Complex-time approach for semi-classical quantum tunneling

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ABSTRACT

The complex-time method for quantum tunneling is studied. In one-dimensional quantum mechanics, we construct a reduction formula for a Green function in the number of turning points based on the WKB approximation. This formula yields a series, which can be interpreted as a sum over the complex-time paths. The weights of the paths are determined.

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The imaginary-time method is quite useful for study of the tunneling phenomena in quantum field theories. Existence of the solutions of the equation of motion, instanton and bounce, allows one to apply the semi-classical approximation for path-integral. It is known to lead to valid results, which one can confirm in the WKB approximation in quantum mechanical models. Its range of applicability is, however, somewhat limited: In the case when there are degenerate vacua, the ordinary instanton calculation gives the right level-splitting only for the lowest-lying states. In the case of the decay of the metastable states, the decay formula is valid for the lowest meta-stable state, the false “vacuum”. These points were investigated by many authors in recent years, especially in relation with tunneling phenomena in high energy scattering, namely, the baryon and lepton number violation.\cite{1} As a result, interacting-instanton method\cite{2} and valley methods\cite{3–5} became known to be useful.

Rubakov, et. al.\cite{6} proposed use of a complex-time method as an alternative. In such a formalism, the external lines “live” in real-time, while the tunneling is carried out in imaginary time, thus the interplay between the initial conditions and the tunneling configuration is expected to be straightforward,\cite{7} unlike the cases when the time is purely imaginary.

Complex-time method is studied extensively in toy models in the one-dimensional quantum mechanics.\cite{8−13} It was argued to overcome the many shortcomings of the imaginary time method.\cite{14} However, even in the simple toy models, the formalism is full of the ambiguities and mysteries. It is the purpose of this letter to expose those points and solve those mysteries, thereby establishing the sound basis of the complex-time method, on which decent treatment of the quantum field theory should be done.

In its most successful formulation,\cite{15} one considers the analytic continuation of the time-integral in Fourier-transform of the the fixed-energy Green functions (resolvents). We consider the one-dimensional quantum mechanics of a particle of unit mass in a potential $V(x)$ assumed to be smooth enough to allow WKB
approximation. We assume that it has asymptotic regions I and II and also in a wide intermediate region III as in Fig.1. The retarded resolvent (the fixed-energy Green function) is defined by the following;

\[
G^R(x_i, x_f; E) = \langle x_f | \frac{1}{E + i\delta - H} | x_i \rangle = -i \int_0^{\infty} dT e^{i(E+i\delta)T} \langle x_f | e^{-iHT} | x_i \rangle .
\]  

(1)

This is useful as energy spectra is obtained from the poles and cuts of the above. Complex-time is introduced by deforming the \(T\)-integration contour in (1): If any saddle point(s) exist in the complex \(T\)-plain, one tries to deform the integration contour so that it goes through the saddle point(s).

Easiest to find among the saddle points are the physical ones: Using the path-integral expression

\[
\langle x_f | e^{-iHT} | x_i \rangle = i \int_{x(0)=x_i}^{x(T)=x_f} Dx e^{iS},
\]  

(2)

The resolvent (1) is written as a double-integral over \(T\) and \(x(t)\). One then requires saddle-point condition for both \(T\) and \(x(t)\). The former leads to the energy conservation law and the latter the equation of motion. If the initial point \(x_i\) is in the allowed region, a solution \(x(t)\) starts from \(t = 0\) and moves along the real axis of \(t\). When it hits a turning point, it can turn around or start moving into the forbidden region with \(t\) moving along the imaginary axis. Corresponding to the choice of the move at turning points, there are infinite of such saddle points. It was proposed that all such saddle points should be taken into account with specific weights.

Closer look of this method reveals many unanswered questions. The complex \(T\)-plane is plagued with singularities and infinite number of saddle points. Among saddle points, there are the ones that cannot be obtained from the above procedure (which we shall call “unphysical saddle points”). Both of the physical and unphysical saddle points are distributed on infinite lattice structures. How the
path is deformed to avoid the singularities and go through only the physical saddle points is unknown. Instead, one simply assumes that all the physical saddle points contribute. Even so, the weight of each saddle point is a mystery. They are determined so that results agree with that of the WKB approximation. It is not known how they come about from the path.

