Path Decomposition for Multidimensional Tunneling

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(Received 24 February 1984)

In order to solve multidimensional tunneling problems that cannot be treated by the normal instanton techniques, we introduce the path decomposition expansion formalism, and show its usefulness by solving three generic examples: the symmetric and asymmetric double well, and the decay problem. The technique allows us to handle excited states and backscattering effects in nonseparable potentials.

PACS numbers: 03.65.Sq, 03.65.Db

Multidimensional quantum mechanical tunneling phenomena, such as the splitting between the symmetric and antisymmetric states in a symmetric double well or the decay of a metastable state, cannot be treated by use of standard perturbation theory. Recently, however, instanton techniques,[1] which are in a sense multidimensional generalizations of the WKB method, have been successfully applied to a number of these problems. The basic idea of this approach is that ground-state tunneling effects are dominated by paths in the vicinity of classical paths which involve infinite imaginary time, which is to say the zero-energy classical motions in the inverted potential.

There are serious limitations to this technique as it involves paths only in the classically forbidden region of configuration space, and contains little information about the classically allowed regions. Thus, it does not lend itself to problems involving tunneling from an initially excited state of a potential well nor to problems in which backscattering final-state effects are significant (i.e., the effect of the spectrum of final states[2]). In one dimension these difficulties can be surmounted elegantly by summing over complex-time classical paths[3] which traverse both the allowed and forbidden regions. The classical path analysis in the classically allowed region[4] is, however, enormously complicated in more than one dimension; it appears quite intractable for nonseparable potentials.

Here, we outline a method that can avoid these difficulties. The technique is based on the observation that, although the contribution of the allowed region is hard to calculate from a classical path analysis, it can often be calculated with other conventional techniques (e.g., low-order perturbation theory). We work with a path-integral representation of the Green's function. We introduce a new multidimensional connection formula, which we call the path decomposition expansion (PDX). This enables us to break configuration space into regions (which we will normally choose to be the various allowed "well" and forbidden "barrier" regions) and to calculate the contribution of different regions separately. In particular, it allows us to use the classical path analysis in the forbidden region, where it is relatively simple, without being forced to handle the permitted region in the same cumbersome fashion.

We wish to consider the effects of tunneling in a potential $V(x)$ where x is a vector in an N-dimensional configuration space, Q. We therefore

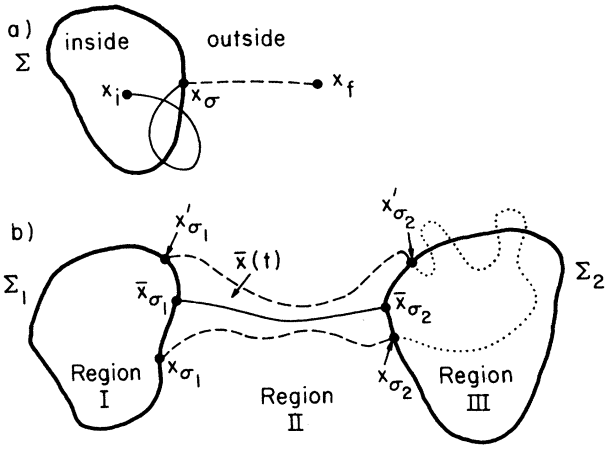

FIG. 1. (a) Schematic representation of the path decomposition in Eq. (2). The solid path contributes to $G(x_\sigma,x_i;E)$ and the dashed path to $G^{(r)}(x_f,x_\sigma;E)$. (b) Path decomposition for G^b in a double-well tunneling problem. Regions I and III are classically allowed, $V(x)<E$. The solid path $\bar{x}(t)$ is the instanton path which dominates G^b. The other path is a typical path from x_{σ_1} to x'_{σ_1} where the dashed pieces contribute to the two G^{II}'s, and the dotted pieces to G^{III}

express the Green's function, G, as the Laplace transform of the Feynman path integral

$$G(x_f,x_i;E)=\int_0^\infty dT\int_{x(0)=x_i}^{x(T)=x_f}\mathscr{D}x\exp((i/\hbar)\{S[x]+(E+i\epsilon)T\}), \tag{1a}$$

where S is the action functional

$$S[x]=\int_0^T dt[\tfrac{1}{2}m\dot{x}^2-V(x)]. \tag{1b}$$

Our first step is to derive the decomposition formula which allows us to isolate the contribution to G from some region of Q. We therefore consider a closed surface Σ in Q which breaks Q into two regions, an "inside" and an "outside." See Fig. 1(a). All paths which start at a point x_i inside Σ, and end at a point x_f outside Σ must pass through at least one point $x_\sigma\in\Sigma$. We can decompose all paths into an initial segment which starts at x_i and ends at x_σ (although it may cross Σ many times), and a final segment which goes directly from x_σ to x_f. The sum over these segments (from x_σ to x_f) is called the restricted Green's function $G^{(r)}$. To obtain the sum over all paths we must integrate over points x_σ. The result is the path-decomposition formula,

