (\lim_{N\to\infty} K_N^{(\tau-\tau_1)}), \tag{2.10}$$

where the limits are taken in the strong sense. The operators K_N^τ are uniformly bounded (in N) by 1. Using the fact that the product of two strongly convergent, uniformly bounded sequences of operators in a Hilbert space is itself strongly convergent, converging to the product of the limits, one concludes

$$K^\tau\psi = \lim_{N\to\infty}(K_N^{\tau_1}K_N^{(\tau-\tau_1)}\psi) \quad \forall\ \Psi \in L^2(R). \tag{2.11}$$

This lemma extends to finite products. Consider any rectifiable contour Γ possessing property (2.6), and select any polygonal approximation of Γ, with vertices ($\tau_0 \equiv 0, \tau_1, \ldots, \tau_{M-1}, \tau_M \equiv t_0$) lying upon Γ. The extension of the lemma applies, yielding

$$K^{t_0}\psi = K^{\tau_1}K^{(\tau_2-\tau_1)}\cdots K^{(\tau_M-\tau_{M-1})} = \lim_{N\to\infty}[K_N^{\tau_1}K_N^{(\tau_2-\tau_1)}\cdots K_N^{(\tau_M-\tau_{M-1})}]. \tag{2.12}$$

Since the same operator K^{t_0} is obtained for finer and finer polygonal approximations, we may pass to the limit. Thus, for contours Γ satisfying (2.6), we have the notion of a path integral representation of K^{t_0} along Γ, along with the fact that such representations actually are contour independent. As long as the path integral exists for real t_0,[19,20] the above results immediately extend to include contours Γ satisfying

$$\mathrm{Im}\,\tau(S_1) \le \mathrm{Im}\,\tau(S_2), \quad S_1 > S_2. \tag{2.6'}$$

3. BARRIER PENETRATION FORMULAS

In this section, armed with this notion of contour independence, we define a contour Γ appropriate to the problem of barrier penetration and extract from the path integral along Γ the asymptotic behavior. Throughout this section we assume that $V(\cdot)$ is smooth enough to guarantee needed existence, uniqueness, and analyticity properties (Appendix).

We consider Eq. (2.5) for the critical path $\bar{x}(\tau)$ and seek those contours in the t plane along which the analytic function $\bar{x}(\tau)$ has constant (in fact no) imaginary part. To describe these contours, we first solve the intitial value problem at energy $\xi = \xi_R + i\xi_I$,

$$\tau(\bar{x}) = \sqrt{\frac{m}{2}}\int_{x'}^{\bar{x}} dz\,[\xi - V(z)]^{-1/2}, \quad z, x', \bar{x} \in R. \tag{3.1}$$

As long as $\xi_I \neq 0$, the branch point of the square root lies off the real z axis. We restrict ourselves to $\xi_I > 0$ and, without loss of generality, fix $x > x'$. Select that branch of the square root defined by

$$(\xi - V)^{1/2} = +\left(\frac{(\xi_R - V) + [(\xi_R - V)^2 + \xi_I^2]^{1/2}}{2}\right)^{1/2} + i\left(\frac{-(\xi_R - V) + [(\xi_R - V)^2 + \xi_I^2]^{1/2}}{2}\right), \tag{3.2}$$

where all radicals are positive. Under these restrictions, contours defined by (3.1) have decreasing imaginary parts (as $\bar{x}$ increases from x' to x).

Define D, a subset of the t plane, by

$$D \equiv \{t \in C^- \mid t = \sqrt{m/2}\int_{x'}^{x} dz\,[\xi - V(z)]^{-1/2}; \ x, x', z \in R; x > x'; \ \text{for some } \xi = \xi_R + i\xi_I, \xi_I > 0\}. \tag{3.3}$$

Consider any $t_0 \in D$. Define $\xi = \xi(t_0)$ by

$$t_0 = \sqrt{m/2}\int_{x'}^{x} dz\,[\xi(t_0) - V(z)]^{-1/2}. \tag{3.1'}$$

Further, define a contour Γ by

$$\Gamma : \tau(\bar{x}) \equiv \sqrt{m/2}\int_{x'}^{\bar{x}} dz\,[\xi(t_0) - V(z)]^{-1/2}. \tag{3.1''}$$

Γ satisfies (2.6) and defines $\bar{x}(\tau)$, a real-valued solution of (2.5). Since Γ satisfies (2.6), the results of Sec. 2 justify selecting it as a contour along which path to integrate.

But now, by construction, the critical path of this function space integral $\bar{x}(\tau)$ is real on Γ, hence, a member of the class of paths P. Expanding the action functional $S[x(\cdot), t_0]$ about $\bar{x}(\cdot)$ while retaining terms through second order, we approximate the path integral by

$$K(x, t_0\,|\,x', 0) \simeq \bar{K}(x, t_0\,|\,x', 0) \quad \text{as } \hbar \to 0, \tag{3.4}$$

where

$$\bar{K}(x, t_0\,|\,x', 0) \equiv \exp\left\{\frac{i}{\hbar}\int_{\Gamma^0}^{t_0}\left[\frac{m}{2}\left(\frac{d\bar{x}}{d\tau}\right)^2 - V(\bar{x}(\tau))\right]d\tau\right\} \times \int_{P(0,t_0\,|\,0,0)} \mathfrak{D}x(\cdot)$$

$$\times \exp\left\{\frac{i}{2\hbar}\int_0^{t_0}\left[m\left(\frac{dx}{d\tau}\right)^2 - \alpha(\tau)x^2\right]d\tau\right\},$$

$$\alpha(\tau) \equiv \left(\frac{d^2V}{dx^2}\right)_{x=\bar{x}(\tau)}. \tag{3.5}$$

This path integral, being Gaussian, may be calculated explicitly to yield

$$\tilde{K}(x,t_0|x',0) = \left(\frac{m}{2\pi i\hbar}\right)^{1/2}\left|\frac{\partial^2 S(x,t_0|x',0)}{\partial x\partial x'}\right|^{1/2}$$
$$\times \exp[(i/\hbar)\,S(x,t_0|x',0)],$$
$$S(x,t_0|x',0) = \int_{\Gamma^0}^{t_0} d\tau\left[\frac{1}{2}m\left(\frac{d\bar{x}}{d\tau}\right)^2 - V(\bar{x}(\tau))\right]. \tag{3.6}$$

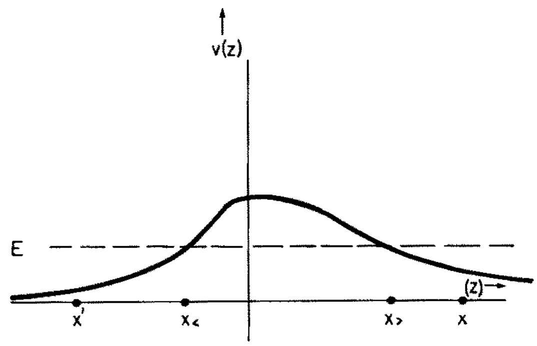

FIG. 3. A typical barrier.

