Quasilinearization method applied to multidimensional quantum tunneling

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We apply the quasilinearization method of Bellman and Kalaba *[Quasilinearization and Nonlinear Boundary-Value Problems* (Elsevier, New York, 1965)] to find approximate solutions for the multidimensional quantum tunneling for separable as well as nonseparable wave equations. By introducing the idea of the complex "semiclassical trajectory" which is valid for the motion over and under the barrier, and which, in the proper limit, reduces to the real classical trajectory in the allowed region, we obtain an eigenvalue equation for the characteristic wave numbers. This eigenvalue equation is similar to the corresponding equation obtained from the WKB approximation and yields complex eigenvalues with negative imaginary parts. When the barrier changes very rapidly as a function of the radial distance, we can replace the concept of the semiclassical trajectory, which may not be applicable in this case, by the concept of a complex "quantum trajectory." The trajectory defined either way depends on a constant of integration, and by minimizing the action with respect to this constant we can obtain the minimum escape path. The case of two-dimensional tunneling is discussed as an example of this method.

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I. INTRODUCTION

The pioneering work of Kapur and Peierls [1] on the penetration into potential barriers in several dimensions and subsequent contributions by Banks and collaborators [2,3] and by others [4] are all based on generalizations of WKB approximation. In their work Kapur and Peierls obtained the Euler-Lagrange equations for the most probable escape path in Cartesian coordinates for real energy eigenvalues and bypassed the problems of imposing the condition that the wave function under the barrier should be single valued, and that the energies of these metastable states are, in general, complex. However, there are physical systems for which the potential barrier does not possess spherical or cylindrical symmetry and the wave equation cannot be reduced into uncoupled partial waves, but the symmetry-breaking part of the interaction is small compared to the central potential. This occurs, e.g., in the problem of α decay [5] with noncentral forces, or in the theory of molecular reactions [6], and the decay of the false vacuum [7,8]. For these systems the preferred coordinate system is not Cartesian but a system with angular variables, and then the question of the periodicity of the wave function under the barrier should be addressed, even if this difficulty is confined to a small part of space. In order to appreciate the complexity of the problem, consider the two-dimensional tunneling where the Schrödinger equation is not separable. If it is expressed in terms of the curvilinear coordinate (ξ,ϕ), the boundary conditions on the wave function assume a simple form; e.g., at the origin $\xi=0$ and on a closed curve $\xi=R$. Then even if the multidimensional tunneling is approximated by a separable wave equation, it still involves a two-point boundary-condition problem with complex eigenvalues, where the complex eigenvalue appears nonlinearly in the differential equation. The complex energy eigenvalue is related to the well-known result that in the case of resonant scattering, the scattering matrix has a pole at a complex value of momentum and the imaginary part of the energy is proportional to the width of the resonant state. In cases where the barrier is high and/or wide, this imaginary part is small and can be ignored, but there can also be resonant states where the imaginary part is not small. The requirements of a single-valued wave function and complex energy are not compatible with real classical trajectories for the motion under the barrier.

In this work we apply the method of quasilinearization [9] to find an approximate solution of the quantum tunneling in two dimensions for a general nonseparable potential barrier. However, it is not difficult to apply the same method to three-dimensional tunneling problems. The layout of the paper is as follows. In Sec. II we illustrate the method of quasilinearization as applied to an exactly solvable example of the Hamiltonian-Jacobi equation. In Sec. III we observe that for a separable wave equation in polar coordinates the partial wave Schrödinger equation can be viewed as a two-point boundary-condition problem with complex eigenvalues. We have not been able to find an accurate and stable numerical method for solving the differential equation for the complex eigenvalues, however, using the WKB approximation we have found a relatively simple eigenvalue equation which can be solved numerically.

Barriers with sharp boundaries are of common occurrence in one-, two-, or three-dimensional problems such as the electron tunneling in metal-insulator-metal junctions [10]. We consider the partial wave Schrödinger equation for situations like these where the connection formulas are exact, and in order to get a better approximation we need to determine the wave function in each region more accurately. This can be achieved if we use the method of quasilinearization to find the wave function above or below the barrier. In Sec. IV we study a barrier of the form $v(r,\phi)$, where the wave equation is not separable. Again applying the method of quasilinearization we find an iterative scheme for calculating the logarithm of the wave function which is a complex quantity. This is done by introducing the concept of the "complex path" and by imposing the condition that the wave function must be single valued. In Sec. V we study two separable examples where the eigenvalue equation can be determined exactly. In Sec. VI we investigate the important question of the escape path of the particle. Finally in Sec. VII we conclude the paper by presenting some numerical results.

II. QUASILINEARIZATION OF THE HAMILTON-JACOBI EQUATION

The theory of quasilinearization developed and expounded by Bellman and Kalaba [9] discusses a method of finding the solution of nonlinear ordinary or partial differential equations subject to prescribed boundary conditions by replacing them by an infinite sequence of linear equations. In the present work we apply the method of quasilinearization to solve the nonlinear separable equations of the Hamilton-Jacobi type by considering them as the limit of an infinite set of linear partial differential equations. We then integrate the first few equations of the set using the method of characteristics, and then obtain an approximate solution for the nonseparable problem. Let us start with a very simple example of a solvable one-dimensional Hamilton-Jacobi equation;

$$(dS/dx)^2=k^2-v(x)-\varepsilon w(x)=q^2-\varepsilon w(x) , \tag{2.1}$$

where S is the characteristic function, k^2 is the total energy, and $v(x)-\varepsilon w(x)$ is the potential energy with $\varepsilon w(x)$ a small perturbation. We replace the nonlinear equation (2.1) by the following sequence of linear equations:

$$2\left[\frac{dS_n}{dx}\right]\left[\frac{dS_{n-1}}{dx}\right]-\left[\frac{dS_{n-1}}{dx}\right]^2=k^2-v(x)-\varepsilon w(x) , \tag{2.2}$$

so that in the limit of $n\to\infty$, $S_n(x)$ tends to $S(x)$, i.e., S_n converges to the solution of (2.1). To start the iterative solution of (2.1) we take S_0 to be a solution of

$$(dS_0/dx)^2=k^2-v(x)=q^2(x) , \tag{2.3}$$

and then using (2.2) we calculate (dS_1/dx), $(dS_2/dx),\ldots,(dS_n/dx)$;

$$\left[\frac{dS_1}{dx}\right]=\left[\frac{dS_0}{dx}\right]-\frac{(\varepsilon/2)w(x)}{q(x)} , \tag{2.4}$$

$$\left[\frac{dS_2}{dx}\right]=\left[\frac{dS_1}{dx}\right]-\frac{(\varepsilon^2/8)w^2(x)}{q(x)[q^2-\varepsilon w(x)/2]} , \tag{2.5}$$

$$\left[\frac{dS_3}{dx}\right]=\left[\frac{dS_2}{dx}\right]+\frac{(\varepsilon^4/128)w^4(x)}{q(x)[q^2-\varepsilon w(x)/2][q^2-\varepsilon w(x)/2)^2-(\varepsilon^2w^2/8)]} , \tag{2.6}$$

and so on. This sequence converges faster than the expansion of $[q^2-\varepsilon w(x)]^{1/2}$ in powers of ε, since (dS_2/dx) already contains $(-\varepsilon^3/16)w^3(x)$, and (dS_3/dx) includes the contribution of $\varepsilon^4w^4(x)$. The question of the convergence of a sequence like (2.2) to the solution of (2.1) is discussed in detail by Bellman and Kalaba [9].

