Wentzel-Kramers-Brillouin method in multidimensional tunneling

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The WKB method is commonly used in semiclassical approximations to the wave function in both the classically allowed and the forbidden regions of a one-dimensional potential. In a multidimensional space, the method can be adapted to construct wave functions in an "allowed" region from classical trajectories or wave normals. However, in the "forbidden" region the WKB wave function is in general specified by two sets of wave fronts, the equiphase and the equiamplitude surfaces or equivalently by two sets of paths defined to be normal to these surfaces, respectively. We present a Huygens-type construction for obtaining these wave fronts and paths, which reveals that for non-normal incidence the paths are coupled to each other. The analysis enables us to answer some of the basic questions concerning tunneling in multidimensional nonseparable potentials. A special and important case occurs when the incident wave is normal to the turning surface. We show that for normal incidence the path equations are decoupled and are equivalent to Newton's equations of motion for the inverted potential and energy.

I. INTRODUCTION

Multidimensional tunneling processes can be important in many areas of quantum physics, such as nuclear reactions[1] and fission,[2,3] the tunneling of the false vacuum state in field theory,[4,5] chemical reactions,[6,7] and electron tunneling, e.g., in the scanning tunneling microscope[8–13] (STM) and point-contact junction devices.[14] In principle, to study these phenomena, one should solve the Schrödinger equation or other appropriate partial differential equations (PDE). However, in practice, we rarely have exact analytical solutions to those equations. Approximations are therefore often employed both in the calculations and the formal analysis of tunneling processes in a multidimensional space.[15–24]

A convenient formalism for introducing approximations to tunneling theories is the Feynman path-integral formulation of quantum mechanics.[25,26] In this approach, for a single particle, one constructs the Green's function $G(\mathbf{r}_f,\mathbf{r}_i;t)$ by summing over all the possible paths connecting points $\mathbf{r}_i$ and $\mathbf{r}_f$, i.e.,

$$G(\mathbf{r}_f,\mathbf{r}_i;t)=\int_{\mathbf{r}_i}^{\mathbf{r}_f}\exp\{iS[\mathbf{r}(t)]/\hbar\}D[\mathbf{r}(t)]\ , \tag{1.1}$$

where the action functional is defined by

$$S[\mathbf{r}(t)]=\int_0^t L(\dot{\mathbf{r}},\mathbf{r},\tau)d\tau\ , \tag{1.2}$$

and

$$L(\dot{\mathbf{r}},\mathbf{r},t)=\tfrac{1}{2}m\dot{\mathbf{r}}^2-V(\mathbf{r}) \tag{1.3}$$

is the Lagrangian. The symbol $D[\mathbf{r}(t)]$ denotes summation over all paths. As $\hbar\to 0$, the leading term S_0 in the expansion of the action S in a power series in $\hbar$ (known as the WKB method) gives[26]

$$G_{\mathrm{WKB}}(\mathbf{r}_f,\mathbf{r}_i;t)=\sum_\alpha[i/(2\pi\hbar)]^{d/2}\left|\det\frac{\partial^2 S_{0\alpha}}{\partial\mathbf{r}_f\partial\mathbf{r}_i}\right|^{1/2}\times\exp[i(S_{0\alpha}/\hbar-n\pi/2)]\ , \tag{1.4}$$

where α labels the classical paths from $\mathbf{r}_i$ to $\mathbf{r}_f$, d is the dimension of the space, $S_{0\alpha}$ is the action along the αth classical trajectory, and n is the sum of the orders of the focal points along α.

For tunneling, it is more convenient to express the Green's function as a function of energy rather than time. By performing a Fourier transformation, we have

$$\tilde{G}_{\mathrm{WKB}}(\mathbf{r}_f,\mathbf{r}_i;E)=i\sum_\alpha[i/(2\pi\hbar)]^{d/2-1}\sqrt{|\tilde{D}_\alpha|}\times\exp(iW_{0\alpha}/\hbar-in\pi/2)\ . \tag{1.5}$$

Here, $\tilde{G}$ is the Fourier transform of G, and $\tilde{D}_\alpha$ and $W_{0\alpha}$ are defined as follows:

$$\tilde{D}_\alpha\equiv\frac{\det(\partial^2 S_{0\alpha}/\partial\mathbf{r}_f\partial\mathbf{r}_i)}{\partial^2 S_{0\alpha}/\partial t^2}\ , \tag{1.6}$$

$$W_{0\alpha}(\mathbf{r}_f,\mathbf{r}_i;E)=S_{0\alpha}+Et\ . \tag{1.7}$$

It can be shown that $S_{0\alpha}$ satisfies the Hamilton-Jacobi equation, and the Hamilton characteristic function $W_{0\alpha}$ satisfies the following time-independent equation:

$$\frac{1}{2m}(\nabla W_{0\alpha})^2+V(\mathbf{r})=E\ . \tag{1.8}$$

The solution of Eq. (1.8) is the lowest-order WKB approximation to the phase of the Green's function. It is not difficult to recognize that Eq. (1.8) also appears in classical mechanics. As is shown in Sec. II, it is also the zeroth-order approximation to the phase of the wave function. In an allowed region, Eq. (1.8) can be solved by the "method of characteristics."[27] This method expresses

a first-order PDE in terms of a set of second-order ordinary differential equations (ODE). Specifically, the solution for $W_{0\alpha}$ can be written as an integral

$$W_{0\alpha}=\int_{\alpha}\sqrt{2m[E-V(\mathbf{r})]}d\xi\ , \tag{1.9}$$

taken along the classical trajectory labeled α. The classical paths themselves satisfy Newton's equation. This method of characteristics is reasonably successful in the calculation of the wave functions and eigenstates in bound-state problems.[28,29]

In quantum tunneling, a forbidden region always separates any two allowed regions so that they are not linked by any classical trajectory. However, the path-integral formalism allows the existence of trajectories even in the forbidden region. The Green's function can be evaluated by summing over all the possible paths across the forbidden region. In tunneling, it is more convenient to divide space into several regions. It has been shown[30] that the global Green's function can be expressed in terms of the Green's functions of subdomains. This decomposition into local Green's function has also been carried out by Auerbach and Kivelson[21,22] (AK) using path-integral formulation. They refer to this technique as the path decomposition expansion (PDX). The method allows one to calculate independently the local contributions to the global Green's function. Auerbach and Kivelson applied the method to double-well problems and showed that the dominant contribution in the forbidden region comes from a single (instanton) path. This path can be obtained by solving Newton's equations of motion with the inverted potential and energy, i.e., $V(\mathbf{r})\rightarrow -V(\mathbf{r})$ and $E\rightarrow -E$.[31]

The method of AK has the additional flexibility of allowing the calculation of the local or site restricted Green's functions in different approximations. This enables them to circumvent the problem of the turning surfaces which characterize the WKB method. Here we should emphasize that we are concerned with the extension of the WKB method to multidimensional nonseparable potentials. In this we differ from AK who are concerned with a calculation of the Green's function for tunneling and not especially with the WKB method.