Finally, we relate this calculation to the problem of barrier penetration. Returning to Eq. (1.2) and the case where no real classical path at energy E connects x and x', we deform the path of integration of the Fourier transform to pass through the region D. In this region we replace K with its asymptotic approximation (3.6), and find that the integrand which results possesses a critical point t_0 in D, namely

$$t_0 = \sqrt{\frac{m}{2}}\int_{x'}^{x} dz\,(\xi - V)^{-1/2}, \qquad \xi = E + i\epsilon,\ \epsilon > 0. \tag{3.7}$$

The dominant behavior of G will be given by a neighborhood of t_0 and may be calculated by the saddle point method to yield

$$\tilde{G}(x,x'|E+i\epsilon) = e^{(-3\pi i)/4}\left[\left(\frac{m}{2}\right)\left(\frac{\partial^2 S}{\partial x\partial x'}\right)\left(\frac{\partial^2 S}{\partial t_0^2}\right)^{-1}\right]^{1/2}$$
$$\times \exp\{(i/\hbar)\,[(E+i\epsilon)t_0 + S]\}, \quad S \equiv S(x,t_0|x',0). \tag{3.8}$$

When (3.8) is specialized to a single barrier (Fig. 3), (3.7) is used to express t_0 in terms of ξ, and ϵ is set at zero, $\tilde{G}$ becomes

$$\tilde{G}(x,x'|E) = -m[k(x)k(x')]^{-1/2}\left[\exp\left(\frac{i}{\hbar}\int_x^{x_<} k(x)dx - \frac{1}{\hbar}\right.\right.$$
$$\left.\left.\times \int_{x_<}^{x_>} K(x)dx + \frac{i}{\hbar}\int_{x_>}^{x'} k(x)dx\right)\right],$$

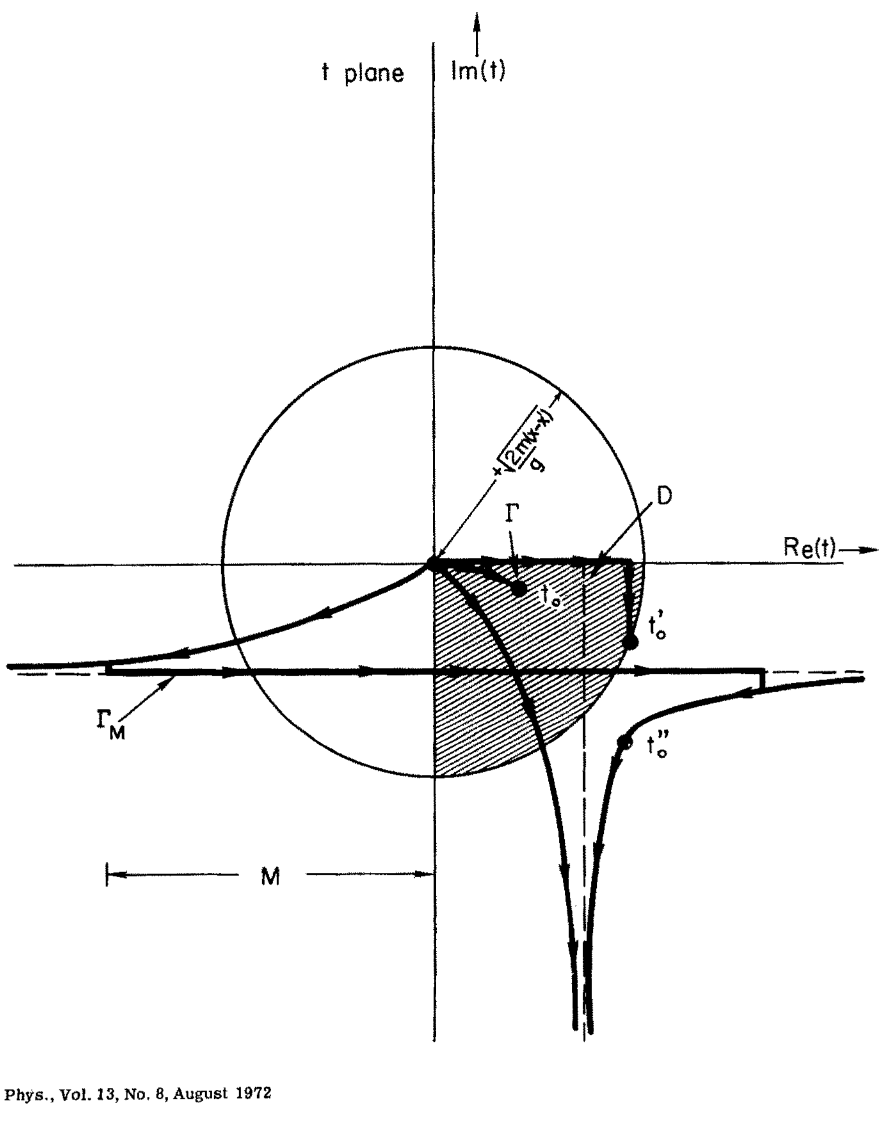

FIG. 4. Region D with typical contours Γ and Γ_M, linear potential.

$$\text{where}\quad k(x) \equiv +\{2m[E - V(x)]\}^{1/2},$$
$$K(x) \equiv +\{2m[V(x) - E]\}^{1/2},$$
$$x' < (x_<) < (x_>) < x'. \tag{3.9}$$

Here the turning points are defined as $x_<$ and $x_>$ (Fig. 4).