III. QUASILINEARIZATION AND THE WKB APPROXIMATION

In this section we consider the application of the quasilinearization method to the tunneling problem, and compare it to the WKB approximation. But first let us consider the two-dimensional tunneling in polar coordinates with a central potential barrier $v(r)$ for which the reduced Schrödinger equation for the mth partial wave reads as

$$u''+[k^2-v(r)-(m^2-\tfrac{1}{4})/r^2]u=0 , \tag{3.1}$$

where primes denote derivatives with respect to r. This equation is subject to the boundary conditions

$$u(r=0)=0 ,$$
$$(u'/u)_{r=R}=\{d[\ln(r^{1/2}H_m^{(1)}(kr))]/dr\}_{r=R} , \tag{3.2}$$

where $H_m^{(1)}(kr)$ is the Hankel function, and R is the range of the potential, i.e., for $r>R$, $v(r)$ becomes negligible. Thus we have a two-point boundary-condition problem where the eigenvalue k appears both in the differential equation as well as the boundary condition. To transform this equation to the normal form of an eigenvalue equation where the boundary conditions are independent of k, we change $u(r)$ to $\chi(r)$ where

$$u(r)=r^{1/2}H_m^{(1)}(kr)\chi(r) . \tag{3.3}$$

By substituting (3.3) in (3.1) we find

$$\chi''+2(d\{\ln[r^{1/2}H_m^{(1)}(kr)]\}/dr)\chi'-v(r)\chi=0 , \tag{3.4}$$

as the wave equation with the boundary conditions

$$\chi(0)=0,\quad \chi'(R)=0 . \tag{3.5}$$

In Eq. (3.4) the eigenvalue k will be complex, since it appears in the argument of the complex function $H_m^{(1)}(kr)$. This is in contrast with the one-dimensional tunneling where the boundary conditions are given at $x=\pm\infty$, and k is real and is not a discrete eigenvalue. Apart from the cases of rectangular and δ-function barriers, Eq. (3.4) has to be solved numerically, and even this is not simple.

Therefore let us consider the semiclassical solution of the tunneling for the central potentials. Since k^2 is complex, the classical turning points cannot be defined as the roots of $k^2-v(r)-(m^2-\frac{1}{4})/r^2=0$. But for calculating the lowest eigenvalues, the imaginary part of k^2 is small, and we can replace k^2 by $\mathrm{Re}k^2$ to define the turning points.

For a simple barrier there are three distinct turning points, a, b, and c with $c>b>a$ for a given energy k^2. For $r>c$ the wave function u_4 approaches the outgoing free particle wave function as $r\to\infty$, i.e.,

$$u_4=\left[\frac{2D}{\sqrt{K_0}}\right]\exp\left\{i\left[\int_c^r K_0(r)dr-\left[\frac{\pi}{4}\right]\right]\right\}, \tag{3.6}$$

where D is a constant, and $K_0(r)$ is a complex quantity (since k is complex), with a small imaginary part and is defined by

$$K_0(r)=[k^2-v(r)-(m^2-\tfrac{1}{4})/r^2]^{1/2}. \tag{3.7}$$

Under the barrier K_0 has a large imaginary part, therefore we replace it by the complex quantity $\mathcal{K}_0(r)$;

$$\mathcal{K}_0(r)=[v(r)+(m^2-\tfrac{1}{4})/r^2-k^2]^{1/2}, \tag{3.8}$$

and we write the wave function for $b<r<c$ as

$$u_3=(D/\sqrt{\mathcal{K}_0})\left[e^{-L}\exp\left[\int_b^r\mathcal{K}_0dr\right]-2ie^{L}\exp\left[-\int_b^r\mathcal{K}_0dr\right]\right], \tag{3.9}$$

where we have used the well-known connection formulas for the WKB approximation, and where L is defined by

$$L=\int_b^c\mathcal{K}_0(r)dr. \tag{3.10}$$

Between the two turning points a and b, the wave function is oscillatory, and again by using the connection formulas we find

$$u_2=\left[\frac{2D}{i\sqrt{K_0}}\right]\left[\left[e^L-\tfrac{1}{4}e^{-L}\right]\exp\left\{i\left[\int_r^b K_0dr-\left[\frac{\pi}{4}\right]\right]\right\}+\left[e^L+\tfrac{1}{4}e^{-L}\right]\exp\left\{-i\left[\int_r^b K_0dr-\left[\frac{\pi}{4}\right]\right]\right\}\right]. \tag{3.11}$$

If the centripetal force $(m^2-\frac{1}{4})/r^2$ is absent in (3.1) (as in the case of three-dimensional tunneling for the S wave), then there are only two turning points b and c. In this case by demanding that u_2 must vanish at $r=0$, we find the eigenvalue equation to be

$$e^{2L}=\frac{(-i/4)\cos(2\delta_0)}{1+\sin(2\delta_0)}, \tag{3.12}$$

where

$$\delta_0=\int_0^b K_0(r)dr. \tag{3.13}$$

In the presence of the centripetal force, we need to find the wave function for $r<a$. This wave function must satisfy the boundary condition $u_1(r=0)=0$. Let T denote the logarithmic derivative of the wave function at $r=a$;

$$T=\frac{(du_1/dr)_{r=a}}{ku_1(a)}. \tag{3.14}$$

Matching this logarithmic derivative with $(du_2/dr)_{r=a}/[ku_2(a)]$ gives us the following eigenvalue equation:

$$e^{2L}=\frac{(i/4)[(\beta^2-T^2)\cos(2\delta)+2T\beta\sin(2\delta)]}{[(\beta^2+T^2)+(T^2-\beta^2)\sin(2\delta)+2\beta T\cos(2\delta)]}, \tag{3.15}$$

where

$$\delta=\int_a^b K_0(r)dr, \tag{3.16}$$

and β is defined by

$$\beta=K_0(a)/k. \tag{3.17}$$

Since a is a turning point, β is zero, therefore if $T(a)$ is not zero, (3.15) reduces to (3.12) except that δ replaces δ_0. However, if we use the WKB approximation we find the following expressions for $u_1(r)$ and for T:

$$u_1(r)=[C/\mathcal{K}_0(r)^{1/2}]\sinh\left[\int_0^r\mathcal{K}_0(r)dr\right] \tag{3.18}$$

and

$$T=[\mathcal{K}_0(a)/k]\coth\left[\int_0^a\mathcal{K}_0(r)dr\right]. \tag{3.19}$$

Thus T also vanishes at $r=a$, and the right-hand side of (3.15) becomes indeterminate. Noting that

$$(\beta/T)\to\pm i\tanh\gamma, \tag{3.20}$$

where

$$\gamma=\int_0^a\mathcal{K}_0(r)dr, \tag{3.21}$$

then (3.15) reduces to

$$e^{2L}=\frac{(i/4)[-(1+\tanh^2\gamma)\cos(2\delta)\pm2i\tanh(\gamma)\sin(2\delta)]}{[(1-\tanh^2\gamma)+(1+\tanh^2\gamma)\sin(2\delta)\pm2i\tanh(\gamma)\cos(2\delta)]}. \tag{3.22}$$

Equations (3.12) and (3.22) have complex roots $k=k_r-ik_i$, but only the roots with $k_i>0$ are acceptable. The quantities k_r and k_i can have only discrete values, therefore only after solving Eq. (3.22) can one determine whether or not the effective height of the barrier, $v(r)+[m^2-\frac{1}{4}]/r^2$, is greater than the real part of k^2, i.e., one is dealing with proper quantum tunneling. Also when $\mathrm{Re}k^2$ is comparable to the height of the potential the semiclassical approximation may not be reliable.