In comparing the approaches of AK with ours one has to recall that, in contrast with the one-dimensional WKB approximation, the multidimensional semiclassical approximation is a solution of a partial differential equation and hence cannot be discussed without references to specific boundary conditions. We are concerned with the tunneling transmission of an incident wave (including a plane wave from infinity). On the other hand, AK are concerned with a particle tunneling from a well. In the latter case, one can always demonstrate that there are classical paths normally incident on the turning surface. For these paths, the transmission probability is exponentially larger than for the obliquely incident paths. This contrasts with the obliquely incident beam where the boundary conditions exclude normal incidence. In this case, the Hamilton characteristic function W must be complex. This, however, is excluded by AK in their semiclassical treatment, which leads to a purely imaginary W. Thus the semiclassical treatment of AK is more restricted than our approach.

In this paper, we show that two coupled sets of paths, the R and I paths, are required to characterize the general complex action W. An extended Huygens construction is proposed to determine these paths and the associated wave fronts. The method, while not easy, is the only WKB-type approximation available for the general obliquely incident beam. However, it reduces to the simpler version of the semiclassical approximation advocated *inter alia* by AK when the WKB wave is normally incident on the turning surface. A detailed analysis is presented in Sec. II. A discussion of the results and conclusions are given in Sec. III.

II. WKB APPROXIMATION IN MULTIDIMENSIONAL SPACE

We could start the formal development with Eq. (1.8), which is the lowest-order WKB approximation. However, an equivalent but somewhat more transparent approach is to expand the wave function in a power series in $\hbar$. This approach is similar to one of the standard developments of the one-dimensional approximation.[32]

A. Asymptotic series expansions in $\hbar$

In the stationary-state Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r})+V(\mathbf{r})\Psi(\mathbf{r})=E\Psi(\mathbf{r})\ , \tag{2.1}$$

let

$$\Psi(\mathbf{r})=\exp[iW(\mathbf{r})/\hbar]\ . \tag{2.2a}$$

Hence

$$\frac{1}{2m}[\nabla W(\mathbf{r})]^2-i\frac{\hbar}{2m}\nabla^2 W(\mathbf{r})+V(\mathbf{r})-E=0\ . \tag{2.2b}$$

Expanding $W(\mathbf{r})$ in a formal power series in $\hbar$,

$$W(\mathbf{r})=W_0(\mathbf{r})+W_1(\mathbf{r})+\cdots\ , \tag{2.3}$$

substituting Eq. (2.3) into Eq. (2.2), and collecting the coefficients of equal powers in $\hbar$, we obtain the following equations:

$$[\nabla W_0(\mathbf{r})]^2-2m(E-V)=0+O(\hbar)\ , \tag{2.4}$$

$$2\nabla W_0(\mathbf{r})\cdot\nabla W_1(\mathbf{r})-i\hbar\nabla^2 W_0(\mathbf{r})=0+O(\hbar^2)\ , \tag{2.5}$$

where $O(x)$ denotes a quantity which has the same order of magnitude as the argument x. Equation (2.4) is identical to Eq. (1.8). Therefore the zeroth-order approximation of the wave function is also the lowest-order approximation in the path-integral formalism. As seen from Eq. (2.4), $W_0(\mathbf{r})$ may in general be complex. Hence we may write

$$W_0(\mathbf{r})=W_{0R}(\mathbf{r})+iW_{0I}(\mathbf{r})\ ,$$

and Eq. (2.4) becomes a pair of coupled equations

$$[\nabla W_{0R}(\mathbf{r})]^2-[\nabla W_{0I}(\mathbf{r})]^2=2m[E-V(\mathbf{r})]\ , \tag{2.6a}$$

$$[\nabla W_{0R}(\mathbf{r})]\cdot[\nabla W_{0I}(\mathbf{r})]=0\ . \tag{2.6b}$$

The simultaneous solution of Eqs. (2.6), discussed below, constitutes the zeroth-order WKB approximation of the complex phase of the wave function Eq. (2.2a).

B. Zeroth-order solutions in a classically allowed region

In a classically allowed region, a particle can be described by a real $W(\mathbf{r})$, i.e., $\nabla W_{0I}=0$, and Eq. (2.6a) reduces to

$$[\nabla W_{0R}(\mathbf{r})]^2=2m[E-V(\mathbf{r})]\ , \tag{2.7a}$$

or

$$\nabla W_{0R}(\mathbf{r})=\hbar k\hat{\mathbf{e}}=\hbar\mathbf{k}(\mathbf{r})\ , \tag{2.7b}$$

where $\hat{\mathbf{e}}$ is the unit vector and

$$k(\mathbf{r})^2=\frac{2m}{\hbar^2}[E-V(\mathbf{r})]\ . \tag{2.8}$$

It is well known that by integrating Eq. (2.7b) along a classical path, one obtains the expression for $W_{0R}(\mathbf{r})$, which is given in Eq. (1.9).[17,31] The above derivation shows that the zeroth-order approximation, in $\hbar$, of $W(\mathbf{r})$ reduces the solution of the Schrödinger equation to the solution of a first-order PDE, that is, Eq. (2.7a). As stated in the introduction, a first-order PDE is equivalent to a set of ODE's. Rather than proceed with the method of characteristics, we present a formal constructive procedure that will facilitate the comparison with the solution in the forbidden region, which is presented in Sec. II D.

Equation (2.7) can be solved by constructing equiphase $[W_{0R}(\mathbf{r})=\text{const}]$ surfaces. We assume that the ith equiphase surface (with phase equal to W_{0R}) is known. The $(i+1)$st surface (with phase $W_{0R}+\Delta W_{0R}$) is constructed pointwise from the ith surface; the (new) point, on the $(i+1)$st surface, is a distance $\Delta\xi=\Delta W_{0R}/\hbar k(\mathbf{r})$ away from the initial point on the ith surface in the direction of $\hat{\mathbf{e}}$. This is the analog to Huygens construction of traveling waves in optics.[33] Besides the equiphase surfaces, the construction also determines a set of paths each one of which is perpendicular to all W_{0R} surfaces. It is easy to show that these paths satisfy the Euler-Lagrangian equations obtained from the Hamilton variational principle, which in terms of the time independent action reduces to $\delta W_{0R}(\mathbf{r})=0$, i.e.,

$$2[V(\mathbf{r})-E]\frac{d^2x_i}{d\xi^2}+\frac{dx_i}{d\xi}\sum_j\frac{dx_j}{d\xi}\frac{\partial V(\mathbf{r})}{\partial x_j}=\frac{\partial V(\mathbf{r})}{\partial x_i}\ , \quad i=1,2,3\ , \tag{2.9}$$

where $x_i=x,y,z$. The proof of this assertion is presented in Appendix A. We note that Eq. (2.9) can be also derived directly from Newton's second law.

