Eur. Phys. J. C 18, 195–201 (2000)
Digital Object Identifier (DOI) 10.1007/s100520000514

The European Physical Journal C
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Springer-Verlag 2000

Classical paths and the WKB approximation

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Received: 6 June 2000 / Published online: 27 October 2000 – © Springer-Verlag 2000

Abstract. Recently, new connection formulas for the WKB method have been proposed, without justification, for quantum tunneling problems. We show that these formulas can be associated with diagrammatic rules within the complex time framework of the path integral formalism and then we express the relevant Green functions in terms of a sum of contributions coming from (easily interpreted) classical paths. The method is applied to barrier penetration and the double well.

1 Introduction

Approximation methods are a necessary industry in physics because exactly soluble problems are few and generally unrealistic. In this respect, it is a very satisfying consolation that one of the oldest approximation schemes in quantum theory, the WKB method, continues to find applications in the broad front of present-day research [1]. The method, however, is plagued with a chronic difficulty: it breaks down when the local particle momentum $p = \hbar k = \sqrt{2m[E - V(x)]}$ is small, and is completely inapplicable when $p = 0$ [2]. The well-known way to circumvent this problem is to connect the approximate wave functions across regions where the method fails: a simple way to implement this is to replace the actual potential $V(x)$ by a linear one at the neighborhood of the classical turning points [3]. In virtue of this simple remedy the WKB method has indeed been an effective tool in dealing with wave-propagation problems.

Effective as the conventional WKB method maybe, the resulting connection formulas, that relate the wave functions across turning points, do not allow freedom for the possibility of wave function suppression on the classical forbidden zone(s) and they constrain the reflection phase to a single value for all energies. In very recent developments, the method has been relieved of these shackles by the introduction of new connection formulas that leave the amplitude and phase unspecified to some extent [4]. Consistency is then built into the new formulas by imposing continuity across the turning points. As offshoots of these developments, certain tunneling and potential reflection problems, previously inaccessible or only unsatisfactorily solved by the conventional theory, have now been successfully addressed [4, 5]. One sees hope in being able to handle the case when p is consistently small.

From another direction it has been shown that the WKB results can be derived by a semi-classical approximation of the path integral [6]. This led to the cross-fertilization of the two approaches culminating in a diagrammatic reformulation of the complex-time path integral formalism for tunneling which is equivalent to the conventional WKB theory [7]. Since, as is well known, path-integral methods lend themselves readily to generalization into field theory and carry considerable physical insight into the entire spectrum of quantum systems, these results are interesting in their own right [8]. The path integral within the semi-classical approximation has in fact received further boost from recent mathematical developments [9].

The issue we seek to address here is a generalization of the complex-time formalism to encompass the generalized WKB connection formulas mentioned above. It is only to be expected that the boon now being enjoyed by the WKB method should also be a boon for the semi- classical path integral approach. Also we may observe that the above-mentioned connection formulas had not been derived; they were simply postulated based on the old conventional form. Although we are unable to provide a first-principles derivation of these formulas, we indicate where the new elements might be from. We also obtain a new diagrammatic rendition of the Green function which can be interpreted in terms of rules for propagation factors, and phases and weights at the turning points. These are consistent with the new connection formulas. Many efforts toward improving the WKB method have been made recently, such as the semiclassically modified Born approximation [10], but we will focus attention on those of references 4 and 5.

The rest of the paper is structured as follows. In Sect. 2 we review the semi-classical path integral approach and show how the new connection formulas emerge. These formulas give rise to diagrammatic rules that we apply to the Green function in Sect. 3. There we show that the Green functions can be interpreted as sums over complex time classical paths consistent with the new connection formu-

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las. Two applications follow in Sect. 4, that demonstrate the directness of the method. A new formula for the lifetime in a double well is obtained. Finally, in Sect. 5 we conclude by indicating directions for future work

2 New connection formulas

Let us begin by deriving the new connection formulas within the context of the semi-classical limit of the Green function $G(x_f, x_i, E)$ for propagation of a particle of mass m, and energy E through a potential $V(x)$ from a point x_i to x_f [6, 11]:

$$G(x_f, x_i, E) = \frac{1}{\hbar}\sum\sum_{x_{cl}} \left[e^{i\pi}\dot{x}_{cl}(0)\dot{x}_{cl}(T_s)\right]^{-1/2} \times e^{iW_{cl}(T_s)} , \qquad (1)$$

where the particle is understood to follow a classical path $x_{cl}(t)$, T_s is the time of transit, $\dot{x}_{cl}(t)$ is the velocity at time t and $S_{cl} = S[x_{cl}] = \int_0^{T_s} dt[\frac{1}{2}m\dot{x}^2 - V(x)]$ is the action evaluated along the classical path. Note that

$$W_{cl}(T_s) = [S_{cl}(T_s) + E_{cl}(T_s)]/\hbar . \qquad (2)$$

The classical energy is given by

$$E_{cl} = -\frac{\partial S_{cl}}{\partial T} . \qquad (3)$$

The sum in (1) is over all classical paths x_{cl} connecting the end points and over times compatible with these paths. Because E_{cl} is the sum of kinetic and potential energies

$$W_{cl}(T_s) = \frac{1}{\hbar}\int_0^{T_s} dx_{cl}(t)p_{cl}(t) , \qquad (4)$$

so that W_{cl} is the usual WKB phase.