Next let us consider the solution of this problem when the barrier has sharp boundaries using the method of quasilinearization. For $r>c$ we write the wave function as

$$u_4=\left[\frac{1}{\sqrt{K(r)}}\right]\exp\left[i\int K(r)dr-i\left[\frac{\pi}{4}\right]\right], \tag{3.23}$$

and substitute this in (3.1) to obtain a differential equation for $K(r)$;

$$\frac{1}{2}\frac{K''}{K}-\frac{3}{4}\left[\frac{K'}{K}\right]^2+K^2-K_0^2(r)=0 . \tag{3.24}$$

If we neglected the first two terms of (3.24) we find $K_0(r)$, where K_0 is defined by (3.7). Let us now apply the method of quasilinearization to (3.24) and write

$$\frac{1}{2}\frac{K''_{n-1}}{K_{n-1}}-\frac{3}{4}\left[\frac{K'_{n-1}}{K_{n-1}}\right]^2+2K_nK_{n-1}-K_{n-1}^2-K_0^2(r)=0 , \tag{3.25}$$

where, for $n=0$,

$$K_{n=0}=K_0 . \tag{3.26}$$

By substituting $K_{n=0}$ in (3.25) we obtain K_1,

$$K_1(r)=K_0(r)+\frac{1}{8}\left[\frac{v_e''}{K_0^3}\right]+\frac{5}{32}\left[\frac{(v_e')^2}{K_0^5}\right] . \tag{3.27}$$

Here v_e is the effective potential;

$$v_e=v(r)+(m^2-\tfrac{1}{4})/r^2 . \tag{3.28}$$

The iteration can be continued by substituting for K_1 in (3.25) and calculating K_2 and so on. Inside the barrier the wave function is a linear combination of the two solutions

$$u_\pm=[1/\sqrt{\mathcal{K}(r)}]\exp\left[\pm\int\mathcal{K}(r)dr\right] . \tag{3.29}$$

Again if we substitute (3.29) in (3.1) we obtain a differential equation for $\mathcal{K}(r)$;

$$\frac{1}{2}\frac{\mathcal{K}''}{\mathcal{K}}-\frac{3}{4}\left[\frac{\mathcal{K}'}{\mathcal{K}}\right]^2-\mathcal{K}^2-K_0^2(r)=0 , \tag{3.30}$$

which can be solve in the same way as Eq. (3.24). We can join the solutions $u_4(n,r)$ obtained from (3.23) with $K=K_n$ and $u_3(n,r)$ found from the linear combination of u_+ and u_-, Eq. (3.29) with $\mathcal{K}=\mathcal{K}_n$, by requiring that their logarithmic derivatives at the turning point c be equal, i.e.,

$$\left[\frac{d\ln[u_3(n,r)]}{dr}\right]_c=\left[\frac{d\ln[u_4(n,r)]}{dr}\right]_c , \tag{3.31}$$

and this is the eigenvalue equation.

IV. TWO-DIMENSIONAL TUNNELING

In scattering theory the semiclassical approximation is applied to calculate the radial part of the wave function, but if it is used to calculate the angular part, in certain cases, the resulting solution may not be physically acceptable. For instance, in the case of resonant scattering we need to calculate the wave function in a part of space where the total energy is lower than the height of the barrier. Here we have a physically acceptable approximate solution if we use Cartesian coordinates, but the wave function will not be single valued in spherical or cylindrical coordinates unless we allow for the complex solutions of the classical Hamilton-Jacobi equation. To illustrate this let us consider the tunneling under the separable potential barrier

$$V(x,y)=V_0-\tfrac{1}{2}M\omega^2(x^2+y^2) , \tag{4.1}$$

where V_0, M, and ω are constants. If we write the wave function as

$$\psi=e^{-S(x,y)/\hbar} , \tag{4.2}$$

then in the limit of $\hbar\to 0$ we have the Hamilton-Jacobi equation

$$\left[\left[\frac{\partial S}{\partial x}\right]^2+\left[\frac{\partial S}{\partial y}\right]^2\right]=2M[V_0-E-\tfrac{1}{2}M\omega^2(x^2+y^2)] , \quad V_0>E \tag{4.3}$$

with $S(x,y)$ a real quantity under the barrier. Thus the wave function is given by

$$\psi=\exp\left[\left[\pm\int[2M(\alpha-\tfrac{1}{2}M\omega^2x^2)]^{1/2}dx-\int[2M(V_0-\alpha-E-\tfrac{1}{2}M\omega^2y^2)]^{1/2}dy\right]\Big/\hbar\right] , \tag{4.4}$$

where $\alpha>0$ is the separation constant. However, consider the approximate solution of the same problem in polar coordinates, i.e.,

$$\left[\left[\frac{\partial S}{\partial r}\right]^2+\left[\frac{1}{r^2}\right]\left[\frac{\partial S}{\partial\phi}\right]^2\right]=2M[V_0-E-\tfrac{1}{2}M\omega^2r^2], \quad V_0>E \tag{4.5}$$

with the corresponding wave function

$$\psi=\exp\left[\left[-p_\phi\phi\pm\int\{2M[V_0-E-\tfrac{1}{2}M\omega^2r^2-(p_\phi/r)^2]\}^{1/2}\right]\Big/\hbar\right]dr\ . \tag{4.6}$$

Here the wave function is not single valued, unless the separation constant p_ϕ is pure imaginary, i.e., a complex solution to the classical equation (4.3) is required for a physically meaningful wave function.

If the potential barrier depends on the radial as well as the angular variable, i.e., $v=v(r,\phi)$, then in general the problem is not separable and therefore not reducible to the solution of an ordinary differential equation. For this case the Schrödinger equation

$$\nabla^2\psi+[k^2-v(r,\phi)]\psi=0 \tag{4.7}$$

can be solved by the method of quasilinearization. To this end let us write

$$\psi=\exp(iS)\ , \tag{4.8}$$

where S, measured in units of $\hbar$, satisfies the nonlinear partial differential equation

$$(\nabla S)^2-[k^2-v(r,\phi)]-i\nabla^2 S=0\ . \tag{4.9}$$

Using the method of quasilinearization we replace (4.9) by a set of first-order partial differential equations:

$$2(\nabla S_n\cdot\nabla S_{n-1})=[k^2-v(r,\phi)]+i(\nabla^2 S_{n-1})+(\nabla S_{n-1})^2,\quad n=1,2,3,\dots\ . \tag{4.10}$$

As we observed in Sec. II, $S(r,\phi)$ will be the limit of $S_n(r,\phi)$ as $n\to\infty$.