C. First-order solution in a classically allowed region

The first-order correction can be easily obtained once the zeroth-order solution is available. With $W_{0I}(\mathbf{r})=0$, Eq. (2.6a) reduces to Eq. (2.7a). Using Eq. (2.7b), Eq. (2.5) becomes

$$\nabla W_1(\mathbf{r})\cdot\hat{\mathbf{e}}=\frac{\hbar}{2}i(k^{-1}\hat{\mathbf{e}}\cdot\nabla k+\nabla\cdot\hat{\mathbf{e}})\ . \tag{2.10}$$

Integrating this equation along the classical trajectory from $\mathbf{r}_1$ to $\mathbf{r}_2$ yields

$$W_1^{(2)}-W_1^{(1)}=\tfrac{1}{2}i\hbar\left[\int_1^2 k^{-1}\frac{dk}{d\xi}d\xi+\int_1^2(\nabla\cdot\hat{\mathbf{e}})d\xi\right]\ . \tag{2.11}$$

Here, as noted above, $\hat{\mathbf{e}}(\mathbf{r})$ is the unit vector tangent at a point $\mathbf{r}$ to the classical trajectory, ξ is the arc length, and the superscripts 1 and 2 denote, respectively, the initial and final points. The integration in the first term on the right-hand side of Eq. (2.11) can be easily carried out. To evaluate the second term, we consider a tube formed by classical paths as shown in Fig. 1. Let $\sigma(\xi)$ be the cross section of the tube. In the limit of small σ,

$$\nabla\cdot\hat{\mathbf{e}}\sigma(\xi)\Delta\xi=\nabla\cdot\hat{\mathbf{e}}\Delta V\ . \tag{2.12}$$

Hence, applying the Gauss theorem to the element of tube with volume $\Delta V=\sigma\Delta\xi$, we obtain

$$\nabla\cdot\hat{\mathbf{e}}\Delta V=\sigma(\xi+\Delta\xi)-\sigma(\xi)=\sigma'(\xi)\Delta\xi\ . \tag{2.13}$$

Note that only the surfaces perpendicular to the paths contribute to Eq. (2.13). This in fact is the consequence of the conservation of flux. Combining Eqs. (2.12) and (2.13) we have

$$\nabla\cdot\hat{\mathbf{e}}d\xi=\frac{\sigma'(\xi)}{\sigma(\xi)}d\xi\ . \tag{2.14}$$

With the help of Eq. (2.14), the integral in the second term of Eq. (2.11) can now be evaluated to obtain an expression for $W_1(\mathbf{r})$. With the result obtained in Sec. II B, and on substituting the expressions for $W_{0R}(\mathbf{r})$ and $W_1(\mathbf{r})$ into Eq. (2.2a), the wave function including the zeroth- and the first-order approximations is

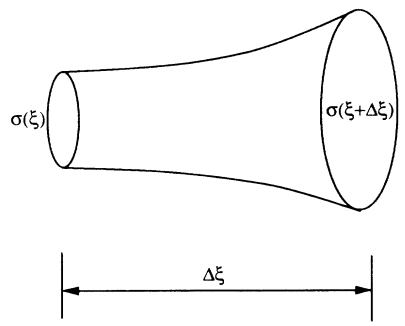

FIG. 1. A tube element formed by $\hat{\mathbf{e}}$ field. σ is the cross-section area and ξ is the arc length.

$$\Psi(\mathbf{r})=\frac{C}{\sqrt{k(\mathbf{r})\sigma(\mathbf{r})}}\exp\left[i\int^{r}k(\xi)d\xi\right], \tag{2.15}$$

where C is the normalization constant. In one dimension, $\sigma(\mathbf{r})$ is a constant, and the expression reduces to the common WKB approximation for the wave function. An alternative representation of the first-order correction can be derived in terms of the Jacobian of the coordinate transformation of $\sigma+\Delta\sigma$ to σ, also referred to as the Jacobian of mapping via rays.[34] Thus, at the top and bottom surfaces of a ray tube denoted respectively by $\sigma(\xi+\Delta\xi)$ and $\sigma(\xi)$, we have

$$\frac{\sigma(\xi)}{\sigma(\xi+\Delta\xi)}=\frac{J(\xi)}{J(\xi+\Delta\xi)}, \tag{2.16}$$

where $J(\xi)$ is the Jacobian at point ξ. Therefore $\sigma(\xi)\propto J(\xi)$.

The first-order correction to the Green's function $\tilde{G}_{\mathrm{WKB}}(\mathbf{r}_f,\mathbf{r}_i;E)$ is similar to the above. It can be shown[35] that $\tilde{D}$ in Eq. (1.6) reduces, in a three-dimensional space, to

$$\tilde{D}\propto\left.\frac{1}{|\mathbf{k}|\sigma}\right|_{\mathbf{r}_f}. \tag{2.17}$$

Here it should be noted that σ and J can be defined also in all other $n\geq 2$ dimensional spaces.

D. Solutions in a forbidden region

In a classically forbidden region, both $W_{0R}(\mathbf{r})$ and $W_{0I}(\mathbf{r})$ may exist. Thus, instead of one set of characteristic surfaces, we have two sets: the equiphase (W_{0R}) surfaces and the equiamplitude (W_{0I}) surfaces as shown in Fig. 2. We shall present a Huygens-type construction for the determination of these wave fronts. First we define the quantities $k_R(\mathbf{r})$, $k_I(\mathbf{r})$, $\hat{\mathbf{e}}_R(\mathbf{r})$, and $\hat{\mathbf{e}}_I(\mathbf{r})$ to satisfy the following relations:

$$\nabla W_{0R}(\mathbf{r})=\hbar k_R\hat{\mathbf{e}}_R=\hbar\mathbf{k}_R(\mathbf{r}), \tag{2.18a}$$

$$\nabla W_{0I}(\mathbf{r})=\hbar k_I\hat{\mathbf{e}}_I=\hbar\mathbf{k}_I(\mathbf{r}). \tag{2.18b}$$

Equations (2.18) also define two corresponding sets of paths, to be called the R and I paths, with unit tangent vectors $\hat{\mathbf{e}}_R$ and $\hat{\mathbf{e}}_I$, respectively. That is, the R and I paths are orthogonal to all constant W_{0R} and constant W_{0I} surfaces, respectively. Substituting Eqs. (2.18) into Eq. (2.6a) yields

$$k_R^2(\mathbf{r})-k_I^2(\mathbf{r})=k(\mathbf{r})^2=\frac{2m}{\hbar^2}[E-V(\mathbf{r})]. \tag{2.19}$$

In the following, we will show that the construction of the W_{0R} and W_{0I} surfaces requires three steps. First, given a W_{0I} surface we construct the surface labeled $W_{0I}+\Delta W_{0I}$. Next we calculate the values of $k_I(\mathbf{r})$ on the second surface from the values of $k_I(\mathbf{r})$ given on the initial surface W_{0I}. Finally, we determine the set of R paths on $W_{0I}+\Delta W_{0I}$ from the corresponding set on the W_{0I} surface.

The reason that we select a W_{0I} surface to start the construction is that the turning surface, which separates the allowed from the forbidden region, can be regarded as a constant W_{0I} surface, and in particular it is the $W_{0I}=0$ surface (see Sec. II E). Assuming the W_{0I} surface is known, to determine the $W_{0I}+\Delta W_{0I}$ surface we use the following equation:

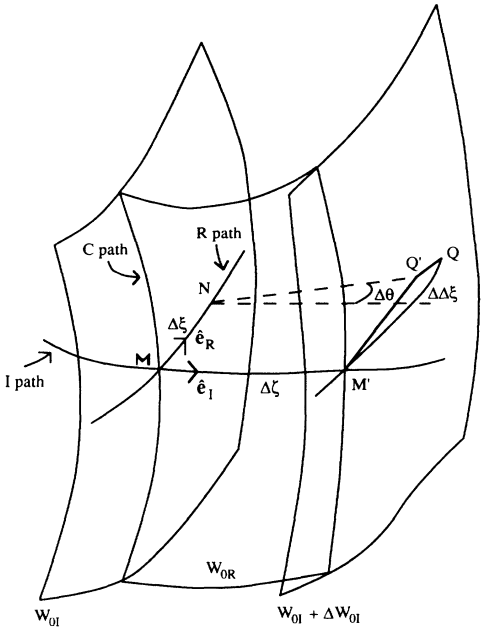

FIG. 2. Schematic representation of two mutually orthogonal wave fronts, i.e., constant W_{0R} and W_{0I} surfaces. Also shown are the orthogonal trajectories or R and I paths and other quantities introduced in Sec. II B. These quantities in general characterize the wave function in the classically forbidden region.