Notice that (3.9) contains the WKB barrier penetration factor, as it should. We have succeeded in obtaining a complex ray description of barrier penetration from the path integral. The entire calculation of Sec. 3 is formal. As with all path integral calculations, no estimate of the error has been made. Nevertheless, Eqs. (3.1′), (6)–(9) provide explicit equations for the complex ray and approximate amplitudes. While we have restricted ourselves to one dimension, it is reasonable to expect that the methods will generalize to higher dimensions. There, of course, the formulas will not be as explicit. We now apply these methods to study several canonical problems in the theory of complex rays, canonical because they are local approximations to many potentials. For these examples we have explicitly verified that the formulas are asymptotic to G.

4. LINEAR POTENTIAL

Let $V(x)$ equal gx, $g > 0$. Further denote the turning point by x_0, $x_0 \equiv (E/g)$, and fix x and x' satisfying $x' < x_0 < x$. In this case the region D (Fig. 4) is the intersection of the fourth quadrant with the interior of the circle centered at the origin with radius r:

$$r^2 \equiv (2m/g)(x - x') \tag{4.1}$$

We remark that for t restricted to the boundary of this circle, the energy ξ for the solution of the classical Eqs. (2.5) is real, while for points t inside D, $\mathrm{Im}\xi > 0$. For points t in D, Γ is given by

$$\Gamma : \tau(\bar{x}) = (2m/g^2)^{1/2}[(\xi - gx')^{1/2} - (\xi - g\bar{x})^{1/2}],$$
$$\xi \equiv \frac{m}{2t^2}\left(\frac{g^2t^4}{4m^2} + \frac{gt^2(x + x')}{m} + (x - x')^2\right). \tag{4.2}$$

Along Γ, formula (3.5) yields

$$\tilde{K}(x,t\,|x',0) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \exp\left[\frac{i}{\hbar}\left(\frac{m}{2}\frac{(x-x')^2}{t} - \frac{g}{2}\right.\right.$$
$$\left.\left.\times\ (x + x')t - \frac{g^2}{24m}t^3\right)\right], \quad t \in D. \tag{4.3}$$

Finally we apply (4.3) in the approximation of the Fourier tranform to obtain

$$\tilde{G}(x,x'\,|\,E) = -m[K(x)k(x')]^{-1/2}$$
$$\exp\left(\frac{i}{\hbar}\int_{x'}^{E/g} k(x)dx - \frac{1}{\hbar}\int_{E/g}^{x} K(x)dx\right), \tag{4.4}$$

where

$$K(x) \equiv +[2m(gx - E)]^{1/2},$$
$$k(x') \equiv +[2m(E - gx')]^{1/2}. \tag{4.5}$$

A similar calculation with x and x' fixed satisfying $x_0 < x' < x$ yields

$$\tilde{G}(x,x'\,|E) = -m[K(x)K(x')]^{-1/2}\exp\left(-\frac{1}{\hbar}\int_{x'}^{x} K(x)dx\right). \tag{4.6}$$

In this simple case it is instructive to verify these formulas by actual application of the method of steepest descent. For the linear potential $\tilde{K}$, formula (3.5) is exact for all t in C^-. [For any t in C^- one need only to calculate the N-fold integral (2.1) explicitly and take the limit to verify K equals $\tilde{K}$.] Fixing $x' < E/g < x$, we consider the Fourier transform

$$G(x,x'\,|\,E + i\epsilon) = e^{-3\pi i/4}\left(\frac{m}{2\pi\hbar}\right)^{1/2}\int_0^\infty \frac{dt}{t^{1/2}}$$
$$\times\ \exp\{(i/\hbar)[(E + i\epsilon)t + S]\}, \tag{4.7}$$
$$S \equiv \frac{m}{2}\frac{(x-x')^2}{t} - \frac{g}{2}(x + x')t - \frac{g^2t^3}{24m}.$$

Except at the origin, the integrand is an analytic function of t. It possesses four critical points

$$\pm(g^2/m)^{1/2}t = \{[(E - gx') + ((E - gx')^2 + \epsilon^2)^{1/2}]^{1/2}$$
$$+ i[-(E - gx') + ((E - gx')^2 + \epsilon^2)^{1/2}]^{1/2}\}$$
$$\pm\{[(E - gx) + ((E - gx)^2 + \epsilon^2)^{1/2}]^{1/2}$$
$$+ i[-(E - gx) + ((E - gx)^2 + \epsilon^2)^{1/2}]^{1/2}\}, \tag{4.8}$$

where all roots are taken to be positive. Of these, denote the one in the fourth quadrant by t_0, and define a contour γ from the origin through t_0 to infinity by the following conditions:

(1) $\mathrm{Re}[S(x,t\,|x',0) + (E + i\epsilon)t]$
$= \mathrm{Re}[S(x,t_0\,|x',0) + (E + i\epsilon)t_0]$ on γ and

(2) γ approaches the asymptote
$\mathrm{Im}(t) = -(3)^{-1/2}\,\mathrm{Re}(t)$ as $t \to \infty$. (4.9)

The contour γ is a line of steepest descent, to which

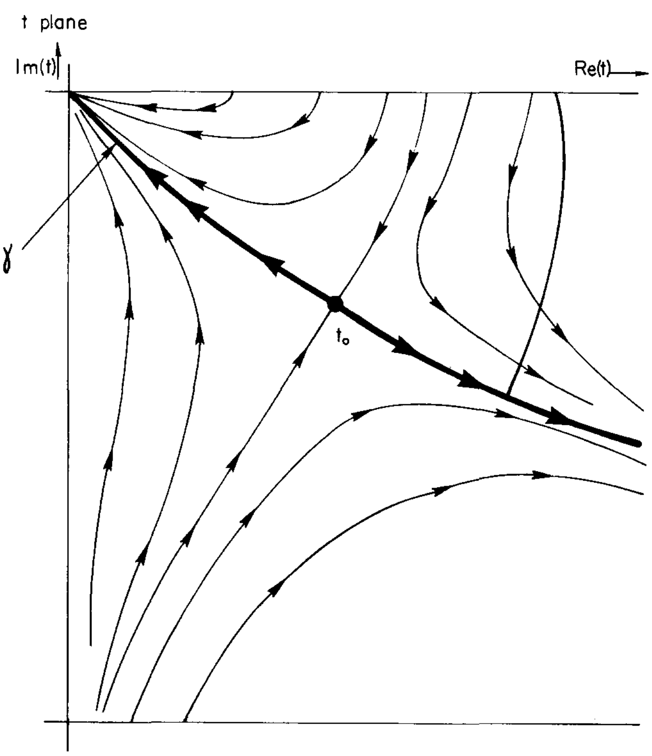

FIG. 5. Lines of constant $\mathrm{Re}(S + Et)$, linear potential, $x' < E/g < x$. Arrows denote direction of increasing $\mathrm{Im}(S + Et)$. t_0 is the critical point.