Following Carlitz and Nicole [6], we study the propagation of the particle in a linear one-dimensional potential

$$V(x) = -\lambda x , \qquad (5)$$

for which the classical path connecting x_i and x_f in a time T is

$$x_{cl}(t) = x_i + \frac{x_f - x_i}{T}t - \frac{\lambda T}{2m}t + \frac{\lambda}{2m}t^2 , \qquad (6)$$

with the corresponding action

$$S_{cl} = \frac{m}{2T}(x_f - x_i)^2 + \frac{\lambda T}{2}(x_f + x_i) - \frac{\lambda^2 T^3}{24m} . \qquad (7)$$

It is convenient to set $E = 0$ so (3) gives the times

$$T_s = \sqrt{\frac{2m}{\lambda}}\left(x_f^{1/2} + x_i^{1/2}\right) , \qquad (8)$$

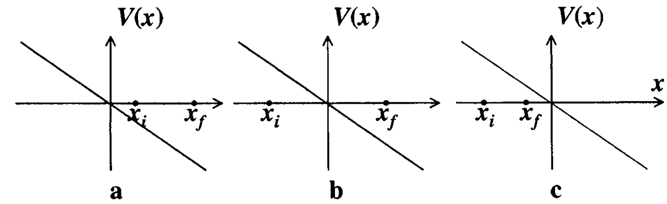

Fig. 1a–c. Linear potential for a particle of mass m, energy $E = 0$, with initial and final points x_i and x_f in **a** the allowed region, **b** in the forbidden and allowed regions, respectively, and **c** in the forbidden region

where all possible signs of the square roots of the x's are permissible. Then the corresponding action may be evaluated, yielding

$$S_{cl} = \frac{2}{3}(2m\lambda)^{1/2}\left[x_f^{3/2} + x_i^{3/2}\right] = \hbar W_{cl} , \qquad (9)$$

and evaluation of (1) gives the Green function

$$G(x_f, x_i, E) = -\sum\frac{e^{i\pi/4}}{\hbar}\left[\frac{e^{-i\pi/2}m}{2\lambda x_i^{1/2}x_f^{1/2}}\right]^{1/2} \times \exp\left[\frac{i}{\hbar}\frac{2}{3}(2m\lambda)^{1/2}\left(x_f^{3/2} + x_i^{3/2}\right)\right] , \qquad (10)$$

where the sum is over the relevant signs of the roots of the x's, as dictated by (8).

We need to study three possible propagation events as depicted in Fig. 1. In Fig. 1a the particle remains in the allowed region all the time and goes from x_i to x_f through two paths: one is direct and the other involves a reflection at the origin while in transit. These yield two times

$$T_s^{(1a)} = \left(\frac{2m}{\lambda}\right)^{1/2}\left(x_f^{1/2} \pm x_i^{1/2}\right) . \qquad (11)$$

The Green function is

$$\begin{aligned} G^{(1a)}&(x_f, x_i, E = 0) \\ &= -\frac{e^{i\pi/4}}{\hbar}\left[\frac{e^{-i\pi/2}m}{-2\lambda x_i^{1/2}x_f^{1/2}}\right]^{1/2} \times \exp\left[\frac{2i}{3\hbar}(2m\lambda)^{1/2}\left(x_f^{3/2} - x_i^{3/2}\right)\right] \\ &\quad -\frac{e^{i\pi/4}}{\hbar}\left[\frac{e^{-i(\pi/2+\alpha)}m}{2\lambda x_i^{1/2}x_f^{1/2}}\right]^{1/2} \times \exp\left[\frac{2i}{3\hbar}(2m\lambda)^{1/2}\left(x_f^{3/2} + x_i^{3/2}\right)\right] \\ &= -\frac{2}{\hbar}\left[\frac{m}{2\lambda(x_i x_f)^{1/2}}\right]^{1/2}\exp\left[\frac{2i}{3\hbar}(2m\lambda)^{1/2}x_f^{3/2}\right] \times e^{i(\pi/4-\alpha/2)} \\ &\quad \times\cos\left[\frac{2}{3\hbar}(2m\lambda)^{1/2}x_i^{3/2} - \frac{\pi}{4} - \frac{\alpha}{2}\right] . \end{aligned} \qquad (12)$$

Here all the $x_f^{1/2}$, $x_i^{3/2}$, etc take the positive sign. Also in the second line, an arbitrary reflection phase of - α is appended in light of the discussion in Sect. 1.