$$\hbar k_I(\mathbf{r})\approx\frac{\Delta W_{0I}}{\Delta\xi}=\hat{\mathbf{e}}_I\cdot\nabla W_{0I}(\mathbf{r}). \tag{2.20}$$

The distance between the W_{0I} surface and the $W_{0I}+\Delta W_{0I}$ surface at point $\mathbf{r}$ is

$$\Delta\xi(\mathbf{r})\approx\frac{\Delta W_{0I}}{\hbar k_I(\mathbf{r})}. \tag{2.21}$$

Using the values $k_I(\mathbf{r})$ on the W_{0I} surface, we can construct the next equiamplitude surface similar to the Huygens construction in the allowed region. However, we also need to calculate $k_I(\mathbf{r})$ on the new surface in order to continue the construction of subsequent surfaces.

To determine $k_I(\mathbf{r})$, let us choose a point M on a W_{0I} surface and introduce a local coordinate system based on the R and I paths passing through the point M. The directional derivative of $k_R(\mathbf{r})$ along the I path is shown (see Appendix B) to be given by

$$\frac{\partial k_R(\mathbf{r})}{\partial \zeta} = -k_R(\mathbf{r})\frac{d\theta}{d\xi} , \tag{2.22}$$

where $d\theta/d\xi$ is the curvature at point M of the curve obtained by projecting the R path onto the plane $(\hat{\mathbf{e}}_I, \hat{\mathbf{e}}_R)$. Note that $d\theta/d\xi$ is not the curvature for the R path. It can be shown that in the classically allowed region, Eq. (2.22) reduces to the equation $F_n(\mathbf{r}) = mv^2/R(\mathbf{r})$, where $F_n(\mathbf{r})$ is the centripetal force and $R(\mathbf{r})$ is the radius of curvature at point $\mathbf{r}$ on the trajectory. Using Eq. (2.22) to eliminate k_R from Eq. (2.19) we finally obtain

$$\frac{\partial k_I(\mathbf{r})}{\partial \zeta} = -\frac{k_I(\mathbf{r})^2 + k(\mathbf{r})^2}{k_I(\mathbf{r})}\frac{d\theta}{d\xi} - \frac{k(\mathbf{r})}{k_I(\mathbf{r})}\frac{\partial k(\mathbf{r})}{\partial \zeta} . \tag{2.23}$$

Equation (2.23) implies that the variation of $k_I(\zeta)$ along an I path depends, in particular, on the curvature $d\theta/d\xi$. Therefore, in addition to the construction of the $W_{0I} + \Delta W_{0I}$ surface and the calculation of $k_I(\mathbf{r})$ on it, the R paths on the surface $W_{0I} + \Delta W_{0I}$ have to be determined in order to evaluate $d\theta/d\xi$, and hence the directional derivative $\partial k_I/\partial \zeta$.

The Huygens type construction of the W_{0I} surface can now proceed as follows. (i) Assume that an equiamplitude surface W_{0I} and the quantities k_R, k_I, $\hat{\mathbf{e}}_R$, and $\hat{\mathbf{e}}_I$ are given (see Sec. II E for details). Choose a point M on a curve in the direction $\hat{\mathbf{e}}_R \times \hat{\mathbf{e}}_I$. Since W_{0R} and W_{0I} are both constant on this curve (see Fig. 2), it is denoted the C path. A point M' corresponding to M, and located on the next equiamplitude $(W_{0I} + \Delta W_{0I})$ surface is a distance $\Delta\zeta$ from M in the direction of $\hat{\mathbf{e}}_I$. Here, it follows from Eq. (2.20) that $\Delta\zeta = \Delta W_{0I}/(\hbar k_I)$. (ii) The curvature $d\theta/d\xi$ at the point M is calculated. (iii) The value of k_I at the new point M' is determined with the help of Eq. (2.23), and k_R is calculated using Eq. (2.19).

This procedure is repeated for a set of points on the starting C path. The locus of the images of these starting points is a new C path on the $W_{0I} + \Delta W_{0I}$ surface. Similarly, other C paths can be constructed. These allow us to determine the new R paths. That is, the normals to all C paths which lie in the new W_{0I} surface. Thus we obtain the new equiamplitude surface as well as the values of k_I, k_R, $\hat{\mathbf{e}}_I$, and $\hat{\mathbf{e}}_R$ at each point on this surface. The determination of these new starting values closes the cycle of the procedure. Subsequent surfaces are constructed by repeating the cycle. To conclude, we have presented a procedure for solving Eqs. (2.6a) and (2.6b) by constructing the equiamplitude surfaces one by one. The equiphase surfaces are obtained automatically in terms of their normals, the R paths.

It is not surprising that the two corresponding sets of paths [the I paths, $x_i = x_i(\zeta)$ and the R paths $x_i = x_i(\xi)$, $i = 1,2,3$] constructed as described above, satisfy the following coupled Euler-Lagrange equations:

$$k_I(\mathbf{r})\frac{d^2x_i}{d\zeta^2} - \frac{dx_i}{d\zeta}\sum_n \frac{\partial k_I(\mathbf{r})}{\partial x_n}\frac{dx_n}{d\zeta} = -\frac{\partial k_I(\mathbf{r})}{\partial x_i} , \tag{2.24a}$$

$$k_R(\mathbf{r})\frac{d^2x_i}{d\xi^2} - \frac{dx_i}{d\xi}\sum_n \frac{\partial k_R(\mathbf{r})}{\partial x_n}\frac{dx_n}{d\xi} = -\frac{\partial k_R(\mathbf{r})}{\partial x_i} , \quad i = 1,2,3 . \tag{2.24b}$$

The two wave vectors in Eq. (2.24) have to satisfy Eqs. (2.18) and (2.19). The derivation of these equations is similar to the one presented in Appendix A for the classical trajectories Eq. (2.9). In the classically allowed region, Eq. (2.24a) is trivially satisfied by $k_I(\mathbf{r}) = 0$. Furthermore, Eq. (2.24b) reduces to Eq. (2.9). This suggests that the I paths are the "continuations" of the classical trajectories into forbidden regions.

Equations (2.24) show that, in a classically forbidden region, in general, the lowest-order approximation of the solution of the Schrödinger equation is not equivalent to the solution of a single set of ordinary differential equations. Equation (2.19) obviously couples I and R paths. In other words, in multidimensional tunneling the WKB approximation generally does not reduce the problem to the solution of a single family of independent path equations such as Newton's equations of motion. There are, however, important cases where the path equations can be decoupled. Some of these cases are presented below.