the path of integration may be deformed (Fig. 5). Along γ we calculate the integral by the method of steepest descent.[21,22] This simple calculation establishes that G is asymptotic to $\tilde{G}$, Eq. (4.4):

$$G(x,x'\,|\,E) \simeq \tilde{G}(x,x'\,|\,E) + O(\hbar^{\delta}\tilde{G}), \qquad 0<\delta<\tfrac{1}{2}, \text{ as } \hbar \to 0. \quad (4.10)$$

Expression (4.10) is not uniformly valid as x and x' approach the turning point (E/g). In our framework, the origin of the nonuniformity is that the critical points "coalesce." As x approaches (E/g) from above, x' fixed, the complex conjugate pairs of critical points approach the real axis, colliding when $x = (E/g)$[23]; as x' approaches (E/g) from below, x fixed, those critical points with identical real parts collide at the imaginary axis; and as both x and x' approach (E/g), all four critical points collide at the origin. In these cases it is unreasonable to expect any one member t_0 of a colliding set to dominate. When two critical points coalesce, both must be taken into account.[24,25] We turn now to a case where colliding critical points play a particularly important role.

Fix x and x' such that $(E/g) < x' < x$. Equations (4.7) and (4.8) still apply. As shown in Fig. 6, the contour γ defined by conditions (4.9) now passes through both critical points in C^-, t_0, and t_0'. Once again the path of integration may be deformed to coincide with γ. Breaking γ at t_0', we separate the Fourier transform into two integrals

$$G(x,x'\,|\,E) = e^{(-3\pi i)/4}(m/2\pi\hbar)^{1/2}[I_1 + I_2], \quad (4.11)$$

where

$$I_1 \equiv \int_{\gamma 0}^{t_0'} \frac{dt}{t^{1/2}} \exp\!\left(\frac{i}{\hbar}(Et+S)\right) \quad (4.12)$$

and

$$I_2 \equiv \int_{\gamma t_0'}^{\infty} \frac{dt}{t^{1/2}} \exp\!\left(\frac{i}{\hbar}(Et+S)\right). \quad (4.13)$$

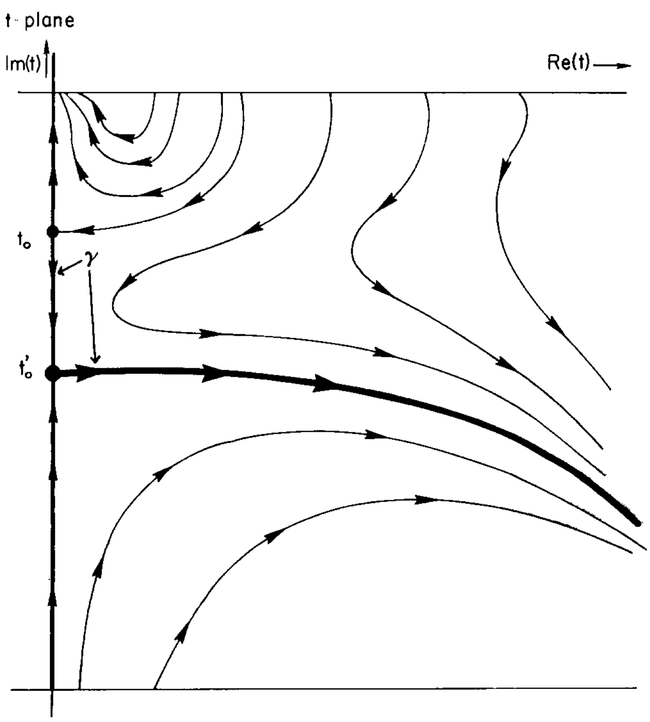

FIG. 6. Lines of constant $\mathrm{Re}(S + Et)$, linear potential, $E/g < x' < x$. Arrows denote direction of increasing $\mathrm{Im}(S + Et)$. t_0 and t_0' denote the critical points.

Applying the method of steepest descent to both I_1 and I_2, noticing that I_2 is only "one-half Gaussian," we obtain

$$G(x,x'\,|\,E)^{1/2} = -m[K(x)K(x')^{-1/2}\left[\exp\!\left(-\frac{1}{\hbar}\int_{x'}^{x} K(x)dx\right) + \frac{e^{(i\pi)/2}}{2}\exp\!\left(\frac{1}{\hbar}\int_{x'}^{E/g} K(x)dx - \frac{1}{\hbar}\int_{E/g}^{x} K(x)dx\right)\right] + 0\left[\hbar^{\delta}\exp\!\left(-\frac{1}{\hbar}\int_{x'}^{x} K(x)dx\right)\right], \quad 0<\delta<\tfrac{1}{2}. \quad (4.14)$$

For fixed $E/g < x' < x$, the second term in (4.14) is exponentially small when compared with the first, and Eq. (4.6) yields the correct asymptotic behavior of G. However, the second factor in (4.14) must be kept if the approximation is to be uniformly valid as x' approaches the turning point E/g. As mentioned above, two critical points coalesce and both contribute to the asymptotic value of G.

The relative factor $\frac{1}{2}\exp(\frac{1}{2}i\pi)$ between the two terms in (4.14) is particularly interesting. Seckler and Keller interpret this factor as the result of a loss of "one half the wave" into the allowed region, together with a phase change due to reflection from the turning point. In their work the factor arises due to the boundary condition of a purely outgoing wave at $(-\infty)$. In our derivation, the $\frac{1}{2}$ may be traced to the fact that I_2 is only "one half a Gaussian," while the $e^{i\pi/2}$ is due to the rotation of γ by $e^{i\pi/2}$ at t_0'.