Note that even in the classical limit, i.e., by ignoring $i\nabla^2 S$ in (4.9), the resulting Hamilton-Jacobi equation is, in general, nonseparable and complex, since k^2 is complex. Denoting the angular average of $v(r,\phi)$ by $\bar{v}$, i.e.,

$$\bar{v}=(2\pi)^{-1}\int_0^{2\pi}v(r,\phi)d\phi\ , \tag{4.11}$$

we find an approximate solution for S, in the classical limit with $\bar{v}(r)$;

$$(\nabla S_0)^2=[k^2-\bar{v}(r)]\ . \tag{4.12}$$

This equation is separable and S_0 is given by

$$S_0(r,\phi)=\nu\phi\pm\int K_0(\nu,r)dr\ , \tag{4.13}$$

where ν is the separation constant. The classical trajectory of the particle in this approximation is found from the relation

$$\frac{\partial S_0}{\partial\nu}=\phi_0=\phi-(\pm)\nu\int\frac{dr}{r^2K_0(\nu,r)}\ , \tag{4.14}$$

where ϕ_0 is a constant. These equations will be used as the starting point for our iterative approach to the solution of Eq. (4.10). For the nth iteration Eq. (4.10) can be solved using the method of characteristic assuming that S_{n-1} is known. Thus the set of equations

$$\frac{dr}{\partial S_{n-1}/\partial r}=\frac{r^2d\phi}{\partial S_{n-1}/\partial\phi}=\frac{2dS_n}{k^2-v(r,\phi)+(\nabla S_{n-1})^2+i(\nabla^2 S_{n-1})} \tag{4.15}$$

gives us both $\phi(r)$ and $S_n(r,\phi)$. Thus after the nth iteration we have

$$\frac{d\phi}{dr}=\frac{\partial S_{n-1}/\partial\phi}{r^2(\partial S_{n-1}/\partial r)} \tag{4.16}$$

as the differential equation of the trajectory. Here even in the classical limit, i.e., when we ignore $i\nabla^2 S$ in Eqs. (4.9) and (4.10), the trajectories are complex, since $\phi(r)$ is needed for all values of r, $0\le r<\infty$, and not just between the classical turning points and since k^2 is complex. By substituting $\phi(r)$ in $v(r,\phi)$, we find $S_n(r,\phi)$ from the integral

$$S_n=\tfrac{1}{2}\int dr\left[\frac{k^2-v(r,\phi(r))+(\nabla S_{n-1})^2+i(\nabla^2 S_{n-1})}{\partial S_{n-1}/\partial r}\right]\ . \tag{4.17}$$

Next let us consider the solution of these equations to the first order of iteration. Again denoting the classical turning points by a, b, and c, as before, we observe that for $a<r<b$, or $r>c$,

$$\mathrm{Re}k^2\ge\bar{v}(r)+(\nu/r)^2\ , \tag{4.18}$$

and $S_0(r,\phi)$ is given by (4.13) which we now write as

$$S_0^{\mathrm{I}}(r,\phi)=\nu\phi\pm\int K_0(\nu,r)dr\ , \tag{4.19}$$

where $K_0(\nu,r)$ is defined by (3.7) and the superscript indicates the motion in the region satisfying the condition (4.18). On the other hand, if

$$\mathrm{Re}k^2<\bar{v}(r)+(\nu/r)^2\ , \tag{4.20}$$

then

$$S_0^{\mathrm{II}}(r,\phi)=\nu\phi\pm i\int\mathcal{K}_0(\nu,r)dr\ , \tag{4.21}$$

the superscript II here means that the motion is under the barrier. Using these two expressions we can calculate $\nabla^2 S_0$,

$$\nabla^2 S_0^{\mathrm{I}}=\pm[K_0'+(K_0/r)]\ , \tag{4.22}$$

and

$$\nabla^2 S_0^{\mathrm{II}}=\pm i[\mathcal{K}_0'+(\mathcal{K}_0/r)]\ . \tag{4.23}$$

By substituting (4.19), (4.21), (4.22), and (4.23) in (4.17) we find

$$S_1^{\mathrm{I}}(r,\phi)=\pm\int Q_0(\nu,r)dr+\nu\phi+(i/2)\ln(K_0r)\ , \tag{4.24}$$

and

$$S_1^{\mathrm{II}}(r,\phi)=\pm i\int \mathcal{Q}_0(\nu,r)dr+\nu\phi+(i/2)\ln(\mathcal{K}_0 r)\ , \qquad (4.25)$$

where

$$Q_0(\nu,r)=K_0(\nu,r)+[\bar{v}-v(r,\phi(r))]/[2K_0(\nu,r)]\ , \qquad (4.26)$$

and $\mathcal{Q}_0(\nu,r)$ is defined by a similar relation,

$$\mathcal{Q}_0(\nu,r)=\mathcal{K}_0(\nu,r)-[\bar{v}-v(r,\phi(r))]/[2\mathcal{K}_0(\nu,r)]\ . \qquad (4.27)$$

Using Eq. (4.16), with $n=1$, we can rewrite (4.24) in the form

$$S_1^{\mathrm{I}}(r,\phi)=\pm\int K_0(\nu,r)dr+\nu\phi$$
$$+(1/2\nu)\int[\bar{v}(r(\phi))-v(r(\phi),\phi)]r^2(\phi)d\phi$$
$$+(i/2)\ln(K_0 r)\ , \qquad (4.28)$$

and we find a similar relation for $S_1^{\mathrm{II}}(r,\phi)$ by starting from Eq. (4.25). Continuing the iteration we can determine $S_2,S_3,\ldots,S_n$. For instance for $S_n(r,\phi)$ we have

$$S_n(r,\phi)=S_{n-1}(r,\phi)+\tfrac{1}{2}\int\left[\frac{k^2-v(r,\phi(n-1,r))-(\nu/r)^2-(\partial S_{n-1}/\partial r)^2}{\partial S_{n-1}/\partial r}\right]dr+\left[\frac{i}{2}\right]\ln\left[r\left|\frac{\partial S_{n-1}}{\partial r}\right|\right]\ , \qquad (4.29)$$

where $\phi(n-1,r)$ is the solution of (4.16)

$$\frac{d\phi(n-1,r)}{dr}=\frac{\nu}{r^2(\partial S_{n-1}/\partial r)}\ . \qquad (4.30)$$

Both of these equations are valid for the classically allowed region or when the particle moves under the barrier.

The rate of convergence of the iteration given by (4.29) depends on the relative magnitude of the second term in (4.29) compared to the first term. Thus in the first order this condition is

$$\left|\int_{r_1}^{r_2}\frac{[v(r,\phi(1,r))-\bar{v}(r)]dr}{2\{\bar{v}(r)+(\nu/r)^2-k^2\}^{1/2}}\right|<\left|\int_{r_1}^{r_2}dr\left[\bar{v}(r)+\left[\frac{\nu}{r}\right]^2-k^2\right]^{1/2}\right|\ , \qquad (4.31)$$

where r_1 and r_2 are the two turning points, and S is calculated for the motion under the barrier.

So far we have treated ν as an arbitrary parameter. Now we impose the condition that the wave function ψ, Eq. (4.7), has to be single valued, i.e.,

$$\psi(r,\phi)=\psi(r,2\pi n+\phi)\quad (n\ \text{ an integer})\ . \qquad (4.32)$$

Thus from Eq. (4.8) and the approximate form of S_1, Eq. (4.24) or (4.25), we find

$$\nu=m\quad (m \text{ an integer})\ . \qquad (4.33)$$

Alternatively we can impose the condition (4.32) on $S_1(r,\phi)$ given by (4.28). To this end we define the angular part of the wave function by $\Phi(\phi)$, where

$$\Phi(\phi)=\exp\{i\nu\phi+(i/2\nu)\int[\bar{v}(r(\phi))-v(r(\phi),\phi)]\times r^2(\phi)d\phi\}\ , \qquad (4.34)$$

then from (4.32) we have

$$\Phi(\phi)=\Phi(\phi+2\pi n)\ . \qquad (4.35)$$

This equation gives us a set of eigenvalues ν which will be different from (4.33). Depending on the explicit form of $v(r,\phi)$, we may choose either (4.24) or (4.28) to obtain an approximate form of the wave function.