(a) Normal incidence: The incoming flux is incident normally at the turning surface $E - V(\mathbf{r}) = 0$, i.e., k_R vanishes on this surface. From Eq. (2.22), it can be seen that if $k_R = 0$ on some W_{0I} surface, then k_R vanishes on all the subsequent surfaces in the same forbidden region. That is, k_R vanishes in the entire forbidden region. Thus Eq. (2.24a) reduces to Eq. (2.9). The latter has been used to calculate semiclassical trajectories in classically forbidden regions.[13,31] Both the zeroth- and the first-order WKB approximations, developed for the semiclassical trajectories in a classically allowed region, can in this case be used in the forbidden region. An illustrative example of the application of this theory is provided by the analyses of a model STM by Das and Mahanty.[13] A similar example is given by Huang, Cutler, and Feuchtwang.[36]

(b) The separable potential: We will show in Sec. II F that the I and R paths can be determined independently if the potential and the boundary conditions are separable. This result can be extended by an adaption of the perturbation theory of Razavy and Pimpale.[24] These authors have developed a perturbative treatment of the WKB theory for the nearly separable potential, which includes a small additive nonseparable term.

(c) The last example in which independent trajectories may be found without solving Eqs. (2.24) is the complex ray method introduced by Keller.[37] The technique seems to be satisfactory for the discussion of some optical and acoustical diffraction problems,[38,39] when $k(\mathbf{r})$ is piecewise constant.

E. Turning surfaces, caustics, and connection formulas

In the preceding analysis, we have obtained separately the solutions of the Schrödinger equation in classically allowed regions as well as in classically forbidden regions. Now we need to join these solutions smoothly across a surface, called the turning surface, which separates a classically allowed region from a forbidden region. At the turning surface, the first-order correction to the WKB approximation diverges. Specifically, from Eq. (2.15) we observe that the zeroth-order approximation is

always finite while the first-order term diverges if either k or σ vanishes. The divergence of the WKB wave function at zeros of either k or σ defines the turning surface. The surface on which σ is zero is called caustic.[26]

Let us divide space into three regions I, II, and III, with region II being the classically forbidden region and regions I and III being the allowed regions. Sufficiently close to the first turning surface Σ_1 (separating region I from region II), we may formulate a local and linear approximation. We expand the potential in a multidimensional Taylor series, and keep only the constant and linear terms. Clearly, in this approximation, the potential is locally separable. At the turning point, the classical trajectory is normal or tangential to the turning surface corresponding to k or σ equal to zero. In order to satisfy the continuity of flux, the wave vectors of the WKB wave functions should be equal on both sides of the turning surface, i.e., $\mathbf{k}=\mathbf{k}_R$. In the direction normal to the turning surface the separated problem reduces to one-dimensional tunneling that can be treated within the ordinary one-dimensional WKB approximation. Thus the following joining relation holds at the first turning surface:

$$2\cos\left[\int_{\mathbf{r}}^{\mathbf{r}_0} k_\perp dl_\perp - \frac{\pi}{4}\right]\exp\left[i\int_{\mathbf{r}}^{\mathbf{r}_0}\mathbf{k}_\parallel\cdot\mathbf{d}l_\parallel\right] \leftarrow \exp\left[-\int_{\mathbf{r}_0}^{\mathbf{r}} k_I d\xi + i\int_{\mathbf{r}_0}^{\mathbf{r}}\mathbf{k}_r\cdot\mathbf{d}_\xi\right] . \quad (2.25)$$

where on the left-hand side $\mathbf{r}$ is in region I, and on the right-hand side $\mathbf{r}$ is in region II. In the forbidden region, *the wave vector* $\mathbf{k}_I$, being perpendicular to $\mathbf{k}_R$, *is normal to the turning surface.* The same applies to the I paths, which are all parallel to $\mathbf{k}_I$.

The complete analysis of the second turning surface Σ_2, is more complicated because the incident wave function consists of two sets of wave fronts. Two cases are illustrated in Fig. 3, in which the second turning surface is determined by locating the surface which is either the locus of the zeros of k_I or the envelope of the set of crossing paths. In Fig. 3(a), the semiclassical trajectories are normally incident at Σ_1. Hence k_R vanishes in the forbidden region. Just as in the argument presented for Σ_1, the continuity of flux requires that all the classical paths in region III emerge perpendicularly from Σ_2. The second example depicted in Fig. 3(b) has nonzero k_R in region II. At the intersection of two I paths lying on two different W_{0R} surfaces, $\hbar k_R=\Delta W_{0R}/\Delta\xi$ tends to infinity. Hence, by Eq. (2.19), k_I diverges in this case, and one may restrict the analysis to the I paths that are normal to Σ_2. It is evident that the I paths join corresponding trajectories in the two disjoint classically allowed regions. As a consistency check of our theory, we present in the following a discussion of tunneling in a separable potential field.

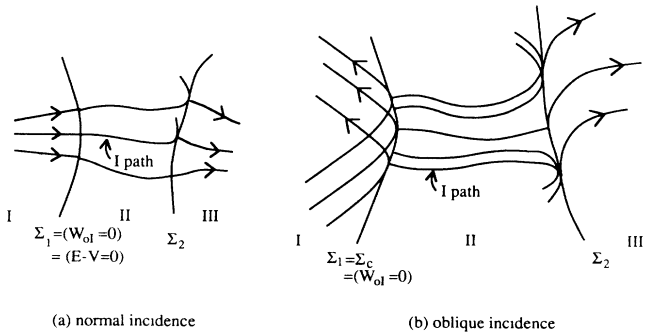

FIG. 3. Two allowed regions I and III separated by a forbidden region II bounded by the turning surfaces Σ_1 and Σ_2. Trajectories in I and III are joined at Σ_1 and Σ_2 to I paths defined in region II. In (a) Σ_1 and Σ_2 satisfy $E-V(\mathbf{r})=0$. In (b) Σ_1 and Σ_2 are also the caustics.

F. Separable potential problem

Consider a potential field given by

$$V(\mathbf{r})=V_1(x)+V_2(y)+V_3(z) , \quad (2.26)$$

which vanishes at infinity. Assume that the potential barrier exists only in the x direction and the incident wave function tends asymptotically, as $x\rightarrow-\infty$, to

$$\Psi(\mathbf{r})=\exp(ik_{0x}x+ik_{0y}y+ik_{0z}z) . \quad (2.27)$$

Here subscript 0 denotes the value as $x\rightarrow-\infty$. In the classically allowed region, the WKB wave function can be described by a set of paths, or rays, which satisfy Newton's equations. The separability requires these paths to be reflected at a surface of constant x on which k_x vanishes. This is the turning surface or the caustic Σ_1 for this problem. To construct the wave function to the right of Σ_1, we notice that the tangential component of the wave vector must be continuous across the turning surface to satisfy the continuity of flux. Then, in the forbidden region, just inside the caustic, we have an equiamplitude surface with known k_y, k_z, and $k_x\sim0$. It is easy to see that in this case $\mathbf{k}_R=\mathbf{k}_y+\mathbf{k}_z$ and $k_I=-ik_x$. These components of the complex wave vector can in this case also be defined, respectively, as the parallel and normal components, relative to the turning surface. In the neighborhood of the turning plane the R paths are straight lines. It follows from Eq. (2.23) that the change in k_x (which here is ik_I) along the x direction is

$$\frac{\partial k_x}{\partial x}=\frac{k}{k_x}\frac{\partial k}{\partial x}=-\frac{m}{\hbar^2 k_x}\frac{dV_1(x)}{dx} . \quad (2.28)$$

Here we have used Eq. (2.26). Hence following the general reasoning described in Sec. II D, we conclude that in the entire forbidden region k_x is a function of x only. Consequently, *the equiamplitude surfaces are planes of constant x.* That is, in the forbidden region, the I paths are parallel to the x axis and the R paths are in the y-z planes. A similar argument can be applied at the second turning surface Σ_2 in order to join the solutions across the boundary. To the right of Σ_2, i.e., in region III, Newton's equations can be used to construct classical paths. This concludes the demonstration of the consistency of the method presented in Sec. II D with the known result for separable potential problems.