Finally this example indicates that the path integral representation may be extended beyond D, and that it must be so extended if uniformly valid approximations are sought. Here $\tilde{K}$ is exact for all t in C^- indicating that the region D is somehow artificial. Noticing that the critical point t_0', lying outside of D, is reached by a change in branches of the t versus E relation, one is tempted to extend D by a switch of branches. In fact, for the linear case, a candidate for the contour Γ [satisfying conditions such as (2.6′)] does exist for points lying outside of D. However, as shown in Fig. 5, it possesses an asymptote which makes it necessary to tie together $(-\infty)$ and $(+\infty)$ in some fashion. One way to accomplish this is to follow Γ_M, also depicted in Fig. 5. Since K^t is a semigroup in C^-, it may be path integrated along Γ_M, the critical path becoming real as $M \to +\infty$. In this way it should be possible to extend the region D.

5. PARABOLIC BARRIER

Let $V(x) = -\frac{1}{2}gx^2$, $g > 0$, denote the turning points by $x_\pm = \pm(\sqrt{2|E|})/g$, and fix $x' < x_- < x_+ < x$. In this case formula (3.9) yields

$$\tilde{G}(x,x'\,|\,E) = -m[k(x)k(x')^{-1/2}\exp\left\{\frac{i}{\hbar}\left[\int_{x'}^{x_-} k(x)dx + \int_{x_+}^{x} k(x)dx + i|E|\pi\left(\frac{m}{g}\right)^{1/2}\right]\right\}, \quad (5.1)$$

where

$$k(x) = +[2m(E + \tfrac{1}{2}gx^2)]^{1/2}. \quad (5.2)$$

Again it is instructive to verify this formula by the method of steepest descent. $\tilde{K}$ is exact for all t in C^-. We consider the Fourier transform

$$G(x,x'\,|\,E+i\epsilon) = e^{(-3\pi i)/4}\left(\frac{(mg)^{1/2}}{2\pi\hbar}\right)^{1/2}\int_0^\infty \times \{\sinh[(g/m)^{1/2}t]\}^{-1/2}\exp\{(i/\hbar)[(E+i\epsilon)t+S]\}dt, \tag{5.3}$$

where

$$S \equiv S(x,t\,|\,x',0) = (\tfrac{1}{4}mg)^{1/2}\{(x^2+x'^2)\coth[(g/m)^{1/2}t] - 2xx'\,\mathrm{csch}[(g/m)^{1/2}t]\}. \tag{5.4}$$

The integrand is an analytic function of t with the exception of the points $t = in\pi(m/g)^{1/2}$, $n\epsilon(0,\pm1,\pm2,\ldots)$. As ϵ vanishes, the critical points are defined by $t_n = t_{nR} + it_{nI}$,

$$t_{nI} = (2n+1)\pi(m/g)^{1/2},$$
$$\frac{2E}{g}\sinh^2((g/m)^{1/2}t_{nR}) = x^2 + x'^2 + 2xx'\cosh(\sqrt{g/m}\,t_{nR}). \tag{5.5}$$

For each value of n, (5.5) admits four solutions (Fig. 7).

We now choose an appropriate contour γ. This choice is not uniquely determined, the only requirement being that one must bound the error along it. In the fourth quadrant the two critical points for $n = -1$, $t_<$ and $t_>$ in Fig. 8, lie closest to the real axis and would be expected to dominate the integral. We define the first part of γ as that line of constant $\mathrm{Re}[Et + S]$ connecting the origin with $t_<$, along which $\mathrm{Im}[Et + S]$ is monotonically decreasing from the origin to $t_<$ (Fig. 8). From $t_<$, γ is defined as the line $(\mathrm{Im}t) = -\pi(m/g)^{1/2}$ through $t_>$ on to infinity. Notice that along this second portion of γ, $\mathrm{Im}[Et + S]$ is constant, and the method of stationary phase is applicable. Once again a standard calculation establishes that the path of integration may be deformed to coincide with γ.

Breaking γ at $t_<$, we separate the Fourier transform into two integrals,

$$G(x,x'\,|\,E+i\epsilon) = e^{-3\pi i/4}\left(\frac{(mg)^{1/2}}{2\pi\hbar}\right)^{1/2}\{I_1 + I_2\}, \tag{5.6}$$

$$I_1 \equiv \int_{\gamma 0}^{t_<}\left[\sinh\left(\sqrt{\frac{g}{m}}\,t\right)\right]^{-1/2}\exp\left(\frac{i}{\hbar}[(E+i\epsilon)t+S]\right), \tag{5.7}$$

and

$$I_2 \equiv \int_{\gamma t_<}^{\infty}\left[\sinh\left(\sqrt{\frac{g}{m}}\,t\right)\right]^{-1/2}\exp\left(\frac{i}{\hbar}((E+i\epsilon)t+S)\right). \tag{5.8}$$

Calculating the first by the method of steepest descent and the second by that of stationary phase, we obtain

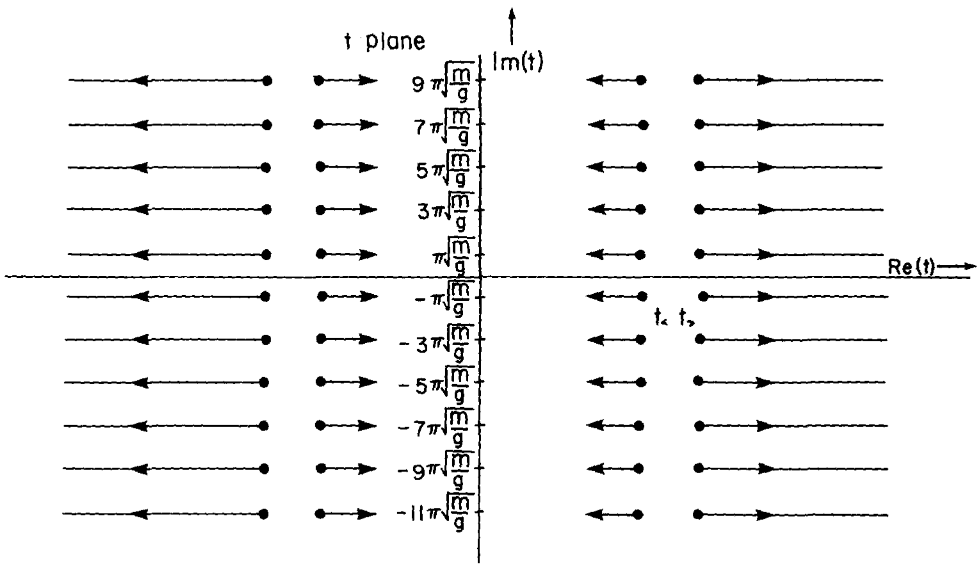

FIG. 7. Critical points for parabolic barrier, $x' < x_- < x_+ < x$. Arrows denote motion of critical points as E approaches the top of the barrier from below. "Outer" critical points coalesce at ∞.