If the potential $\bar{v}(r)$ defined by (4.11) is singular (like a δ function) or changes rapidly, then as before we can use Eq. (4.10) for iteration, but rather than starting with S_0 which is given by (4.13), we use S_0 as the solution of

$$(\nabla S_0)^2-[k^2-\bar{v}(r)]-i\nabla^2 S_0=0\ . \qquad (4.36)$$

This S_0 can be written in terms of the wave function $u(m,r)$, Eq. (3.1). Using the definition (4.8) we have

$$S_0=m\phi-i\ln[u(m,r)/\sqrt{r}\,]\ , \qquad (4.37)$$

where m is an integer. By substituting (4.37) in (4.16) and (4.17), with $n=1$, we find the following equations:

$$\phi(r)=i\int^r m\,dr/(r^2 d\{\ln[u(m,r)/\sqrt{r}\,]\}/dr) \qquad (4.38)$$

and

$$S_1=i\int^r\frac{dr\{i(\nabla^2 S_0)+[k^2-\bar{v}(r)]+\frac{1}{2}[\bar{v}(r)-v(r,\phi)]\}}{d\{\ln[u(m,r)/\sqrt{r}\,]\}/dr}\ . \qquad (4.39)$$

In Eq. (4.38), $\phi(r)$ is a continuous function of r even when the logarithmic derivative of $u(m,r)$ is discontinuous, as in the case of a δ-function potential. This $\phi(r)$ is the quantum analog of the classical equation for the trajectory (4.14), and reduces to it if we replace $\ln[u(m,r)/\sqrt{r}\,]$ by its WKB approximate form

$$\ln[u(m,r)/\sqrt{r}\,]=i\int^r K_0(m,r)dr\ . \qquad (4.40)$$

If we substitute for $k^2-\bar{v}(r)$ from (4.36) in (4.39) and simplify, we find $S_1(r,\phi)$,

$$S_1(r,\phi)=S_0(r,\phi)+\left[\frac{i}{2}\right]\int^r\frac{[\bar{v}-v(r,\phi)]dr}{d\{\ln[u(m,r)/\sqrt{r}\,]\}/dr}\ , \tag{4.41}$$

where in the last integral ϕ in $v(r,\phi)$ is to be replaced by the complex trajectory (4.38) and thus S_1 will depend on the constant of integration ϕ_0 of Eq. (4.38). This point will be discussed in Sec. VI.

V. BARRIERS WITH SHARP BOUNDARIES

Let us now consider those cases where the barrier extends from $r=b$ to $r=c$, and is zero everywhere else. Between these two points the height of the barrier can depend on both r and ϕ. The wave function in the three regions $r<b$, $b<r<c$, and $r>c$ is given by

$$u_2=Ar^{1/2}J_m(kr),\quad r<b \tag{5.1}$$

$$u_3=r^{1/2}\{B\exp[iS_n^{\rm II}(r,b)]+C\exp[-iS_n^{\rm II}(r,b)]\},\quad b<r<c,\quad n=0,1,2,\ldots \tag{5.2}$$

and

$$u_4=2Dr^{1/2}H_m(kr),\quad r>c \tag{5.3}$$

where $S_0^{\rm II}(r,b)$, and $S_1^{\rm II}(r,b)$ are given by (4.21) and (4.25), respectively, with $\phi=0$, and A, B, C, and D are constants. By matching the logarithmic derivatives of u at b and c we find the following relation;

$$e^{2iS_n(c,b)}=\frac{\{d/dr[iS_n^{\rm II}-\ln J_m(kr)]\}_{r=b}\{d/dr[\ln H_m(kr)+iS_n^{\rm II}]\}_{r=c}}{\{d/dr[iS_n^{\rm II}+\ln J_m(kr)]\}_{r=b}\{d/dr[iS_n^{\rm II}-\ln H_m(kr)]\}_{r=c}}\ , \tag{5.4}$$

where $S_n(c,b)=S_n(r=c,\phi=0)-S_n(r=b,\phi=0)$, and these are given by Eq. (4.29). Note that in (5.4) $(\partial S_n^{\rm II}/\partial r)$ is not zero either at b or c since these turning points are not dependent on k. For $m>1$ we can replace u_4 by its WKB approximate form;

$$u_4=\left[\frac{2D}{[k^2-(m^2-\frac{1}{4}/r^2]^{1/2}}\right]\times\exp i\left[\int_c^r\left[k^2-\frac{m^2-\frac{1}{4}}{r^2}\right]^{1/2}dr-\left[\frac{\pi}{4}\right]\right]\ . \tag{5.5}$$

As an example of two-dimensional tunneling with finite-range potentials, let us consider the case where the barrier is given by

$$v(r,\phi)=\bar{v}(r)+f(\phi)/r^2\ , \tag{5.6}$$

where

$$\bar{v}(r)=[v_0-(B/r)]\Theta(r-b)\Theta(c-r)\ . \tag{5.7}$$

In these expressions v_0, B, b, and c are constants, $\Theta(x)$ is the step function

$$\Theta(x)=\begin{cases}1, & x>0\\ 0, & x<0\end{cases} \tag{5.8}$$

and $f(\phi)$ is an arbitrary function of ϕ, subject to the condition

$$\int_0^{2\pi}f(\phi)d\phi=0\ . \tag{5.9}$$

The Schrödinger equation for the potential (5.7) can be found in terms of special functions. Thus the solution of Eq. (3.1) (for $\mu=m$) is given by

$$u_2(\mu,r)=r^{1/2}J_\mu(kr),\quad 0<r<b \tag{5.10}$$

$$u_3(\mu,r)=CW_{\lambda,\mu}(2qr)+DM_{-\lambda,\mu}(2qr)\ , \tag{5.11}$$

and

$$u_4(\mu,r)=Fr^{1/2}H_\mu(kr)\ ,\quad r>c \tag{5.12}$$

where

$$q^2=v_0-k^2\ \text{ and }\ \lambda=B/(2q)\ . \tag{5.13}$$

The functions $W_{\lambda,\mu}(2qr)$ and $M_{-\lambda,\mu}(2qr)$ are two independent solutions of the Whittaker differential equation [11]

$$\frac{d^2W}{dz^2}+\left[-\frac{1}{4}+\left[\frac{\lambda}{z}\right]+\frac{\frac{1}{4}-\mu^2}{z^2}\right]W=0\ , \tag{5.14}$$

and C, D, and F are constants which can be determined by matching the logarithmic derivatives at the boundaries b and c. This results in the following eigenvalue equation for k:

$$[kL_2(kb)W_{\lambda,\mu}(2qb)-2qW'_{\lambda,\mu}(2qb)][2qM'_{-\lambda,\mu}(2qc)-kL_4(kc)M_{-\lambda,\mu}(2qc)]-[kL_4(kc)W_{\lambda,\mu}(2qc)-2qW'_{\lambda,\mu}(2qc)][2qM'_{-\lambda,\mu}(2qb)-kL_2(kb)M_{-\lambda,\mu}(2qb)]=0\ , \tag{5.15}$$

where primes denote derivatives with respect to the argument. The two functions $L_4(kb)$ and $L_4(kc)$ are defined by

$$L_2(kb)=[\partial/\partial z\,\ln\{\sqrt{z}J_\mu(z)\}]_{z=kb}\ , \tag{5.16}$$

and

$$L_4(kc)=[\partial/\partial z\ \ln\{\sqrt{z}H_\mu(z)\}]_{z=kc}\ . \tag{5.17}$$

For $B=0$, Eqs. (5.11) and (5.15) reduce to

$$u_3(\mu,r)=br^{1/2}\{[qJ_\mu(kb)I'_\mu(qb)-kJ'_\mu(kb)I_\mu(qb)]K_\mu(qr)+[kK_\mu(qb)J'_\mu(kb)-qJ_\mu(kb)K'_\mu(qb)]I_\mu(qr)\},\quad b<r<c \tag{5.18}$$

and

$$[qH_\mu(kc)I'_\mu(qc)-kH'_\mu(kc)I_\mu(qc)][qJ_\mu(kb)K'_\mu(qb)-kJ'_\mu(kb)K_\mu(qb)]=[qH_\mu(kc)K'_\mu(qc)-kH'_\mu(kc)K_\mu(qc)][qI'_\mu(qb)J_\mu(kb)-kJ'_\mu(kb)I_\mu(qb)]\ . \tag{5.19}$$

Both of the eigenvalue equations (5.15) and (5.19) have complex eigenvalues.