III. DISCUSSION AND CONCLUSIONS

A. Construction of the WKB wave function in multidimensional space

In this paper, we have investigated the WKB approximation for tunneling calculations in a multidimensional nonseparable potential field. To obtain the wave function in a region including the barrier, we started in a classically allowed region the construction of a family of paths associated with the wave front, on which the boundary conditions are specified. The turning surfaces (caustics) are surfaces on which either the wave vector $\mathbf{k}$ vanishes (i.e., for paths of normal incidence) or the paths cross each other. In the latter case, the family of the paths does not have a unique wave front at the turning surface, which is the envelope of the paths traced in the allowed region. The wave vector $\mathbf{k}$ at the turning surface, when it does not vanish, is tangent to this surface. Furthermore, $\mathbf{k}=\mathbf{k}_R$ just inside the forbidden region.

In order to calculate the wave function in the forbidden region we require, besides $\mathbf{k}_R$, another wave vector $\mathbf{k}_I$, which is always perpendicular to $\mathbf{k}_R$. That is, in this region, we identify two mutually perpendicular sets of rays or paths, the R and I paths with tangent vectors $\mathbf{k}_R$ and $\mathbf{k}_I$, respectively. In contrast to the rays in an allowed region, these paths, in general, cannot be determined independently one by one. As noted above, we propose to use the R and I paths to determine the Hamilton characteristic W. In Sec. II D, we showed how to construct formally the surfaces of constant W_{0I}. This construction is sequential across the forbidden region, in which both R and I paths are determined simultaneously.

As a by-product of this construction, we also obtained two sets of coupled equations satisfied by the R and I paths. Although neither an analytical nor a computational approach to obtain the explicit solution of these equations is available, our geometric construction is a solution of these equations subject to proper boundary conditions. The method is general and applicable to any tunneling problem as long as the WKB approximation, Eqs. (2.3)–(2.5), is valid. In the following we discuss several of the characteristics of multidimensional tunneling that can be deduced from our solution.

B. Tunneling at normal incidence to the turning surface

First we shall consider the use of Newton's equations with inverted potential and energy to obtain the trajectories in the forbidden region. From Sec. II we know that this is justified when the incoming wave is normally incident at the turning surface; in this case the tangential component of the wave vector vanishes on the turning surface, and hence k_R remains zero in the entire forbidden region. Thus one set of wave fronts (i.e., the set of constant W_{0I} surfaces) suffices to describe the WKB wave function in the forbidden region. The wave function can be equivalently described by the I paths, which satisfy Eq. (2.24a). These equations reduce, in this case, to the semiclassical path equations and can be derived from Newton's equations of motion with inverted potential and energy.

The semiclassical treatment of the path decomposition expansion method introduced by AK (Ref. 21) effectively assumes the tunneling particle to be normally incident. In this case, tunneling can be described by the I paths which correspond to the instanton paths in their papers. This treatment is valid for tunneling from a well because for a fixed total energy the normally incident wave has the smallest exponential decrement, and hence dominates the other contributions to the tunneling rate.

C. Turning surfaces in multidimensional tunneling

Next, we consider the determination of the multidimensional turning surfaces. It has been argued[24] that "for nonseparable potentials one cannot uniquely define the kinetic energy for a particular coordinate, thus it is impossible to obtain the turning points." From Eq. (2.15), it is clear that the turning surfaces are determined by *either of two independent conditions:* $k(\mathbf{r})=0$ (normal incidence), or $\sigma(\mathbf{r})=0$ (the cross section of the flux tube vanishes). Evidently in the second case it is impossible to determine the turning surface in terms of only a single classical trajectory. Thus in a multidimensional space one has, in general, to use a family of classical trajectories and to locate the surfaces on which either $k(\mathbf{r})$ or $\sigma(\mathbf{r})$ vanishes in order to obtain the turning surfaces. Note that the turning surfaces are determined not only by the potential field but also by the boundary conditions. That is, different families of classical trajectories do not, in general, have the same turning surface. For example, in a potential field that depends on x only, the turning surface for a plane wave is a flat plane. However, for a point source, the turning surface could be a paraboloid of revolution.

D. Most probable tunneling path

In some multidimensional tunneling theories,[18,31] it is suggested that the tunneling calculation can be performed by evaluating the contributions from single or at most a few locally most probable paths and their respective neighborhoods included in an appropriate flux "tube." Consider the cases presented in Fig. 3. In the first example all trajectories are normal at the incident turning surface. These trajectories are continued by I paths into the forbidden region. Because $k_R=0$, these paths can be determined independently by Eq. (2.9), and a set of these paths can be constructed. The contribution from each of these paths can be evaluated easily and independently. The tube concept does not have in this case any advantage in the calculation of the tunneling current density. In fact, interpreting the tube as a device to introduce a line-shape broadening of the tunneling probability density, we recognize that the tunneling current density may have structure easily missed by the Gaussian line shape.

E. Complex tunneling time

The preceding analysis also allows us to answer the question concerning the complex time in tunneling calcu-

lation.[40,41] Here the intent is to extend the expression

$$t=\int_{\mathbf{r}_1}^{\mathbf{r}_2}\frac{d\xi}{\sqrt{2[E-V(\mathbf{r})]/m}} \tag{3.1}$$

into the forbidden region. But as discussed above, a single trajectory is in general not sufficient to determine the turning surface. In particular, a single trajectory does not determine its intersection with the caustic except when this trajectory is at normal incidence. Only when a family of paths is specified will we be able to separate the allowed from the forbidden region. Therefore, in general, multidimensional tunneling theory can not be formulated in terms of a complex time associated with a single trajectory.

However, if the point $\mathbf{r}_1$ is taken to be the location of a point source, then this boundary condition allows a family of paths to be constructed. All of these paths emerge from the point. Thus the procedure presented in Sec. II D can be followed to obtain the paths in the different regions. Two end points belonging to different classically allowed regions can be joined by two segments of the classical trajectory which are connected by an I path as shown in Fig. 3. The preceding discussion amounts to a generalization of Eq. (3.1) to the complex valued expression

$$t=\int_{\mathbf{r}_1}^{\mathbf{a}}\frac{d\xi}{\sqrt{2[E-V(\mathbf{r})]/m}}+\int_{\mathbf{b}}^{\mathbf{r}_2}\frac{d\xi}{\sqrt{2[E-V(\mathbf{r})]/m}} +i\int_{\mathbf{a}}^{\mathbf{b}}d\xi\frac{m}{\hbar k_I(\mathbf{r})}\ . \tag{3.2}$$

Here, **a** and **b** are adjacent turning points. The third term involves an integral over the forbidden region of the unknown function $k_I(\mathbf{r})$, which has been shown in Sec. II D to depend on the neighboring paths which have to be calculated. It appears that the determination of these additional paths involves a construction similar to that described in Sec. II D. The difficulty of implementing this procedure probably is equal to that of the method presented in that section. Again, if the incidence is normal to the first turning surface, then in the forbidden region we have $k_R=0$ and $k_I=-ik$. Thus in this case the integrand in the third term in Eq. (3.2) is known. In fact, the analysis is not different from that in the allowed region except that time becomes purely imaginary because $E<V(\mathbf{r})$. It has been shown that for one-dimensional tunneling, the complex time method recovers the WKB approximation.[40]

F. Spatial complex trajectories

Finally, we turn to the problem of trajectory with complex spatial coordinates.[42] This is not essentially different from the complex trajectories introduced by the complex time scheme above. Trajectories can be always expressed in terms of a single parameter, either the time or a spatial coordinate. It can be real or complex. We emphasize once more that any attempt to use a single trajectory to describe tunneling in a multidimensional space is bound to fail. This is due to the fact that except for some special cases mentioned above, e.g., normal incidence and separable problems, the phenomenon can be adequately described only in terms of two sets of paths.