$$G(x_f,x_i;E)=\int_\Sigma d\sigma\, G^{(r)}(x_f,x_\sigma;E)[(i\hbar/2m)\overleftrightarrow{\nabla}_\sigma]G(x_\sigma,x_i;E), \tag{2a}$$

where $\int d\sigma$ is the surface integral over Σ, and $(i\hbar/2m)\overleftrightarrow{\nabla}_\sigma$ is the average of the incoming and outgoing velocities at x_σ, which is defined equivalently by the expression

$$f(x_\sigma)\overleftrightarrow{\nabla}_\sigma g(x_\sigma)=\hat{\sigma}[f(x)\partial_x g(x)-g(x)\partial_x f(x)]|_{x=x_\sigma}, \tag{2b}$$

where $\hat{\sigma}$ is the outward normal to Σ at x_σ. This velocity operator is the Jacobian of the transformation from Eq. (1) to (2), as can be seen by a careful analysis of the discrete time-step version of the path integral.[4] $G^{(r)}$ is defined by the expression

$$G^{(r)}(x_2,x_1;E)=\int_0^\infty dT\int_{x(0)=x_1}^{x(T)=x_2}\mathscr{D}^{(r)}x\exp((i/\hbar)\{S[x]+E^\dagger\}), \tag{3}$$

where $\mathscr{D}^{(r)}x$ is the sum over each path which stays strictly outside Σ and does not touch it (except possibly at its initial point x_1 if it is on Σ). We will use the following shorthand for rewriting the decomposition formula in Eq. (2);

$$G(x_f,x_i;E)=\langle x_i|G\,[\Sigma]\,G^{(r)}|x_f\rangle, \tag{4}$$

where $[\Sigma]$ implies the integration over the surface Σ including the appropriate normal derivatives (Jacobian).

Since $G^{(r)}$ is an unfamiliar quantity, it is worthwhile to examine its properties in a little more detail. It is defined by a path integral with the same action as G so it satisfies the same differential equation everywhere outside the surface Σ:

$$[-(\hbar^2/2m)\partial_x^2V(x)-E^\dagger]G^{(r)}(x,x';E)=\hbar\sigma(x-x')\theta(x,\Sigma), \tag{5}$$

where $\theta(x,\Sigma)$ is 1 when x is outside Σ, and 0 for x on Σ. Like G, $G^{(r)}$ is symmetric under interchange of its arguments ($x\leftrightarrow x'$), and it satisfies all the same boundary conditions as G on their common boundary surfaces. In addition, however, it satisfies both the unusual homogeneous boundary conditions on Σ represented by the function θ in Eq. (5), and the integral condition

$$\langle x|G^{(r)}\,[\Sigma]\,G^{(r)}|x'\rangle=0, \tag{6}$$

for any x and x' not inside Σ. Equations (5) and (6) can be viewed alternatively as the definition of $G^{(r)}$ in terms of a differential equation. Since $\mathscr{D}^{(r)}x$ excludes all paths which touch Σ at any point other than the initial point, the boundary conditions on $G^{(r)}$ correspond to a perfectly emitting wall on Σ. In one dimension this can be seen from Eqs. (5) and (6) to yield the boundary condition at point x_σ

$$-i\hbar\,\partial_x\ln G^{(r)}(x',x;E)|_{x=x_\sigma}=+\{2m[E-V(x_\sigma)]\}^{1/2}. \tag{7}$$

It is possible to iterate the PDX [Eqs. (2) or (4)] so as to break configuration space Q into many disjointed regions. We will demonstrate this by considering the double-well potential illustrated schematically in Fig. 1(b). We choose to make the decompositions at the surface of constant energy E, Σ_1 and Σ_2, which defines three regions: regions I and III enclosed by Σ_1, Σ_2, respectively, which are the classically allowed regions, and region II, the forbidden region, which is everywhere else. The different restricted Green's functions are

G^{I}, restricted outside Σ_2; G^{III}, restricted outside Σ_1; and G^{II}, restricted to the outside of both allowed regions. G^{II} is therefore doubly restricted and has a direction corresponding to paths which start on Σ_1 and end on Σ_2, $G^{\mathrm{II}}(\rightarrow)$, or, vice versa, $G^{\mathrm{II}}(\leftarrow)$. In the tunneling problems in which we are interested, E is well below the barrier which separates regions I and III. Because of this, G^{I} is only weakly dependent on the boundary conditions (or even the potential) at Σ_2. Thus, to accuracy $O(e^{-2W/\hbar})$ [where $W(E)$ is the classical action under the barrier, defined below] $G^{\mathrm{I}}(E)$ is well approximated by the Green's function of the single-well problem in which the potential in region III is replaced by a potential $V > E$, so