In Fig. 1b the particle lies initially at the classically forbidden zone and propagates into the allowed zone. Only one path contributes to G, namely the one whose time of transit is

$$T_s^{(1b)} = \left(\frac{2m}{\lambda}\right)^{1/2}\left(x_f^{1/2} - i(-x_i)^{1/2}\right) . \tag{13}$$

As we had noted in Sect. 1, the new WKB approach modifies the connection formulas by introducing suitably generalized phases and amplitudes. In this spirit, we assume that a phase of - $\alpha/2$ accrues as the particle crosses the origin and that a real factor of N acts to control the final amplitude. That is, we expect the phase to be half that for a reflection in Fig. 1a. Then the Green function for this case is

$$\begin{aligned} &G^{(1b)}(x_f, x_i, E=0) \\ &= -\frac{1}{\hbar}\left(\frac{m}{2\lambda(-x_i x_f)^{1/2}}\right)^{1/2} \\ &\quad\times \exp\left[\frac{2i}{3\hbar}(2m\lambda)^{1/2}x_f^{3/2}\right] N e^{i(\pi/4-\alpha/2)} \\ &\quad\times \exp\left[-\frac{2}{3\hbar}(2m\lambda)^{1/2}(-x_i)^{3/2}\right] . \end{aligned} \tag{14}$$

Finally in Fig. 1c the particle starts and ends in the forbidden zone. A direct path contributes together with a path reflecting at the origin. Both evolve in purely imaginary time. As in Fig. 1b, we append an arbitrary amplitude factor of $N/2\bar{N}$ together with an arbitrary phase factor of $e^{-i(\alpha-\bar{\alpha})/2}$ for reflection inside the forbidden zone. The $\bar{N}, \bar{\alpha}$ are arbitrary. Thus, we find

$$\begin{aligned} &G^{(1c)}(x_f, x_i, E=0) \\ &= -\frac{1}{\hbar}\left[\frac{m}{2\lambda(x_f x_i)^{1/2}}\right]^{1/2} \exp\left[-\frac{2}{3\hbar}(2m\lambda)^{1/2}(-x_i)^{3/2}\right] \\ &\quad\times\left\{\exp\left[\frac{2}{3\hbar}(2m\lambda)^{1/2}(-x_f)^{3/2}\right] - e^{i\pi/2}\frac{N}{2\bar{N}}e^{-i(\alpha-\bar{\alpha})/2}\right. \\ &\quad\left.\times \exp\left[-\frac{2}{3\hbar}(2m\lambda)^{1/2}(-x_f)^{3/2}\right]\right\} . \end{aligned} \tag{15}$$

The WKB phase is

$$W(x) = \frac{1}{\hbar}\int_0^x p(x')dx' = \frac{2}{3\hbar}(2m\lambda)^{1/2}x^{3/2} . \tag{16}$$

We can extract the connection formulas by comparing pairs of formulas. It is convenient to define new phase angles as follows $\phi = \pi/2 + \alpha, \bar{\phi} = 3\pi/2 + \bar{\alpha}$. Comparing (12) and (14) we obtain

$$\begin{aligned} &\frac{1}{\sqrt{|p(x)|}}\left(\exp\left[-i\left|\frac{1}{\hbar}\int_0^x p(x')dx'\right|\right]\right. \\ &\qquad\left. + e^{-i\phi}\exp\left[i\left|\frac{1}{\hbar}\int_0^x p(x')dx'\right|\right]\right) \\ &\qquad\to \frac{N}{\sqrt{|p(x)|}}e^{-i\phi/2}\exp\left[-\left|\frac{1}{\hbar}\int_x^0 p(x')dx'\right|\right] , \end{aligned} \tag{17}$$

where $x \geq 0$ on the left-hand expression while $x \leq 0$ on the right-hand expression. Similarly, (14) and (15) yield

$$\begin{aligned} &\frac{1}{\sqrt{|p(x)|}}\left(\exp\left[\left|\int_0^x p(x')dx'\right|\right] - \frac{N}{2\bar{N}}e^{-i(\phi-\bar{\phi})/2}\right. \\ &\quad\left.\times\exp\left[-\left|\int_0^x p(x')dx'\right|\right]\right) \\ &\qquad\to \frac{iN}{\sqrt{|p(x)|}}e^{-i\phi/2}\exp\left[i\left|\int_x^0 p(x')dx'\right|\right] , \end{aligned} \tag{18}$$

Table 1. Phase and weight factors at each turning point

	Phase	Weight
Allowed → allowed	$e^{-i\phi}$	1
Forbidden → forbidden	$-e^{-i(\phi-\bar{\phi})/2}$	$N/2\bar{N}$
Forbidden → allowed	$ie^{-i\phi/2}$	N
Allowed → forbidden	$e^{-i\phi/2}$	N

On the left-hand side $x \leq 0$ while on the right $x \geq 0$. Equation (17) tells us that a particle incident from the allowed region is reflected with a phase - ϕ and unchanged amplitude and transmitted with a phase - $\phi/2$ and transmitted with a phase new amplitude of N. Equation (18) asserts that a particle incident from the forbidden zone undergoes reflection with a phase $-e^{-i(\phi-\bar{\phi})/2}$ and an amplitude of $N/2\bar{N}$ and is transmitted with amplitude N and a phase of $ie^{-i\phi/2}$. These results are gathered together in Table 1. Because a shift in energy is equivalent to a translation in x for a linear potential, these results hold for any value of E. In the older literature, $N = \bar{N} = 1$ and $\phi = -\bar{\phi} = \pi/2$. For expressions for these in the new approach, we refer to references 4 and 5. We will not derive them here.