In order to investigate the situation, we shall construct the Green function from the complete orthonormal set of the WKB-eigenfunctions of the Hamiltonian. For a state with the eigenvalue $\lambda$ in the continuum spectrum, the second-order WKB approximation yields the following;

$$
\psi_\lambda(x) = \frac{1}{\sqrt{2\pi p(x)}} \times \begin{cases} 
A_\lambda e^{i \int_x^{a_1} p(x') dx'} + B_\lambda e^{-i \int_x^{a_1} p(x') dx'}, & \text{for } x \in I, \\
C_\lambda e^{-i \int_x^{b_2} p(x') dx'} + D_\lambda e^{i \int_x^{b_2} p(x') dx'}, & \text{for } x \in II,
\end{cases}
$$

(3)

where $p(x) = \sqrt{2(\lambda - V(x))}$. Among the coefficients $A$, $B$, $C$, and $D$, only two are independent. Their inter-relation can be summarized in the following relation;\(^{[16]}\)

$$
\begin{pmatrix}
A_\lambda \\
B_\lambda
\end{pmatrix} = S(\lambda) 
\begin{pmatrix}
C_\lambda \\
D_\lambda
\end{pmatrix},
$$

(4)

The $2 \times 2$ matrix $S(\lambda)$ is determined by the shape of the potential $V(x)$ in the intermediate region. The flux conservation law allows the following general parametrization;

$$
S(\lambda) = \begin{pmatrix}
e^{i\alpha} \cosh \rho & e^{i\beta} \sinh \rho \\
e^{-i\beta} \sinh \rho & e^{-i\alpha} \cosh \rho
\end{pmatrix},
$$

(5)

where $\alpha$, $\beta$ and $\rho$ are real functions of $\lambda$. For a given value of $\lambda$, there are two eigenfunctions. We can show that one orthonormal choice is the following;

$$
(A_\lambda, B_\lambda, C_\lambda, D_\lambda)^{(1)} = \sqrt{2} \begin{pmatrix}
e^{i\alpha} \cosh \rho, & 0, & 1, & -e^{i(\alpha-\beta)} \tanh \rho
\end{pmatrix},
$$

(6)

$$
(A_\lambda, B_\lambda, C_\lambda, D_\lambda)^{(2)} = \sqrt{2} \begin{pmatrix}
e^{i(\alpha+\beta)} \tanh \rho, & 1, & 0, & e^{i\alpha} \cosh \rho
\end{pmatrix}.
$$

4
The Green function is written as an integration over continuous $\lambda$ and sum over the discrete spectrum. This results in the following expression in case $x_i, x_f \in \Pi$ as in Fig.1:

$$G(x_i, x_f; E) = -|p(x_i)p(x_f)|^{-1/2}e^{-\Delta_i} \left(e^{\Delta_i} + iRe^{-\Delta_i}\right). \quad (7)$$

where the argument is $\lambda = E$ and $R \equiv iS_{21}/S_{22}$ is essentially the (analytically-continued) reflection amplitude for the incoming wave from the right asymptotic region II. The exponents are given by

$$\Delta_{i,f} = \int_{b_2}^{x_{i,f}} dx |p(x)|. \quad (8)$$

Due to the existence of the intermediate region III, the matrix $S$, which connects the regions I and II, can be written in terms of the matrices $S_1$ that connects regions I and III and $S_2$ for III and II. More specifically, we apply the linear WKB connection formula for the latter region and obtain

$$S = S_1 \left( \begin{array}{cc} \frac{1}{2}e^{-\Delta_1} \cos W_2 & e^{-\Delta_1} \sin W_2 \\ -e^{-\Delta_1} \sin W_2 & 2e^{\Delta_1} \cos W_2 \end{array} \right) \quad (9)$$

where $W_2$ and $\Delta_1$ are defined by,

$$W_2 = \int_{a_2}^{b_2} dx p(x), \quad \Delta_1 = \int_{b_1}^{a_2} dx |p(x)|. \quad (10)$$