G. Conclusions and results

We applied the WKB method to tunneling in multidimensional and nonseparable potentials. In the classically allowed regions our method leads to the standard semiclassical approximation. In the classically forbidden region, we introduce two sets of real, mutually perpendicular paths, called I and R paths, which are defined to be normal to the constant (amplitude) W_{0I} surfaces and constant (phase) W_{0R} surfaces, respectively. These paths characterize the WKB-type wave function and its propagation. Classical trajectories, in two disjoint and classically allowed regions, are joined in the forbidden region by corresponding I paths. The I and R paths obey two sets of coupled ordinary differential equations which obviously differ from Newton's equations, though they resemble them. Specifically, if the incidence of all the classical trajectories is normal to the turning surface, the path equations decouple. In this case, the WKB method used in the classically allowed regions is directly applicable in the adjacent forbidden region. This procedure was, in fact, followed by Das and Mahanty[13] and Huang, Cutler, and Feuchtwang.[36] Finally, we note that the path equations, Eq. (2.24), may be interpreted as the Euler-Lagrange equations of the two constained variational principles $\delta W_{0I}=0$ and $\delta W_{0R}=0$ subject to the constaint given by Eq. (2.19). These variational principles reduce, in the classically allowed regions, to the principle $\delta W_0=0$, whose Euler-Lagrange equations are Eqs. (2.9).

We are currently studying two alternative multidimensional WKB-type methods: the complex time scheme described in Sec. III E and the technique of spatially complex trajectories, described in Sec. III F. In both cases, it appears that the role of the real I path in joining classical trajectories across a forbidden region will be assumed by complex trajectories.

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APPENDIX A: PROOF OF EQ. (2.9)

Consider the following integral for a function called $W_{0R}(\mathbf{r})$:

$$W_{0R}(\mathbf{r})=\hbar\int^{\mathbf{r}}k(\mathbf{x})d\xi\ . \tag{A1}$$

If the end point $\mathbf{r}$ changes to $\mathbf{r}+\Delta\mathbf{r}$, W_{0R} will be changed by ΔW_{0R},

$$\Delta W_{0R}(\mathbf{r})=\hbar\Delta\int^{\mathbf{r}}k(\mathbf{x})\sqrt{x_n'x_n'}d\xi\ , \tag{A2}$$

that is,

$$\Delta W_{0R}(\mathbf{r})=\hbar\int^{\mathbf{r}}\left[\frac{\partial k}{\partial x_i}\sqrt{x_n'x_n'}-\frac{d}{d\xi}\left[k(\mathbf{x})\frac{x_i'}{\sqrt{x_n'x_n'}}\right]\right]\delta x_i\,d\xi+\hbar\left[k(\mathbf{x})\frac{x_i'\Delta x_i}{\sqrt{x_n'x_n'}}\right]\Bigg|^{\mathbf{r}}, \tag{A3}$$

where the prime denotes the derivative with respect to ξ. If we require that the change of $\mathbf{r}$ be perpendicular to the constant W_{0R} surface, then $d\mathbf{r}/d\xi$ is in the direction of ∇W_{0R}, and Eq. (2.7b) becomes

$$\nabla W_{0R}=\hbar k\frac{d\mathbf{r}}{d\xi}\ . \tag{A4}$$

Thus substituting Eq. (A4) into Eq. (A3), we conclude that the first term on the right-hand side of Eq. (A3) must vanish. However, since δx_i is arbitrary, the expression enclosed by square brackets must vanish, i.e.,

$$\frac{\partial k}{\partial x_i}\sqrt{x_n'x_n'}-\frac{d}{d\xi}\left[k(\mathbf{x})\frac{x_i'}{\sqrt{x_n'x_n'}}\right]=0,\quad i=1,2,3\ . \tag{A5}$$

These are the Euler-Lagrange equations for the variational principle $\delta W_{0R}=0$, with fixed end points. With the help of Eq. (2.8), Eq. (A5) leads to Eq. (2.9). A completely analogous analysis applies in the classically forbidden region for the two paths, and leads to the two variational principles $\delta W_{0I}=0$ and $\delta W_{0R}=0$, respectively.

APPENDIX B: PROOF OF EQ. (2.22)

First we show that the error in replacing an infinitesimal arc length by a straight line is a third-order quantity. Let the arc length be $\Delta\lambda$, the corresponding straight line length be $\Delta\xi$, and the radius of the curvature of the segment be R, then we have

$$\Delta\lambda=(\Delta\theta)R\ , \tag{B1}$$

where $\Delta\theta$ is the angle subtended by the arc, and

$$\Delta\xi=2R\sin(\Delta\theta/2)=2R\left[(\Delta\theta/2)-\frac{(\Delta\theta/2)^3}{6}+\cdots\right].$$

With the help of Eq. (B1) we have

$$\Delta\xi=\Delta\lambda-\frac{(\Delta\lambda)^3}{24R^2}+\cdots\ . \tag{B2}$$

In the derivation of Eq. (2.22), second-order terms are needed. However, one can still interchange the arc length increment with a straight-line segment approximation.

Through every point M on a W_{0I} surface, there pass a R path and an I path. The intersections of these paths with the $W_{0R}+\Delta W_{0R}$ and $W_{0I}+\Delta W_{0I}$ surfaces are called points N and M', respectively. Using M', we can also define a point Q as the intersection of the R path with the $W_{0R}+\Delta W_{0R}$ surface. The quantities $\Delta\xi$ and $\Delta\zeta$ shown in Fig. 2 can be calculated as follows: $W_{0R}(\mathbf{r})$ at point M can be written as $W_{0R}(\mathbf{r}_1(\xi))$ and at point N as $W_{0R}(\mathbf{r}_1(\xi+\Delta\xi))$, where $\mathbf{r}_1(\xi)$ represents the R path. Using Taylor expansion, we have

$$\begin{aligned}W_{0R}(\mathbf{r}_1(\xi+\Delta\xi))&=W_{0R}(\mathbf{r}_1(\xi))+\left.\frac{\partial W_{0R}}{\partial\xi}\right|_{\xi}\Delta\xi+\left.\frac{\partial^2 W_{0R}}{\partial\xi^2}\right|_{\xi}\frac{\Delta\xi^2}{2}+O(\Delta\xi^3)\\&=W_{0R}(\mathbf{r}_1(\xi))+\hbar k_R(\mathbf{r}_1(\xi))\Delta\xi+\hbar\left.\frac{\partial k_R}{\partial\xi}\right|_{\xi}\frac{\Delta\xi^2}{2}+O(\Delta\xi^3)\ .\end{aligned} \tag{B3}$$