In Table I, the numerical results for the lowest eigenvalues of Eqs. (5.15) and (5.19) are given for different values of v_0, and for the partial wave $\mu=m=2$. In Fig. 1, the real and the imaginary parts of the ground-state wave function are plotted as a function of r for a constant barrier which is slightly larger than $\mathrm{Re}k^2$. We observe that for each partial wave when $\mathrm{Re}k^2<v_0+(m^2-\frac{1}{4})/r^2$, the wave function approximates a wave packet for a particle trapped to the left of the barrier. The current associated with the two-dimensional tunneling, unlike the current in the one-dimensional case, is not constant. For instance, if the barrier is independent of ϕ, then the radial component of current is given by

$$j_r(r)=-((\mathrm{Im}k^2)\int_0^r|u(\mu,r)|^2dr\geq 0\ . \tag{5.20}$$

This current flows radially outward since $\mathrm{Im}k^2<0$. In Fig. 2 the radial current is shown for a constant barrier.

The concept of the "complex trajectory" under the barrier for this problem will be discussed in the next section.

VI. THE MOST PROBABLE ESCAPE PATH

Kapur and Peierls [1] have shown that the most probable escape path, or the path of minimum opacity [12] in the semiclassical regime, can be found by minimizing the classical action, S_c under the barrier (see also Banks and co-workers [2,3]). Their formulation is applicable when the action is given in terms of the rectangular coordinates, when k and S_c are real quantities. However, in cylindrical (or spherical polar) coordinates, we require a different approach due to the quantization condition for the variable ϕ, and the fact that $\mathrm{Im}k^2\neq 0$. In the present method the wave function defined in terms of $S(\phi,r)$ is completely determined once the potential $v(r,\phi(r))$ is known. Now according to (4.14) or (4.38), $\phi(r)$ is known up to an arbitrary constant ϕ_0. This constant can be found by requiring that $\phi(r)$, to any order of iteration n, be the same as the most probable escape path to the order $n-1$.

Noting that the amplitude of the wave function under the barrier has the form $\psi=\exp(-\mathrm{Im}S)$, the most probable escape path is obtained by minimizing $\mathrm{Im}S(m,\phi_0)$ with respect to the continuous variable ϕ_0 for a given m, i.e., by finding a complex number ϕ_0^M such that

$$\mathrm{Im}S(m,\phi_0^M)=\min\mathrm{Im}(m,\phi_0)\ . \tag{6.1}$$

Since $\phi(r)$ is a complete quantity, ϕ_0^M is also a complex number, and for this value of ϕ_0, $\mathrm{Im}S(m,\phi_0^M)$ should be bounded and positive. The potential $v(r,\phi)$ is a periodic function of ϕ, $v(r,\phi)=v(r,\phi+2\pi)$, therefore we only need to consider those roots satisfying the relation $0\leq\mathrm{Re}\phi_0^M\leq 2\pi$. This condition may not be sufficient for a unique solution to Eq. (6.1). Let us consider the condition given by (6.1) for the trajectory of the outgoing (or the ingoing) wave for the two iteration schemes discussed in Sec. III. From Eqs. (4.25) and (4.41) we have

$$\mathrm{Im}S_1^{\mathrm{II}}=\mathrm{Im}S_0^{\mathrm{II}}\pm\tfrac{1}{2}\mathrm{Re}\int_b^c\frac{[v(r,\phi)-\bar{v}(r)]dr}{\mathcal{H}_0(r)}+\tfrac{1}{2}\mathrm{Re}[\ln(r\mathcal{H}_0)]\ , \tag{6.2}$$

and

$$\mathrm{Im}S_1=\mathrm{Im}S_0\pm\tfrac{1}{2}\mathrm{Re}\int_b^c\frac{[\bar{v}(r)-v(r,\phi)]dr}{d/dr\{\ln[u(m,r)/\sqrt{r}\,]\}}\ . \tag{6.3}$$

TABLE I. Complex eigenvalues for the potential $\bar{v}(r)=[v_0-(B/r)]\Theta(2-r)\Theta(r-1)$ for the two cases of $B=0$, and $B=1(l^{-1})$ are given for different heights of the barrier v_0. The approximate value of the real part of $k\,(l^{-1})$ is calculated using Eq. (7.8).

$v_0(l^{-2})$	14	20	24	28
$B=0$(exact)	$3.8347-0.0286i$	$4.0596-0.0059i$	$4.15873-0.0022i$	$4.2341-0.0008i$
$B=0$(appr.)	3.7892	4.00921	4.1080	4.1848
$B=1$(exact)	$5.0050-0.381i$	$4.0330-0.0055i$	$4.13939-0.0021i$	$4.2189-0.0008i$
$B=1$ (appr.)	3.7889	3.9798	4.0857	4.1672

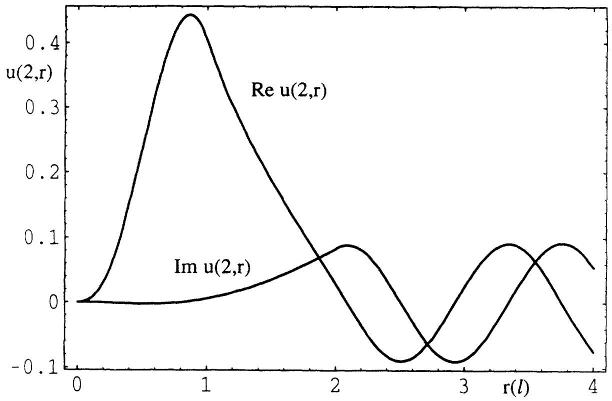

FIG. 1. The wave function $u(2,r)$, for the rectangular barrier $\bar{v}(r)=14\Theta(2-r)\Theta(r-1)(l^{-2})$ [Eqs. (5.1), (5.3), and (5.18)], is plotted as a function of r (in units of l), for the lowest eigenvalue $k=(3.8357-0.0286i)l^{-1}$.