Using the above, we arrive at the following expressions;

$$iR = \frac{i}{2} \frac{1 - \tilde{R}_2 e^{2iW_2}}{1 + \tilde{R}_2 e^{2iW_2}} = \frac{i}{2} + (-i\tilde{R}_2)e^{2iW_2} + (-i)(-i\tilde{R}_2)^2e^{4iW_2} + ..., \quad (11)$$

$$-i\tilde{R}_2 = -i \frac{1 - \frac{1}{2}R_1 e^{-2\Delta_1}}{1 + \frac{1}{2}R_1 e^{-2\Delta_1}} = (-i) + (iR_1)e^{-2\Delta_1} + \frac{i}{2}(iR_1)^2e^{-4\Delta_1} + ..., \quad (12)$$

where $R_1$ is the reflection amplitude at the turning point $b_1$. 
We prove that the reduction formula (11) and (12) is equivalent to summation over the classical complex-time paths: Let us first look at the expansions of the resolvents in (11). [The convergence of this expansion is guaranteed by $\delta$.] The phase $W_2$ is equal to $ET + S$ of the real-time solution between the turning points $a_2$ and $b_2$. The factor $i/2$ is the phase and weight at the turning point, where the path approaches from the forbidden region and turns around. When the path hits the turning point from the allowed region and turns around, it picks up the phase $-i$. Thus the series can be understood as the sum over the paths that goes through the allowed region $(a_2, b_2)$ different times (see Fig.2). Similarly, $\Delta_1$ is $-E\tau + S_E$ and the expansion in (12) can be understood as the summation over paths for the forbidden region $(b_1, a_2)$ (Fig.3). The reflection coefficient $R_1$ itself can be expressed as the sum over the oscillation in $(a_1, b_1)$. Combined, they produce the sum over the different ways the paths goes back and forth between $(a_1, b_2)$. We thus prove that the sum is only over the physical paths. At the same time, the weights and phases are completely determined by these expansions. We have also looked at the case when $x_i$ and $x_f$ belong to different asymptotic regions. We have proven also that it can be obtained by the sum over the physical paths with the specified formula for the phase and the weight.

As a summary, we have shown the Green function is cast in the form of sum only over the physical paths. We have derived the general rule for the weights and phases for each paths. These coincide the rules assumed by Carlitz and Nicole and correctly reproduce the WKB energy-level condition and the decay formula. As the above procedure is reductive in its nature, our proof is valid for potentials with more turning points. Although we have used the linear WKB connection formula in this letter, using the quadratic formula, for the purpose of investigating the lower energy spectrum, should be straightforward, as our method is solely based on the reduction of the matrix $S$. We should stress that the weight $1/2$ for the turn around in the allowed region is problematical for the path-integral: How it is obtained from a path that goes through all the saddle points is unknown. What we have done here is to justify a hybrid method, where we apply the path-integral
method for the elementary processes and then combine them using the knowledge of the wavefunction. In view of the fact that the weights are now fixed by our analysis, the path-integral method should be more seriously considered, as this should open ways for decent treatment of the tunneling phenomena in field theories. Detail of the analysis will be published in near future.\cite{17}
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FIGURE CAPTIONS

1) A potential $V(X)$ with asymptotic region I and II and wide intermediate region III, where WKB approximation is valid.

2) Diagrammatic view of the expansion of (11) in terms of $\tilde{R}_2$.

3) Diagrammatic view of the expansion of (12) in terms of $R_1$. 
Fig. 1

$V(x)$

$I$  $II$  $III$

$E$

$x$

$a_1$  $b_1$  $a_2$  $b_2$  $x_f$  $x_i$

$iR$

$a_1$  $b_1$  $a_2$  $b_2$  $x_f$  $x_i$
\[
\begin{align*}
\alpha_1 b_1 a_2 b_2 x_f x_i &= -i \tilde{R}_2 \\
\Rightarrow &= -i + iR_1 + iR_1 + \frac{i}{2} + \cdots
\end{align*}
\]