We may now establish contact with the generalized connection formulas in the literature [4]. From (17) we have

$$\begin{aligned} &\frac{2}{\sqrt{|p(x)|}}\cos\left(\left[\left|\int_0^x p(x')dx'\right|\right] - \frac{1}{2}\phi\right) \\ &\qquad\to \frac{N}{\sqrt{|p(x)|}}\exp\left[-\left|\int_0^x p(x')dx'\right|\right] , \end{aligned} \tag{19}$$

which is one of the connection formulas. Next we rewrite (18) in the form

$$\begin{aligned} &\frac{1}{\sqrt{|p(x)|}}\left(\exp\left[\left|\int_0^x p(x')dx'\right|\right] - \frac{N}{2\bar{N}}e^{-i(\phi-\bar{\phi})/2}\right. \\ &\quad\left.\times\exp\left[-\left|\int_0^x p(x')dx'\right|\right]\right) \to 2\frac{iN}{\sqrt{|p(x)|}}e^{-i\phi/2} \\ &\quad\times\left\{\frac{e^{-i\bar{\phi}/2}}{e^{-i\phi} - e^{-i\bar{\phi}}}\cos\left[\left|\int_x^0 p(x')dx'\right| - \frac{1}{2}\bar{\phi}\right]\right. \\ &\quad\left. - \frac{e^{-i\phi/2}}{e^{-i\phi} - e^{-i\bar{\phi}}}\cos\left[\left|\int_x^0 p(x')dx'\right| - \frac{1}{2}\phi\right]\right\} . \end{aligned} \tag{20}$$

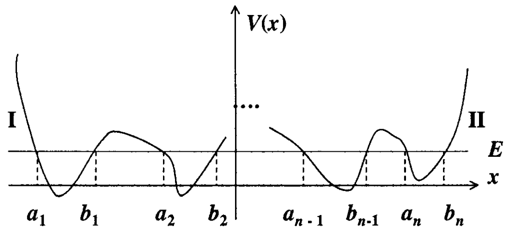

Fig. 2. A potential $V(x)$ with n wells. The turning points are denoted by a_i, b_i $(i = 1, 2, \ldots, n)$

It is clear that (19) connects the last terms of both sides of (20) provided that $-\frac{N}{2\bar{N}} e^{-i(\phi-\bar{\phi})/2} = i\frac{N^2 e^{-i\phi}}{e^{-i\phi}-e^{-i\phi}}$ or simply

$$N\bar{N} = \sin\frac{1}{2}(\phi - \bar{\phi}) \,. \tag{21}$$

This is the continuity condition of ref. [5]. Now the first terms of both sides of (20) 'connect' provided

$$\frac{1}{\sqrt{|p(x)|}} \exp\left(\left|\int_0^x p(x')dx'\right|\right) \to \frac{1}{\sqrt{|p(x)|}} \frac{1}{\bar{N}} \cos\left(\left|\int_x^0 p(x')dx'\right| - \frac{1}{2}\bar{\phi}\right) \,, \tag{22}$$

which is the second generalized connection formula. We had invoked (21) in writing (22). Formulas (19) and (22) are, in fact, the new generalized connection formulas [4].

3 Diagrammatic representation of the Green function

We now derive a diagrammatic representation for the Green function employing the rules of Table 1. In the case that the energy spectrum is discrete, the retarded Green function can be written as a sum over eigenfunctions, namely,

$$G(x_f, x_i, E) = \sum_k \frac{\Psi_k(x_f)\Psi_k^+(x_i)}{E - E_k}, \tag{23}$$

where we assume implicitly that E has a tiny imaginary part so the poles are in the lower half of the energy plane. Following Aoyama and Harano [7], we replace the wave functions by their WKB forms.