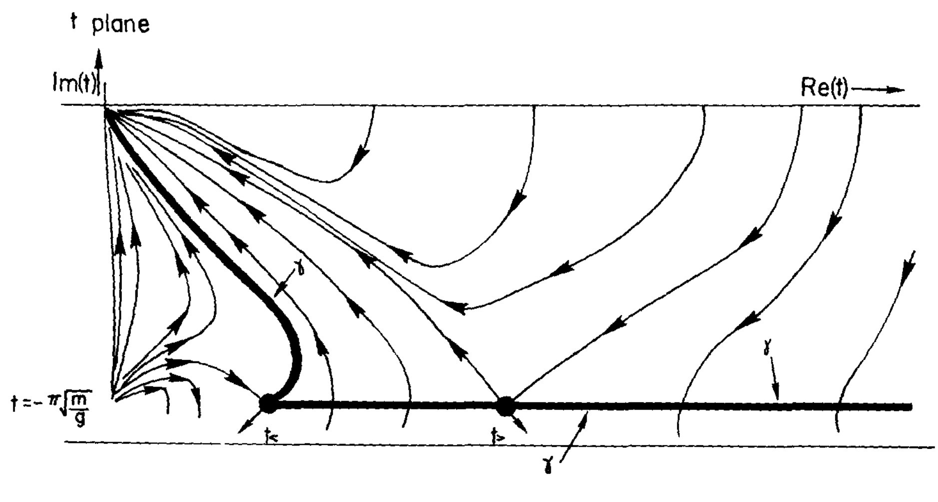

FIG. 8. Lines of constant $\mathrm{Re}(S + Et)$, parabolic potential, $x' < -(2|E|/g)^{1/2} < +(2|E|/g)^{1/2} < x$. Arrows denote direction of increasing $\mathrm{Im}(S + Et)$. $t_<$ and $t_>$ denote the critical points.

$$I_1 = -e^{(i\pi)/4}\exp\left(\frac{i}{\hbar}(Et_< + S)\right)\left\{(\pi\hbar)\left[2\left(\frac{\partial^2 S}{\partial t_<^2}\right)^{1/2}\right.\right.$$
$$\left.\left.\times \sinh\left(\sqrt{\frac{g}{m}}\,t_<\right)\right]^{-1}\right\}^{1/2}[1 + O(\hbar^\delta)],$$
$$0 < \delta < \tfrac{1}{2}, \tag{5.9}$$

and

$$I_2 = e^{(i\pi)/4}\exp\left(\frac{i}{\hbar}(Et_< + S)\right)\left\{(\pi\hbar)\left[2\left(\frac{\partial^2 S}{\partial t_<^2}\right)\right.\right.$$
$$\left.\left.\times \sinh\left(\sqrt{\frac{g}{m}}\,t_<\right)\right]^{-1}\right\}^{1/2}[1 + O(\hbar^\delta)]$$
$$+ e^{(-i\pi)/4}\exp\left(\frac{i}{\hbar}(Et_> + S)\right)\left\{(2\pi\hbar)\left[\left|\frac{\partial^2 S}{\partial t_>^2}\right|\right.\right.$$
$$\left.\left.\times \sinh\left(\sqrt{\frac{g}{m}}\,t_>\right)\right]^{-1}\right\}^{1/2}[1 + O(\hbar^\delta)], \quad 0 < \delta < \tfrac{1}{2}. \tag{5.10}$$

Adding, we compute that G is asymptotic to $\tilde{G}$, Eq. (5.1),

$$G(x,x'\,|\,E) = \tilde{G}(x,x'\,|\,E) + O(\hbar^\delta \tilde{G}), \quad 0 < \delta < \tfrac{1}{2}. \tag{5.11}$$

Here we have used (5.5) to express $t_>$ in terms of E.

This result may be interpreted as a particle traveling in real time until it strikes the turning point where its real time "freezes." It then penetrates the barrier by taking an excursion into complex time. Upon striking the second turning point, its complex time freezes, and it leaves the barrier with increasing real time. Notice that the calculation establishes that $\tilde{G}$ depends only upon $t_>$ and not upon $t_<$. (Physically one might have expected $t_<$ not to contribute since it may be interpreted as arising from a motion "backwards in real time" due to a change in branch of the t versus E relation.)[26]

Finally, we remark that $\tilde{G}$ is not uniformly valid as E vanishes, since one half of the critical points move to infinity, Fig. 8. The change of varible $t' = 1/t$ establishes that the transformed integrand has a countable number of critical points coalescing at the origin. Certainly one member of this set, $t_>^{-1}$, does not dominate the behavior of the integral. However, other techniques[27] show the uniformly valid expansion will depend upon a countable number of these critical points. Since countable numbers of coalescing critical points arise in physical problems involving resonances and "above barrier reflections," it may be necessary to understand such critical point behavior in order to treat these problems with the path integral.

6. TWO ADDITIONAL EXAMPLES

In this section we mention two additional potentials for which the formula may be checked by other methods. First, let $V(x) = V_0[\cosh(\alpha x)]^{-2}$, $\alpha > 0$, $V_0 > 0$. Clearly formula (3.9) applies (x' is to the left) of the barrier, x to the right).

Since in this case no closed form of $K(x,t\,|\,x',0)$ is known, $\tilde{G}$ may not be verified as directly as were the preceding two examples. Nevertheless, the time-independent Schrödinger equation in this potential may be solved terms of hypergeometric functions.[28] By using these to construct G, and then evaluating it asymptotically as $\hbar$ vanishes, one can verify $\tilde{G}$. We mention this only because this potential, due to its behavior at infinity, may provide a better model for above barrier reflection than the parabolic barrier.