$$G^{\mathrm{I}}(x,x';E) \cong \hbar \sum_n \frac{\psi_n^{\mathrm{I}*}(x)\psi_n^{\mathrm{I}}(x')}{E^{\dagger} - E_n^{\mathrm{I}}} + R(xx';E), \tag{8}$$

where R signifies a regular function of E and the poles, E_n^{I}, and residues, $\psi_n^{\mathrm{I}}(x)$, are the spectrum and eigenstates, respectively, of the corresponding single-well problem. Note that in cases of practical interest, we cannot actually compute G^{I}'s exact poles and residues with accuracy remotely approaching $O(e^{-2W/\hbar})$. Nevertheless, we will see that small errors in calculating G^{I} only produce proportionate errors in the tunneling effects we shall consider This is the power of the PDX approach, in that it allows us to use any suitable approximation to calculate G^{I}.

In order to sum over all paths contained in G it is convenient to define a composite quantity called the "bounce," G^b, which is the sum over all single return trip paths to region III which begin and end on Σ_1 but never enter region I [see Fig. 1(b)],

$$G^b(x'_{\sigma_1},x_{\sigma_1};E) = \langle x_{\sigma_1} | G^{\mathrm{II}}(\rightarrow)\,[\Sigma_2]\,G^{\mathrm{III}}\,[\Sigma_2]\,G^{\mathrm{II}}(\leftarrow) | x'_{\sigma_1} \rangle. \tag{9}$$

G^b contains two surface integrations on Σ_2. Finally, G is obtained by summing over all bounces. For example if x and x' are both in region I,

$$\begin{aligned} G(x,x';E) &= \hbar \sum_{nn'} \frac{\psi_n^{\mathrm{I}*}(x)\psi_{n'}^{\mathrm{I}}(x')}{E^{\dagger} - E_n^{\mathrm{I}}} \sum_{N=0}^{\infty} \left[\mathcal{G}^b(E) \left[\frac{1}{E^{\dagger} - \epsilon^{\mathrm{I}}} \right] \right]_{nn'}^{N} + R(E) \\ &= \hbar \sum_{nn'} \psi_n^{\mathrm{I}*}(x) \left[\frac{1}{E^{\dagger} - \epsilon^{\mathrm{I}} - \hbar \mathcal{G}^b(E)} \right]_{nn'} \psi_{n'}^{\mathrm{I}}(x') + R(E), \end{aligned} \tag{10}$$

where we have used the ψ_n^{I} basis to define the various matrices

$$\mathcal{G}^b(E)_{nn'} = \psi_n^{\mathrm{I}*}\,[\Sigma_1]\,G^b\,[\Sigma_1]\,\psi_{n'}^{\mathrm{I}}, \tag{11a}$$

$$\epsilon^{\mathrm{I}}_{nn'} = \delta_{nn'} E_n^{\mathrm{I}}. \tag{11b}$$

The poles of G occur at energies E_n where

$$\mathrm{Det}[E_n^{\dagger} - \epsilon^{\mathrm{I}} - \hbar \mathcal{G}^b(E_n)] = 0. \tag{12}$$

Typically $\mathcal{G}^b(E)$ is small compared with the splitting between energy levels, $\Delta E^{\mathrm{I}} = |E_n^{\mathrm{I}} - E_{n'}^{\mathrm{I}}|$, and hence the sum over bounces produces only a small shift in the energy which can be computed with use of low-order perturbation theory in $\mathcal{G}^b$. In the case of resonant tunneling, when $G^{\mathrm{III}}(E)$ [and hence $\mathcal{G}^b(E)$] has a pole at energy E_n^{III} which is nearly equal to E_n^{I}, Eq. (12) must be solved with use of near degenerate perturbation theory; the sum over bounces produces important effects (see examples below).

Equations (10)–(12) are our principal results. They permit us to employ a hybrid approximation scheme, in which only G^{II} need be computed with use of a semiclassical approximation. We now conclude by briefly illustrating how this scheme works by examples. Many technical considerations are deferred for future publication.[5]

As a demonstration we consider the symmetric and asymmetric double well in an arbitrary number of dimensions [see Figs. 1(a) and 1(b)] and study the effect of asymmetry on the poles and residues of G. In the symmetric case regions I and III are equivalent so G^{III} has the same poles as G^{I}. (This is the simplest example of resonant tunneling.) Thus, combining Eqs. (9) and (12) for the case of a large barrier (G^{II} small), we find that each energy level E_n splits into a symmetric and an antisymmetric state

$$E_n^{\pm} = E_n^{\mathrm{I}} \pm \Delta_n + O(\mathcal{G}^2/\Delta\epsilon^{\mathrm{I}}) \tag{13}$$

where the splitting

$$\Delta_n = \hbar |\psi_n^{I*}[\Sigma_1]\, G^{II}(\rightarrow)\,[\Sigma_2]\,\psi_n^{I}|. \tag{14}$$

Δ_n is a relatively straightforward object to compute semiclassically. It is dominated in most practical examples by a single path $\bar{x}(t)$ which minimizes the action $W = S + ET$ from Σ_1 to Σ_2 [$G^{II} = O(\hbar e^{-W/\hbar})$].