To fix our discussion, consider the propagation of a particle of mass m from x_i in region II to x_f in region I as shown in Fig. 2. The points a_1 and b_n denote the turning points nearest to these initial and final points. The WKB wave functions can be cast as

$$\frac{1}{\sqrt{|p|}}\left\{A_E \exp\left(i\int_x^{a_1} p(x')dx'\right) + B_E \exp\left(-i\int_x^{a_1} p(x')dx'\right)\right\}, x \in I,$$
$$\frac{1}{\sqrt{|p|}}\left\{C_E \exp\left(-i\int_{b_n}^{x} p(x')dx'\right) + D_E \exp\left(i\int_{b_n}^{x} p(x')dx'\right)\right\}, x \in II, \tag{24}$$

with the coefficients related by a 2×2 matrix $S(E)$ determined by the potential and the energy [12]:

$$\begin{pmatrix} A_E \\ B_E \end{pmatrix} = S(E) \begin{pmatrix} C_E \\ D_E \end{pmatrix}. \tag{25}$$

It will be useful to have an explicit form for the matrix $\tilde{S}(E)$ connecting region II to the region (b_{n-1}, a_n) [this differs from $S(E)$ of (25) which connects regions I and II]. Toward this end, we start with the wave function in II (we omit the factor $|p|^{1/2}$, for convenience),

$$\Psi_{II}(x) = C \exp\left(\int_{b_n}^{x} K(x')dx'\right) + D \exp\left(-\int_{b_n}^{x} K(x')dx'\right),$$
$$K = \sqrt{\frac{2m}{\hbar^2}(V - E)} \,. \tag{26}$$

By the connection formulas (19) and (22) we can write the wave function in the region (a_n, b_n) adjacent to II:

$$\begin{aligned}\Psi_{(a_n,b_n)}(x) &= \frac{C}{\bar{N}}\left[-\frac{\sin(W_n - \frac{1}{2}(\phi - \bar{\phi})}{\sin\frac{1}{2}(\phi - \bar{\phi})} \cos\left(\int_{a_n}^{x} p(x')dx' - \frac{1}{2}\bar{\phi}\right) + \frac{\sin(W_n - \bar{\phi})}{\sin\frac{1}{2}(\phi - \bar{\phi})} \cos\left(\int_{a_n}^{x} p(x')dx' - \frac{1}{2}\phi\right)\right] \\ &+ \frac{2D}{N}\left[\frac{\sin(W_n - \frac{1}{2}(\phi + \bar{\phi})}{\sin\frac{1}{2}(\phi - \bar{\phi})} \cos\left(\int_{a_n}^{x} p(x')dx' - \tfrac{1}{2}\phi\right) + \frac{\sin(W_n - \phi)}{\sin\frac{1}{2}(\phi - \bar{\phi})} \cos\left(\int_{a_n}^{x} p(x')dx' - \tfrac{1}{2}\bar{\phi}\right)\right]\end{aligned} \tag{27}$$

where $W_n = \int_{a_n}^{b_n} p(x')dx'$. A second application of the connection formulas now yields the wave function in the next adjacent zone, $\Psi_{(b_{n-1},a_n)}(x)$, from which we can extract the required matrix

$$\tilde{S}(E) = \begin{pmatrix} \frac{N}{2\bar{N}} \frac{\sin(W_n - \bar{\phi})}{\sin\frac{1}{2}(\phi - \bar{\phi})} e^{-\Delta_{n-1}} & \frac{\sin(W_n - \frac{1}{2}(\phi + \bar{\phi})}{\sin\frac{1}{2}(\phi - \bar{\phi})} e^{-\Delta_{n-1}} \\ -\frac{\sin(W_n - \frac{1}{2}(\phi + \bar{\phi})}{\sin\frac{1}{2}(\phi - \bar{\phi})} e^{\Delta_{n-1}} & -\frac{2\bar{N}}{N} \frac{\sin(W_n - \phi)}{\sin\frac{1}{2}(\phi - \bar{\phi})} e^{\Delta_{n-1}} \end{pmatrix} \tag{28}$$

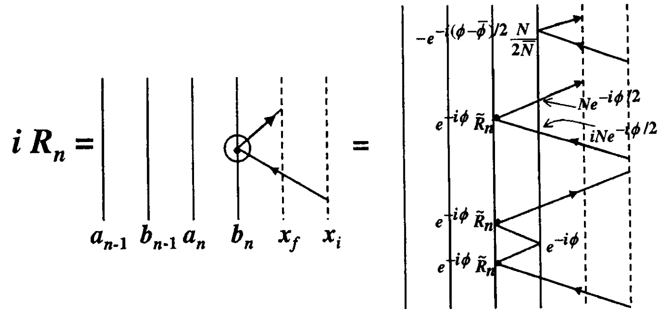

Fig. 3. Diagrammatic representation of iR_n (35). Physically the particle undergoes reflection at b_n (top diagram, right) and oscillates in the region (a_n, b_n) [remaining diagrams]

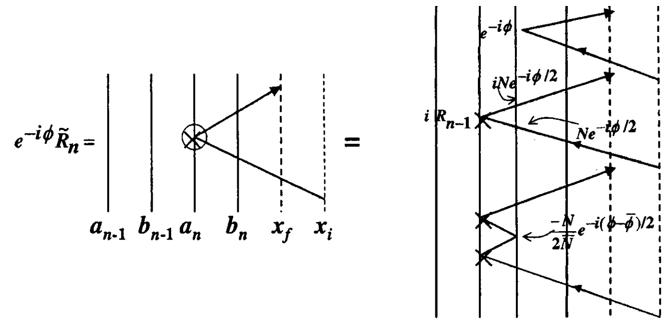

Fig. 4. Diagrammatic representation of $e^{-i\phi}\tilde{R}_n$ (36). Physically, the particle reflects at a_n and also undergoes tunneling reflections in the region (b_{n-1}, a_n)

where $\Delta_{n-1} = \int_{b_{n-1}}^{a_n} |p(x')dx'|$.