Rather than present the details of this verification, we prefer to consider an example involving the radial Schrödinger equation. Let $V(r)$ be a repulsive potential, and let the energy E be high enough that the effective potential $[l(l+1)\hbar^2]/(2mr^2) + V(r)$ has only one turning point r_0. Fix $r' > r_0 > r$. We seek the asymptotic behavior of G as $\hbar$ vanishes:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right)G(r,r'\,|E,l) = -\delta(r - r'). \tag{6.1}$$

Following Langer,[29] we transform the singularity at the origin to infinity by the change of variable $r = e^{-x}$,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + W(x) + L\right)g(x,x'\,|E,L) = -\delta(x - x'), \tag{6.2}$$

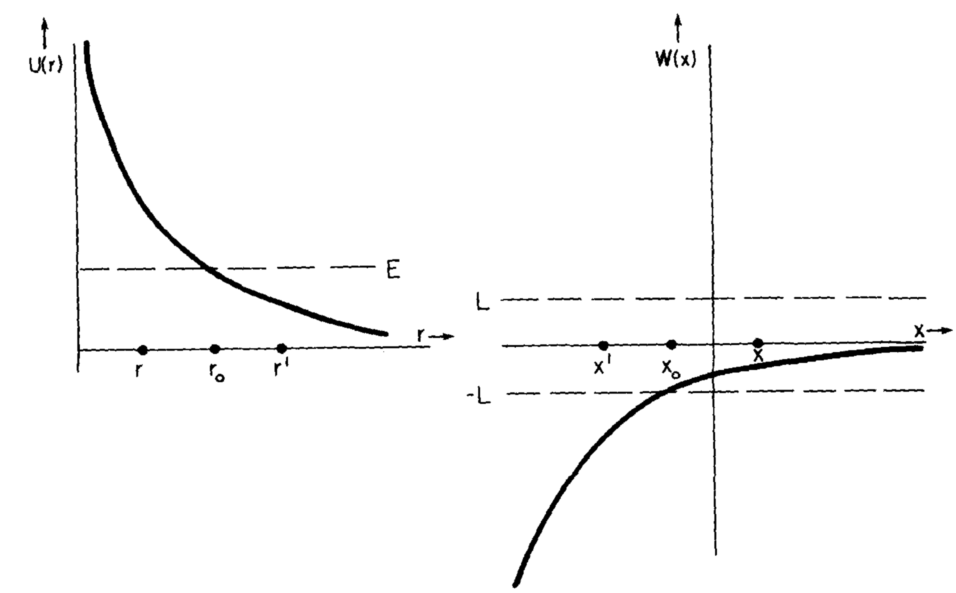

FIG. 9. (a) $U(r) = [l(l+1)\hbar^2/2mr^2] + V(r)$; (b) $W(x) = [V(e^{-x}) - E]e^{-2x}$.

where

$$r' = e^{-x'}, \quad r_0 = e^{-x_0}, \quad L = \frac{\hbar^2}{2m}\left(l + \frac{1}{2}\right)^2,$$
$$W(x) = [V(e^{-x}) - E]e^{-2x}, \quad \text{and} \quad g = (r'r)^{-1/2}G. \tag{6.3}$$

In order to place (6.3) in a form suitable for path integration,[30] we Fourier transform on the variable L. The transform $\hat{g}$ satisfies

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + W(x) - i\hbar\frac{\partial}{\partial\lambda}\right)\hat{g}(x,x'|E,\lambda) = 0 \tag{6.4}$$

$$\lim_{\lambda\to 0+}\hat{g}(x,x'|E,\lambda) = \delta(x-x'), \quad \hat{g}\equiv 0, \ \lambda < 0,$$

and may be represented as a path integral,

$$\hat{g}(x,x'|E,\lambda) = \int_{x(\cdot)\in P(x,\lambda|x',0)} \mathfrak{D}x(\cdot)\ \exp\left(\frac{i}{\hbar}S(x(\cdot),\lambda)\right),$$

$$S(x(\cdot),\lambda) = \int_0^\lambda \left[\frac{1}{2}m\left(\frac{dx}{d\tau}\right)^2 - W[x(\tau)]\right]d\tau. \tag{6.5}$$

g is then given by

$$g(x,x'|E,L) = \frac{i}{\hbar}\int_0^\infty d\lambda\ \exp\left(-\frac{i}{\hbar}\lambda L\right)\hat{g}(x,x'|E,\lambda). \tag{6.6}$$

We seek to evaluate this "λ-path" integral asymptotically as $\hbar$ vanishes, L fixed. The situation is sketched in Fig. 9, from which it is clear that there is no real critical path. However, the technique of Sec. 3 applies with λ playing the role of time. In this case, formula (3.8) becomes

$$\tilde{g}(x,x'|E,L) = m[K_w(x)k_w(x')]^{-1/2}$$
$$\times \exp\left(\frac{i}{\hbar}\int_{x'}^{x_0} k_w(x)dx - \frac{1}{\hbar}\int_{x_0}^{x} K_w(x)dx\right), \tag{6.7}$$

where

$$K_w(x) = +\{2m[L + W(x)]\}^{1/2},$$
$$k_w(x') = +\{2m[-L - W(x')]\}^{1/2}. \tag{6.8}$$

Returning to the physical variables r, r', and l, we obtain

$$\tilde{G}(r,r'|E,l) = m[K(r)k(r')]^{-1/2}$$
$$\exp\left(-\frac{i}{\hbar}\int_{r'}^{r_0} k(r)dr + \frac{1}{\hbar}\int_{r_0}^{r} K(r)dr\right), \tag{6.7'}$$