In both of these expressions, the second term on the right-hand side depends on ϕ_0, therefore ϕ_0^M can be obtained by minimizing

$$\left|\mathrm{Re}\int_b^c [v(r,\phi)-\bar{v}(r)]dr/D(r)\right| ,$$

where $D(r)$ is given by $\mathcal{K}_0(r)$, or $-d/dr\{\ln[u(m,r)/\sqrt{r}\,]\}$, depending on the starting function $S_0(m,r)$. Having obtained ϕ_0^M, the classical path of minimum opacity for the outgoing wave is given by Eq. (4.14);

$$\phi(r)=\phi_0^M-i\nu\int_b^r dr/\{r^2\mathcal{K}_0(\nu,r)\},\quad \nu=[m^2-\tfrac{1}{4}]^{1/2} . \tag{6.4}$$

The quantum version of this path of minimum opacity (again for the outgoing wave) is given by

$$\phi(r)=\phi_0^M+i\int_b^r m/(r^2 d/dr\{\ln[u(m,r)/\sqrt{r}\,]\})dr . \tag{6.5}$$

As an application of the present approach, let us consider the following two simple nonseparable examples;

$$v_1(r,\phi)=v_0\Theta(r-b)\Theta(c-r)(1+\varepsilon\cos\phi) \tag{6.6}$$

and

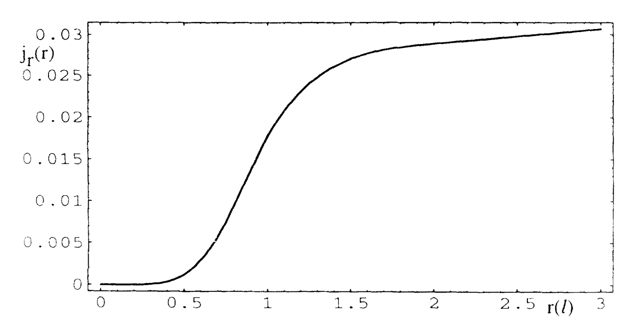

FIG. 2. The radial component of the current $j_r(r)$, Eq. (5.20), is calculated for the potential $\bar{v}(r)=14\Theta(2-r)\Theta(r-1)(l^{-2})$.

$$v_2(r,\phi)=\lambda\delta(r-b)+\varepsilon v_0\Theta(r-b)\Theta(c-r)\cos\phi , \tag{6.7}$$

where ε is a small positive number and λ and v_0 are constants. For these cases $\bar{v}_1(r)$ and $\bar{v}_2(r)$ are given by a rectangular and a δ-function barrier, respectively. In the case of $\bar{v}_1(r)$ we can obtain the path of minimum opacity either using the semiclassical approach, Eq. (4.21) or the quantal approach, Eq. (4.41). For either of these potentials we have

$$\min(\mathrm{Im}S_1)=\min\left[\tfrac{1}{2}\mathrm{Re}\left|\int_b^c \varepsilon v_0\cos[\phi(r)]dr/D(r)\right|\right] , \tag{6.8}$$

for the two approximate ways of calculating ϕ_0^M and hence the most probable escape path to the first order.

In Fig. 3 the "path" $\phi(r)$ which is found by the semiclassical method is shown as a function of r, and in Figs. 4 and 5 the same $\phi(r)$ but calculated by the quantum method is plotted as a function of r. Note that in each case the lowest eigenvalue is determined using the appropriate zeroth-order approximation, therefore the corresponding zeroth-order wave functions for the two cases are very different, even asymptotically. Since the limits of integration in Eq. (6.8) are independent of ϕ_0, this equation can be written as

$$\min(\mathrm{Im}S_1)=\min[\mathrm{Re}(A\cos\phi_0+B\sin\phi_0)] , \tag{6.9}$$

where A and B are both complex numbers given by the integral in (6.8). The real and the imaginary parts of ϕ_0^M are found by minimizing (6.9), and once ϕ_0^M is known, Eq. (6.4) [or (6.5)] gives us the most probable escape path.

The concept of complex trajectories defined by (6.4) is consistent with the idea of using imaginary time to calculate the *trajectory under the barrier* [12]. To show this consider the classical Lagrangian for two-dimensional motion in a central potential $V(r)$;

$$L=\tfrac{1}{2}M[(dr/dt)^2+r^2(d\theta/dt)^2]-V(r) , \tag{6.10}$$

where r and θ (not ϕ) are the polar coordinates, and M is the mass of the particle. The reason for this change of

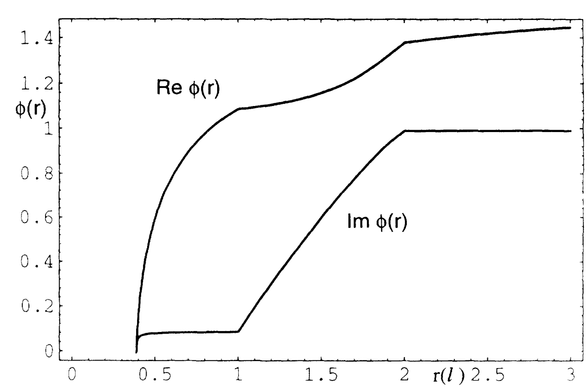

FIG. 3. The "semiclassical" trajectory for penetration through the barrier $\bar{v}(r)=24\Theta(2-r)\Theta(r-1)(l^{-2})$ is shown for the approximate eigenvalue $k=(4.9987-0.0385i)l^{-1}$, and $m=2$.

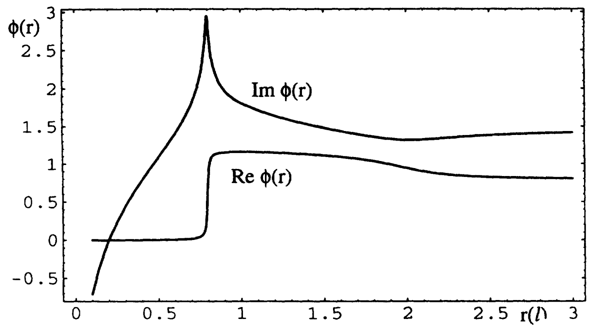

FIG. 4. The "quantum trajectory" for the rectangular barrier $\bar{v}(r)=14\Theta(2-r)\Theta(r-1)$, and for $m=2$, is shown when the lowest eigenvalue $k=(3.8347-0.0286i)l^{-1}$ is used in the calculation.

notation will be seen later. Changing the variable t to $i\tau$, we have

$$L=-\tfrac{1}{2}M[(dr/d\tau)^2+r^2(d\theta/d\tau)^2]-V(r) . \quad (6.11)$$

The conserved quantity corresponding to the energy of the system calculated from (6.11) is given by

$$E=V(r)-\tfrac{1}{2}M(dr/d\tau)^2-[p_\theta^2/(2Mr^2)] , \quad (6.12)$$

where p_θ is the momentum conjugate to the variable θ,

$$p_\theta=-Mr^2(d\theta/d\tau) . \quad (6.13)$$

From Eqs. (6.12) and (6.13) it follows that

$$d\theta=\frac{-(\pm i)(p_\theta dr/Mr^2)}{((2/M)\{V-E-[p_\theta^2/(2Mr^2)]\})^{1/2}} . \quad (6.14)$$

Now if we replace θ by $i\phi$, and p_θ by $-ip_\phi=i\nu$, then (6.14) agrees with (6.4).

VII. RESULTS

The numerical solutions of the eigenvalue equations such as those given by Eqs. (3.12), (3.15), (5.15), and (5.19) are by no means trivial. Since the eigenvalues are complex numbers it is difficult to arrange them in a definite

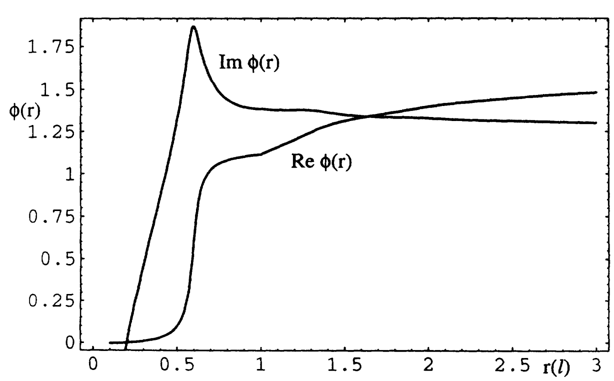

FIG. 5. The "quantum trajectory" defined by Eq. (6.5), for a δ-function potential $\bar{v}(r)=5\delta(r-1)(l^{-2})$, and for $m=2$. The lowest eigenvalue $k=(5.135-0.299i)l^{-1}$ has been used in this calculation.