Aoyama and Harano [7] have calculated (23) for the retarded Green function for propagation from x_i to x_f where both points are in the forbidden zone in II and $x_i > x_f$. Their result is

$$G^R\left(x_i^{II}, x_f^{II}, E\right) = -\left|p(x_i)p(x_f)\right|^{-1/2} e^{-\Delta_i}\left(e^{\Delta_f} + iR_n e^{-\Delta_f}\right), \quad (29)$$

where the reflection coefficient has been defined by

$$R_n = i\frac{S_{21}^{(n)}}{S_{22}^{(n)}}, \quad (30)$$

and $\Delta_{i,f} = \int_{b_n}^{x_{i,f}} |p(x')dx'|$. The superscript n reminds us that there are n wells in the potential. If x_i and x_f lie on opposite sides of the wells, then, their result is

$$G^R(x_i^{II}, x_f^{I}, E) = -\left|p(x_i)p(x_f)\right|^{-1/2} T_n e^{-\Delta_i} e^{-\Delta'_f}, \quad (31)$$

where $\Delta'_f = \int_{x_f}^{x_i} |p(x')dx'|$ and the transmission coefficient has been introduced,

$$T_n = \frac{1}{S_{22}^{(n)}}\,. \quad (32)$$

In the above, the matrix $S^{(n)}$ connects regions I and II and it can be written as a product of the matrix $S^{(n-1)}$ which connects region I to the region (b_{n-1}, a_n) and the matrix $\tilde{S}(E)$ which links the region (b_{n-1}, a_n) with region II.

We calculate the reflection coefficient R_n and the transition amplitude T_n and show that their diagrammatic representations consistent with Table 1 can be drawn. The importance of diagrams has been noted by Carlitz and Nicole and by Millard [6]: through them we have a physical criterion with which to study the dominant scattering mechanism and to adequately strengthen the weakness inherent in the stationary phase approximation. We start with the reflection coefficient defined by (30):

$$R_n = i\left\{S_{21}^{(n-1)}\tfrac{N}{2\bar{N}}\sin\left(W_n - \bar{\phi}\right)e^{-\Delta_{n-1}} - S_{22}^{(n-1)}\right.$$
$$\left.\times\sin\left[W_n - \tfrac{1}{2}\left(\phi + \bar{\phi}\right)\right]e^{\Delta_{n-1}}\right\}\Big/\left\{S_{21}^{(n-1)}\right.$$
$$\times\sin\left(W_n - \tfrac{1}{2}(\phi + \bar{\phi})\right)e^{-\Delta_{n-1}} - S_{22}^{(n-1)}\tfrac{2\bar{N}}{N}$$
$$\left.\times\sin\left[W_n - \phi\right]e^{\Delta_{n-1}}\right\}$$
$$= i\frac{N}{2\bar{N}}e^{-i(\phi-\bar{\phi})/2}\frac{1 - \tilde{R}_n e^{2iW_n}e^{-i(\phi+\bar{\phi})}}{1 - \tilde{R}_n e^{2iW_n}e^{-2i\phi}}, \quad (33)$$

where

$$\tilde{R}_n = \frac{1 - \frac{N}{2i\bar{N}}e^{i(\phi-\bar{\phi})}R_{n-1}e^{-2\Delta_{n-1}}}{1 - \frac{N}{2i\bar{N}}e^{-i(\phi-\bar{\phi})}R_{n-1}e^{-2\Delta_{n-1}}}. \quad (34)$$

If we now expand (33) in the form

$$iR_n = -\frac{N}{2\bar{N}}e^{-i(\phi-\bar{\phi})/2}e^{-i(\phi-\bar{\phi})/2} + \left(e^{-i\phi}\tilde{R}_n\right)e^{2iW_n}\left(iN^2e^{-i\phi}\right) + \left(e^{-i\phi}\tilde{R}_n\right)^2 e^{4iW_n}\left(iN^2e^{-i\phi}\right)e^{-i\phi} + \ldots \quad (35)$$

we obtain immediately the diagrammatic representation given in Fig. 3. The first at the top (right diagram) corresponds to a direct reflection at the turning point b_n. The other paths have oscillations in the nth well; $e^{-i\phi}\tilde{R}_n$ contains information on the region left of a_n. Similarly for (35):