This path, which we call the instanton path, is a classical path with energy $-E$, in the inverted potential from an initial point $\bar{x}_{\sigma_1}$ on Σ_1 to a final point $\bar{x}_{\sigma_2}$ on Σ_2. It will necessarily start and end with zero velocity. In terms of this path all integrations in Eq. (14) can be carried out by the steepest-descent method to obtain Δ to leading order in $\hbar$:

$$\Delta_n = \hbar |\psi_n^{I}(\bar{x}_{\sigma_1})|^2 \exp\{-\hbar^{-1}\int_{\bar{x}_{\sigma_1}}^{\bar{x}_{\sigma_2}} [2m(V(\bar{x}) - E_n^{I})]^{1/2} d\bar{x}\} A_n. \tag{15}$$

A_n is a factor of order $\hbar^0$ with dimensions of (time)$^{-1}$ (distance)^N, arising from the quantum fluctuations around the instanton path and the two surface integrations. In the near future a full discussion of A_n will be published.[5] Subtleties due to the fact that $\bar{x}_\sigma$ is a classical turning point[2] can be handled in a way analogous to the usual WKB connection formula. In many cases of physical interest, A_n can be calculated to good approximation in closed analytic form. For the present we just point out that in the separable case the effect of A_n is to renormalize the potential $V(\bar{x})$ in Eq. (15) to $V^{ren}(\bar{x}) = V + E_\perp(m_\perp)$, where $m_\perp$ are the quantum numbers of the directions not coupled to the tunneling coordinate. Note that as we commented earlier, small errors in the computation of ψ_n^I and E_n^I produce only small fractional errors in Δ_n.

In the asymmetric double well, when $\mathcal{G}^b(E)$ is regular near E_n^I, it is clear from Eq. (12) that there is an eigenstate with energy negligibly shifted from E_n^I, $E_n = E_n^I + O(e^{-2W/\hbar})$. This eigenstate has an amplitude (which we can calculate) in region III of $O(e^{-W/\hbar})$; the tunneling probability is of $O(e^{-2W/\hbar})$. In contrast, in cases of resonance when $|E_n^I - E_m^{III}| \lesssim \Delta_n$, $\mathcal{G}^b(E)$ is singular [$\mathcal{G}^b(E) \sim e^{-2W/\hbar}/(E - E_m^{III})$], and hence an energy splitting of $O(e^{-W/\hbar})$ is obtained, just as in the symmetric case. This resonance effect cannot, in general, be obtained by normal instanton techniques.

The decay rate Γ_n of a metastable state is determined by the imaginary part of the pole, $\mathrm{Im}(E_n) = \hbar\Gamma_n/2$. A finite decay rate can only occur if there is a continuum of states, $\psi_E^{III}(x)$, in region III. Formally, a continuum of states in region III implies that G^{III} has a finite imaginary part proportional to the density of states,

$$\mathrm{Im}\, G^{III}(x,x';E) = \hbar\pi\psi_E^{III}(x)\psi_E^{III*}(x')\rho^{III}(E).$$

It is apparent from Eq. (12) that this gives rise to a complex pole with

$$\hbar\Gamma_n/2 = \pi\hbar^2 |\psi_n^I(\bar{x}_{\sigma_1})|^2 |\psi_{E_n}^{III}(\bar{x}_{\sigma_2})|^2 \rho^{III}(E_n)(A_n)^2 \exp\left[-\frac{2}{\hbar}\int_{\bar{x}_{\sigma_1}}^{\bar{x}_{\sigma_2}} [2m(V - E_n)]^{1/2} d\bar{x}\right]. \tag{16}$$

We have shown that the PDX provides a method for isolating the important factors in tunneling processes in a way that enables us to develop controlled approximations to solve problems involving many coupled degrees of freedom. In future publications we will demonstrate the usefulness of this technique for specific problems of physical interest. For instance we are currently completing a calculation of the cross section for photoinduced soliton pair production in polyacetylene, including the effects of simultaneous phonon emission.

We would like to acknowledge important discussions with and encouragement from Professor S. Chakravarty, Dr. D. Stone, and Dr. J. Sethna. Two of us (S.K.) and (A.A.) would also like to thank Dr. P. B. Allen. This work was supported in part by National Science Foundation Grants No. NSF-NMR 81-29154 and No. NSF-DMR-8318051.

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