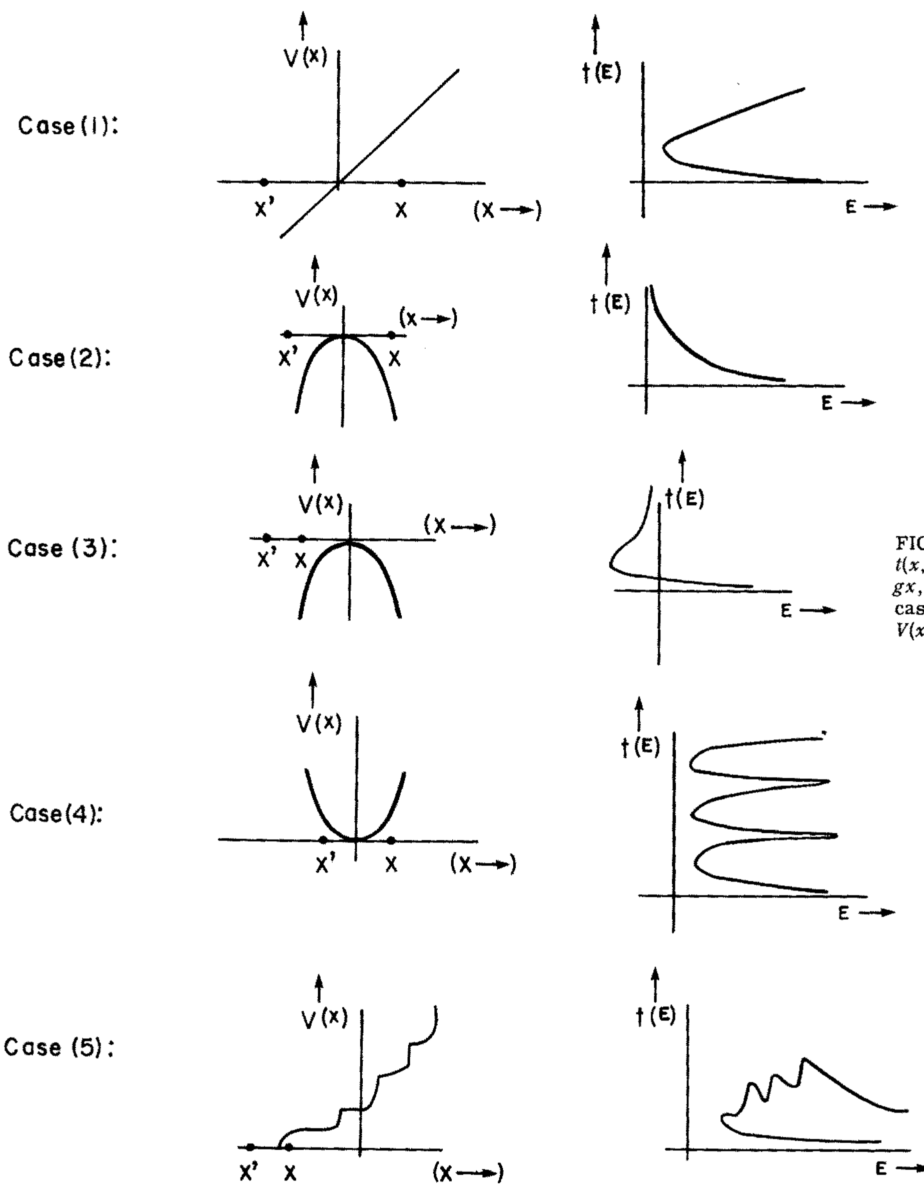

FIG. 10. Sketches of potentials and their $t(x,x'|E)$ vs E relation. Case (1): $V(x) = gx$, $g > 0$; case (2): $V(x) = -\frac{1}{2}gx^2$, $g > 0$; case (3): $V(x) = -\frac{1}{2}gx^2$, $g > 0$; case (4): $V(x) = \frac{1}{2}gx^2$, $g > 0$.

where

$$K(r) = +\left[2m\left(-E + V(r) + \frac{(l+\frac{1}{2})^2}{2mr^2}\hbar^2\right)\right]^{1/2},$$

$$k(r') = \left[2m\left(E - V(r') - \frac{(l+\frac{1}{2})^2}{2mr'^2}\hbar^2\right)\right]^{1/2}. \qquad (6.8')$$

For $V(r) = g/r$, $g > 0$, we have verified formula (6.7′) by solving (6.1) in terms of Whittaker functions and then evaluating its asymptotic expansion.

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APPENDIX

Even for real t_0 the two-point boundary value problem (2.5) may possess none, one, or several solutions.[31] Which possibility occurs depends upon the potential V, the boundary point t_0, and the boundary values x and x'. For a given potential V and fixed x and x', a particularly direct way to understand the situation is to solve the initial value problem at energy E for the time of flight t between x and x'. If one then plots the $t\ V_s\ E$ relation, intersections of this relation with the line $t = t_0$ count the multiplicity of solutions of (2.5). (Intersections of the relation with the line $E = E_0$ count the times the solution crosses the point x.) It is amusing to sketch the $t\ V_s\ E$ relationship for several simple potentials (Fig. 10).

Note added in proof: Since this work was submitted, Karl Freed[31] has published results on barrier penetration obtained by an analytic continuation of the sum over classical paths. His approach, which is similar to one we employed earlier,[32] does not continue the function space integral, but rather its asymptotic approximation.

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An $O(2, 1) \times O(3)$ Solution to a Generalized Quantum Mechanical Kepler Problem

M. J. Cunningham

Physics Department, University of Canterbury, Christchurch, New Zealand

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A differential equation directly related to the generalized Kepler equation of Infeld and Hull is solved in an $O(2, 1) \times O(3)$ group scheme. This equation contains as special cases the Schrödinger, Klein–Gordon, and Dirac (two forms) hydrogen atoms. A generalized Pasternack and Sternheimer selection rule exists and some matrix elements can be evaluated group theoretically.

I. INTRODUCTION

In an earlier paper[1] hereafter written as I, the author examined the nonrelativistic hydrogen atom according to the group scheme $O(4, 2) \supset O(2, 1) \times O(3)$ of Barut and Kleinert[2] and was able to give a group theoretical derivation of the selection rule of Pasternack and Sternheimer[3] on radial matrix elements. Here the method is used on a more general differential equation directly related to the generalized Kepler equation of Infeld and Hull.[4] This allows a unified treatment of all quantum mechanical Kepler problems in an $O(2, 1) \times O(3)$ scheme, since the Schrödinger, Klein–Gordon, and Dirac hydrogen atoms, the latter diagonalized in the usual k scheme (see, for instance, Bethe and Salpeter[5]) or the S scheme of Biedenharn,[6] are special cases of this equation.