$$e^{-i\phi}\tilde{R}_n = e^{-i\phi} + ie^{-i\phi}N^2(iR_{n-1})e^{-2\Delta_{n-1}} - \frac{N}{2\bar{N}} \times e^{-i(\phi-\bar{\phi})/2}ie^{-i\phi}N^2(iR_{n-1})e^{-4\Delta_{n-1}} + \ldots \quad (36)$$

which is shown in Fig. 4. As with the case of Fig. 3, each diagram corresponds to a group of paths that oscillate in the forbidden zone (b_{n-1}, a_n). The explicit case of iR_1 is

$$iR_1 = -\frac{N}{2\bar{N}}e^{-i(\phi-\bar{\phi})/2} + \left(iN^2e^{-i\phi}\right)e^{-i\phi}e^{2iW_n} + \left(iN^2e^{-i\phi}\right)\left(e^{-i\phi}\right)^3 e^{4iW_n} + \ldots \quad (37)$$

which is easily rendered in diagrammatic form and is omitted.

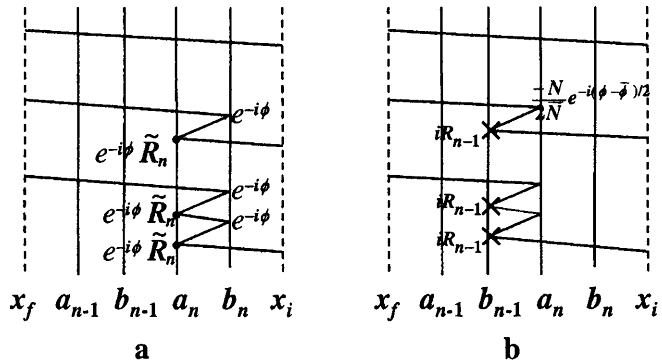

Fig. 5a,b. Interpretation of the factors in (39) in terms of classical paths involving passage through **a** the nth well and **b** tunneling within the $(n-1)$st barrier

Let us next look at the transmission coefficient:

$$T_n = iN^2 e^{-i\phi} \frac{e^{-\Delta_{n-1}}}{1 - \frac{N}{2i\bar{N}} R_{n-1} e^{-2\Delta_{n-1}} e^{-i(\phi-\bar{\phi})/2}} \cdot \frac{e^{iW_n}}{1 - \tilde{R}_n e^{2iW_n} e^{-2i\phi}} T_{n-1}, \tag{38}$$

$\Delta_{n-1} = \int_{b_{n-1}}^{a_n} |p(x')|\, dx'$, whose factors can be rendered diagrammatically as shown in Fig.5a and b, respectively:

$$\frac{e^{iW_n}}{1 - \tilde{R}_n e^{2i(W_n-\phi)}} = e^{iW_n} + \tilde{R}_n e^{-2i\phi} e^{3iW_n} + (\tilde{R}_n e^{-2i\phi})^2 e^{5iW_n} + ...,$$
$$\frac{e^{-\Delta_{n-1}}}{1 - \frac{N}{2i\bar{N}} R_{n-1} e^{-2\Delta_{n-1}} e^{-i(\phi-\bar{\phi})/2}} = e^{-\Delta_{n-1}} + \frac{N}{2i\bar{N}} R_{n-1} e^{-3\Delta_{n-1}} e^{-i(\phi-\bar{\phi})/2} + \left(\frac{N}{2i\bar{N}}\right)^2 R_{n-1}^2 e^{-5\Delta_{n-1}} e^{-i(\phi-\bar{\phi})} + ... \tag{39}$$

The first factor above involves oscillations in the allowed region (a_n, b_n) while the second tunneling back and forth in the forbidden zone (b_{n-1}, a_n). We also have an expansion for T_1:

$$T_1 = iN^2 e^{-i\phi} e^{iW} \left[1 + e^{-2i\phi} e^{2iW} + e^{-4i\phi} e^{4iW} + ...\right] \tag{40}$$

As the diagrams show, both R_n and T_n can be given diagrammatically in terms of classical paths.

4 Applications

We give two examples of the use of the above methods. To distinguish the phases and weights at the left and right turning points we append the subscripts l and r.

For the transmission of a particle through a potential barrier $V(x)$ with two classical turning points x_l and x_r with $V(x)$ approaching constant values as $x \to \pm\infty$, we have the diagrams given in Fig. 6. From Table 1 the corresponding expression for the transmission amplitude is the geometric series

$$T = e^{-i\phi_l/2} N_l e^{-\Delta} i e^{-i\phi_r/2} N_r + N_l e^{-i\phi_l/2} e^{-\Delta} \times \left(\frac{N_r}{2\bar{N}_r}\right)\left(-e^{-i(\phi_r-\bar{\phi}_r)}\right) e^{-\Delta} \left(\frac{N_l}{2\bar{N}_l}\right)\left(-e^{-i(\phi_l-\bar{\phi}_l)}\right) \times e^{-\Delta} i e^{-i\phi_r/2} N_r + ... = \frac{iN_l N_r}{e^{\Delta} e^{i(\phi_l+\phi_r)/2} - \frac{N_l}{\bar{N}_l}\frac{N_r}{\bar{N}_r}\frac{1}{4\Delta} e^{i(\bar{\phi}_l+\bar{\phi}_r)}}. \tag{41}$$