order. The most interesting states of such a system are the low-lying states with very small imaginary parts (corresponding to the long lifetime of these levels). For these states we use the perturbation theory to calculate the real and the imaginary parts of k. Let us write

$$k=k_r-i\Delta k_i , \quad (7.1)$$

where the imaginary part is assumed to be very small. Substituting this in the expression for L and δ, we have

$$L(k)=L_r+iL_i=L_r+ik_rJ(k_r)\Delta k_i \quad (7.2)$$

and

$$\delta(k)=\delta(k_r)-ik_rI(k_r)\Delta k_i , \quad (7.3)$$

where

$$J(k_r)=\int_b^c dr/[\bar{v}+(\nu/r)^2-k_r^2]^{1/2} , \quad (7.4)$$

and

$$I(k_r)=\int_a^b dr/[k_r^2-(\nu/r)^2-\bar{v}]^{1/2} . \quad (7.5)$$

In the absence of the centripetal barrier, we replace $\delta(k_r)$ by $\delta_0(k_r)$, i.e., we set $a=0$. Here by substituting for L and δ_0 in Eq. (3.12) and separating the real and imaginary parts, keeping only terms linear in Δk_i, we find

$$\Delta k_i=(1/2k_r)\{-\cos[2\delta_0(k_r)]/(IJ)\}^{1/2} \quad (7.6)$$

and

$$\exp(2L_r)=\frac{\{-\cos[2\delta_0(k_r)](I/J)\}^{1/2}}{4\{1+\sin[2\delta_0(k_r)]\}} , \quad (7.7)$$

as the two equations giving us k_r and Δk_i. Since I, J, and k_r are finite quantities, $1+\sin(2\delta_0)$ has to be small to make $\exp(2L_r)$ large and Δk_i small, i.e., as a first approximation we can take $\delta_0(k_r)\approx n\pi+(3\pi/4)$.

For the general case with three turning points, Eq. (3.15), we can also use the perturbation theory to find the lowest complex eigenvalues. When the potential has two sharp boundaries, we can use the approximate form [i.e., Eq. (5.4)] to calculate the complex eigenvalues. For the state with smallest imaginary part, Δk_i, we can simplify the calculation by noting that since the particle is initially trapped behind the barrier, $e^{2iS_n(c,b)}$ must be large, therefore the denominator in (5.4) has to be small independent of the position of the point c. Thus, for $n=0$, the equation

$$\{d/dr[iS_0^{\mathrm{II}}+\ln J_m(kr)]\}_{r=b}=0 \quad (7.8)$$

will give us an approximate value for k_r. For numerical calculation we have chosen an arbitrary unit of length l. The wave numbers are given in units of l^{-1} and the potentials in units of l^{-2}. In Table I, for two cases, the rectangular barrier and for a combination of rectangular and cutoff Coulomb barrier, we have compared the results of the exact calculation using Eqs. (5.15) and (5.19) with the approximate results obtained from (7.8) with $n=0$. The results indicate that the approximate calculation improves as v_0 becomes larger than $\mathrm{Re}k^2$. In the second round of iteration, i.e., for $n=1$, Eq. (4.25) shows that $S_1^{\rm II}(r,b,\phi=0)$ and its derivative $(\partial S_1^{\rm II}/\partial r)$ depend on ϕ_0^M. Thus for $n=1$, using Eq. (5.4), or the simpler approximation given by (7.8), we can find k. However, in the second-order iteration, unlike the first, the roots of Eq. (7.8) will be complex since ϕ_0^M is complex. For the nonseparable rectangular barrier given by (6.6) with $v_0=24$ and $\varepsilon=0.2$ with the semiclassical trajectory shown in Fig. 3. The constant ϕ_0^M calculated from Eq. (6.8) is given by $\phi_0^M=0.1086-5.497i$, whereas for quantum trajectory shown in Fig. 4 ($v_0=14$ and $\varepsilon=0.2$), ϕ_0^M is $0.7168-5.353i$. Now using Eq. (7.8) but with $(\partial S_1^{\rm II}/\partial r)$ rather than $(\partial S_0^{\rm II}/\partial r)$, i.e.,

$$(\partial S_1^{\rm II}/\partial r)_{r=b}\approx Q_0(m,b)\ , \qquad (7.9)$$

we find that the lowest eigenvalue to the first order is given by $4.4568-0.354i\,(l^{-1})$. Note that in this approximation, in the zeroth order, k is real but in the first order the imaginary part Δk_i is larger than the exact result. We obtain a similar result for the δ-function potential, Eq. (6.7), using the quantum trajectory of Fig. 5. The complex eigenvalues describe discrete quasibound states with finite lifetime. From the eigenvalue equation (5.4) we calculate a set of complex eigenvalues $k_r^{(j)}-i\Delta k_i^{(j)}$, $j=0,1,2,\ldots$ where $k_r^{(j)}$ always increases with j and $\Delta k_i^{(j)}$, in general, becomes larger for larger j's. The energy of the jth quasibound states, $E^{(j)}$, is given by

$$E^{(j)}=(k_r^{(j)})^2-(\Delta k_i^{(j)})^2\ , \qquad (7.10)$$

with width $\Gamma^{(j)}$ where

$$\Gamma^{(j)}=4k_r^{(j)}\Delta k_i^{(j)}\ . \qquad (7.11)$$

The concept of the quasibound state is meaningful only if the width of the level is much narrower than the spacing between the adjacent levels [13], $E^{(j+1)}-E^{(j)}$, i.e.,

$$\Gamma^{(j)}\ll E^{(j+1)}-E^{(j)}\ . \qquad (7.12)$$

For large enough barrier this condition is satisfied. For instance, for the complex eigenvalues given in Table I, when $B=0$ and $v_0=14$, $E^{(0)}=14.699(l^{-2})$, $\Gamma^{(0)}=1.675(l^{-2})$, and $E^{(1)}-E^{(0)}=10.548(l^{-2})$, therefore (7.13) is satisfied. When $B=1$ and $v_0=20$, then $E^{(0)}=16.265(l^{-2})$, $\Gamma^{(0)}=0.089(l^{-2})$, and $E^{(1)}-E^{(0)}=13.654$, which again shows the validity of (7.13). These examples show that even when the potential is not very high and very wide one can define quasistationary states.

Let us summarize the main points discussed in this paper.

(a) We have shown that one- or two-dimensional tunneling problems can be solved approximately using the method of quasilinearization.

(b) To the first order this method yields the same result as WKB approximation for one-dimensional tunneling, however, it is easy to include higher-order corrections, at least for barriers with sharp boundaries.

(c) For multidimensional tunneling, there are two ways of using quasilinearization method. If we start with S_0 given by (4.12) then we have a semiclassical approach similar to WKB, but if we choose S_0 as a solution of Eq. (4.36) then the method can be applied to a larger group of potentials.

(d) The "trajectory" of the particle which can be defined semiclassically as in Eq. (6.4) or quantum mechanically as in Eq. (6.5) is complex and depends on a constant of integration.

(e) The most probable escape path is obtained by minimizing a functional relation, (i.e., ImS) with respect to the constant of integration appearing in the equation of the "trajectory." All calculations can be done while preserving the single-valued property of the wave function.

(f) For the nonseparable problems it is difficult to investigate the accuracy of the quasilinearization method for the tunneling problem. However, this method has been tested for nonseparable bound-state problems, where it has been shown to be a reliable method [14].

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