Similarly, the $W_{0R}(\mathbf{r})$ values at points M' and Q satisfy the following relation:

$$W_{0R}(\mathbf{r}_2(\xi'+\Delta\xi'))=W_{0R}(\mathbf{r}_2(\xi'))+\hbar k_R(\mathbf{r}_2(\xi'))\Delta\xi'+\hbar\left.\frac{\partial k_R}{\partial\xi}\right|_{\xi'}\frac{\Delta\xi'^2}{2}+O(\Delta\xi'^3)\ . \tag{B4}$$

Points M and M' have the same W_{0R}, and points N and Q also have the same W_{0R}. Hence we obtain with the help of Eqs. (B3) and (B4),

$$\frac{\partial k_R}{\partial\zeta}=-k_R\frac{\Delta\Delta\xi}{\Delta\zeta\Delta\xi}\ , \tag{B5}$$

where

$$\Delta\Delta\xi\equiv\Delta\xi'-\Delta\xi\ . \tag{B6}$$

Now, let us define a plane based on the points M, M', and N. We may draw a line $M'Q'$ in the plane $MM'N$ to be parallel to MN, and terminate the line at the $W_{0R}+\Delta W_{0R}$ surface. By applying the law of sine to the triangle $M'QQ'$, we obtain

$$\frac{\overline{M'Q'}}{\overline{M'Q}}=\frac{\sin(\pi/2-\Delta\alpha)}{\sin(\pi/2-\Delta\beta)}\ . \tag{B7}$$

Due to the fact that both $M'Q$ and $M'Q'$ are perpendicular to the $W_{0R}+\Delta W_{0R}$ surface as $\Delta\zeta\to 0$, we have $\Delta\alpha\propto\Delta\zeta$, $\Delta\beta\propto\Delta\zeta$, and

$$\overline{M'Q'}=\overline{M'Q}+O(\overline{M'Q}\Delta\zeta^2)\ . \tag{B8}$$

We may write

$$\Delta\Delta\xi=\Delta\theta\Delta\zeta\ , \tag{B9}$$

where $\Delta\theta$ is the angle formed by the lines NQ' and MM'. Note that these two lines are on the plane $MM'N$ and are perpendicular to the R path MN. Substituting Eq. (B9) into Eq. (B5), we have Eq. (2.22).

[1]H. M. Van Horn and E. E. Salpeter, Phys. Rev. **157**, 751 (1967).
[2]T. Ledergerber and H.-C. Pauli, Nucl. Phys. **A207**, 1 (1973).
[3]H. Hofmann, Nucl. Phys. **A224**, 116 (1974).
[4]S. Coleman, Phys. Rev. D **15**, 2929 (1977).
[5]C. G. Gallen, Jr. and S. Coleman, Phys. Rev. D **16**, 1762 (1977).
[6]T. F. George and W. H. Miller, J. Chem. Phys. **57**, 2458 (1972).
[7]W. H. Miller, J. Chem. Phys. **62**, 1899 (1975).
[8]G. Binnig and H. Rohrer, Helv. Phys. Acta **55**, 726 (1982).
[9]T. E. Feuchtwang, P. H. Cutler, and N. M. Miskovsky, Phys. Lett. **99A**, 167 (1983).
[10]A. A. Lucas, H. Morawitz, G. R. Henry, J.-P. Vigneron, Ph. Lambin, P. H. Cutler, and T. E. Feuchtwang, Phys. Rev. B **37**, 10 708 (1988).
[11]J. Tersoff and D. R. Hamann, Phys. Rev. B **31**, 805 (1985).
[12]M. Chung, T. E. Feuchtwang, and P. H. Cutler, Surf. Sci. **187**, 559 (1987).
[13]B. Das and J. Mahanty, Phys. Rev. B **36**, 898 (1987).
[14]N. M. Miskovsky, P. H. Cutler, T. E. Feuchtwang, and A. A. Lucas, Int. J. Infrared Millimeter Waves **2**, 739 (1981).
[15]P. Ring, J. O. Rasmussen, and H. Massmann, Fiz. Elem. Chastits At. Yadra **7**, 916 (1976) [Sov. J. Part. Nucl. **7**, 366 (1977)].
[16]A. Ranfagni, G. Viliani, M. Cetica, and G. Molesini, Phys. Rev. B **16**, 890 (1977).
[17]A. Ranfagni, Phys. Lett. **62A**, 395 (1977).
[18]J. L. Gervais and B. Sakita, Phys. Rev. D **16**, 3507 (1977).
[19]H. J. Korsch and R. Möhlemkamp, Phys. Lett. **67A**, 110 (1978).
[20]S. Y. Lee and N. Takigawa, Phys. Rev. C **28**, 1123 (1983).
[21]A. Auerbach, S. Kivelson, and D. Nicole, Phys. Rev. Lett. **53**, 411 (1984).
[22]A. Auerbach and S. Kivelson, Nucl. Phys. **B257**, 799 (1985).
[23]X. W. Wang and D. L. Lin, J. Phys. A **19**, 1597 (1986).
[24]M. Razavy and A. Pimpale, Phys. Rep. **168**, 305 (1988).
[25]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[26]L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).
[27]R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Wiley, New York, 1962), Vol. 2, Chap. 2.
[28]M. C. Gutzwiller, J. Math. Phys. **8**, 1979 (1967); **10**, 1004 (1969); **11**, 1791 (1970); **12**, 343 (1971).
[29]V. P. Maslov and M. V. Fedoriuk, *Semi-classical Approximation in Quantum Mechanics,* (Reidel, Holland, 1981).
[30]T. E. Feuchtwang, Phys. Rev. B **10**, 4121 (1974).
[31]T. Banks, C. M. Bender, and T. T. Wu, Phys. Rev. D **8**, 3346 (1973); **8**, 3366 (1973).
[32]L. I. Schiff, *Quantum Mechanics,* 3rd ed. (McGraw-Hill, New York, 1968), pp. 268–279.
[33]M. Alonso and E. J. Finn, *Fundamental University Physics,* (Addison-Wesley, Reading, MA, 1967), Vol. II, pp. 774.
[34]N. Bleistein, *Mathematical Methods for Wave Phenomena* (Academic, New York, 1984), p. 260.
[35]M. V. Berry and K. E. Mount, Rep. Prog. Phys. **35**, 315 (1972).
[36]Z. H. Huang, P. H. Cutler, and T. E. Feuchtwang, J. Phys. (Paris) (to be published).
[37]J. B. Keller, in *Calculus of Variations and its Applications* (MacGraw-Hill, New York); Proc. Symp. Appl. Math **8**, 27 (1958); J. Opt. Soc. Am. **52**, 116 (1962).
[38]L. B. Felsen, J. Opt. Soc. Am. A **2**, 954 (1985).
[39]Yu. A. Kravtsov, in *Progress in Optics,* edited by E. Wolf (North-Holland, Amsterdam, 1988), Vol. 26, p. 229.
[40]D. W. McLaughlin, J. Math. Phys. **13**, 1099 (1972).
[41]A. Patrasciouiu, Phys. Rev. D **24**, 496 (1981).
[42]J. Knoll and R. Shaeffer, Ann. Phys. (N.Y.) **97**, 307 (1976).