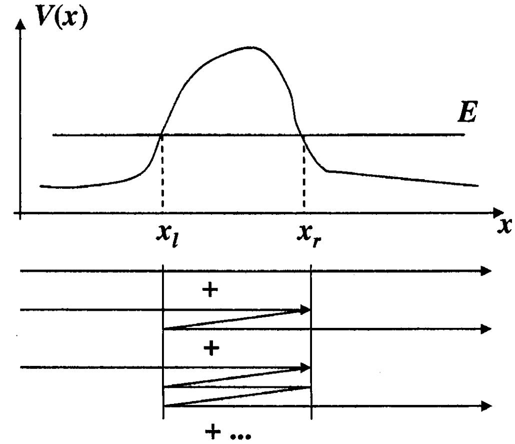

Fig. 6. Tunneling across a potential barrier interpreted as a sum of complex-time paths inside the barrier

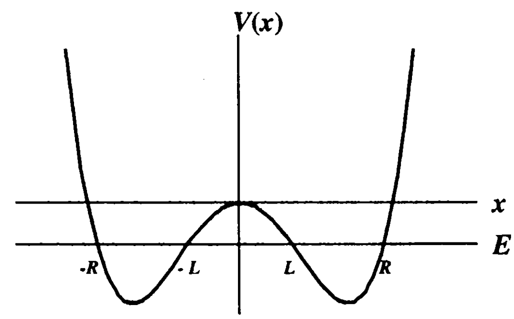

Fig. 7. Particle with energy E in a double well potential with turning points labeled $\pm\, L$ and $\pm.\, R$

Here $\Delta = \int_{x_l}^{x_r} |p(x')|\, dx'$. This is exactly the result of Eltschka et al. [3], which they derived via the classical WKB way (using the generalized connection formulas).

Let us now take the symmetrical double well of Fig. 7. There are four turning points. We assume that at each of these $N = \bar{N}$ and $\phi = -\bar{\phi}$ so that $N\bar{N} = N^2 = \sin\phi$. Using (38) and with $n = 2$, we obtain

$$T_2 = iN_R N_L e^{-i\phi_R/2} e^{-i\phi_L/2} \cdot \frac{e^{-\Delta}}{1 - \frac{1}{2i} R_1 e^{-2\Delta} e^{i\phi_L}} \cdot \frac{e^{iW_1}}{1 - \tilde{R}_2 e^{2iW_1} e^{-i(\phi_L+\phi_R)}} T_1\,, \tag{42}$$

where

$$iR_1 = -\frac{1}{2}\frac{\sin\left[\frac{1}{2}(\phi_L - \phi_R) - W_1\right]}{\sin\left[\frac{1}{2}(\phi_L + \phi_R) - W_1\right]},$$
$$\tilde{R}_2 = \frac{1 - \frac{1}{2i}e^{i\phi_L}R_1 e^{-2\Delta}}{1 - \frac{1}{2i}e^{-i\phi_L}R_1 e^{-2\Delta}},$$
$$T_1 = \frac{N_R N_L}{2\sin\left[\frac{1}{2}(\phi_L + \phi_R) - W_1\right]}, \qquad (43)$$

in which $\Delta = \int_{-L}^{L} |p(x')|\, dx'$, and $W_1 = \int_{L}^{R} |p(x')|\, dx'$. The energy splitting can be computed:

$$\Delta E \cong \frac{1}{\tau}\frac{e^{-\Delta}\left(\sin\phi_L \sin\phi_R\right)^{1/2}}{1 - \frac{1}{8}e^{-2\Delta}\cos(\phi_L + \phi_R)}, \qquad (44)$$

where $\tau = \int_L^R dx\sqrt{\frac{2m}{(E-V)}}$ is the classical period. This is to be compared with Park et al's [5] result. Their result must be in error because when $\phi_L + \phi_R$ is a multiple of 2π theirs gives a lifetime that is proportional to $e^{+\Delta}$.

5 Outlook

We have shown how the generalized connection formulas for tunneling through a potential barrier can be obtained from a semi-classical approximation of the path integral. We also showed that a diagrammatic representation of the Green function in terms of contributions from classical paths is possible. The applications to barrier penetration and the double well in Sect. 4 give an indication of the utility and directness of the method. Where can we go from here? As we had noted in the introduction, the method generalizes the WKB approximation to situations in which the momentum is small. There are a number of interesting situations at present where this is important, for instance ref. [13]. Applications to field theory may also be carried out, as for instance, the study of properties of instantons when they are not infinitely far apart (that is, questions relating to the validity of the 'dilute gas approximation' [8, 14]).

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