Semiclassical theory of nonadiabatic transitions in a two-state exponential model

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A general two-state exponential potential model is solved with use of the Bessel transformation and the WKB (Wentzel-Kramers-Brillouin) type semiclassical approximation. Accurate expressions are obtained for the nonadiabatic transition probability for one passage of the transition point and for the two dynamical phases. Functionalities of these quantities in terms of two basic parameters are the same as those obtained before by Nikitin. The two basic parameters are, however, expressed in more general and accurate forms. Accuracies of these expressions are numerically confirmed. The three quantities, the nonadiabatic transition probability and the two dynamical phases, constitute the nonadiabatic transition matrix and can be used to describe various (spectroscopic as well as scattering) processes not only for a two-state but also for a multichannel system. A possible generalization of the present theory is also briefly discussed to formulate a unified theory that can cover both Landau-Zener-Stueckelberg and Rosen-Zener-Demkov cases within the adiabatic state representation. [S1050-2947(98)07504-0]

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I. INTRODUCTION

It is well known that nonadiabatic transitions present one of the most essential mechanisms of state and/or phase changes in various physical, chemical, and biological systems [1–5]. The most fundamental models among them are the Landau-Zener-Stueckelberg (LZS) type curve crossing and the Rosen-Zener-Demkov (RZD) type noncrossing problems. Recently, the Landau-Zener-Stueckelberg type problem has been completely solved by Zhu and Nakamura; and the compact and accurate analytical formulas have been derived for both Landau-Zener and nonadiabatic tunneling (NT) type crossings [5–8]. They can cover practically the whole ranges of energy and coupling strength. Besides, this theory does not require any nonunique diabatization procedure and information of any coupling, neither diabatic nor nonadiabatic. What is required is the information of adiabatic potentials on the real axis. On the other hand, the most basic model of the Rosen-Zener-Demkov type noncrossing problem, i.e., constant diabatic potentials coupled by an exponential potential, was solved quantum mechanically exactly by Osherov and Voronin [9].

It is interesting to note that the nonadiabatic transition probability for one passage of the transition point at low energies is given by

$$p=e^{-\Delta}, \tag{1.1}$$

where Δ is the imaginary part of complex phase integral, for both LZS and RZD cases [1,2,4,5]. At high energies the probability in the LZS case is still given by Eq. (1.1) and goes to unity in the $E\rightarrow\infty$ limit; in the RZD case, on the other hand, p is given by

$$p=\frac{e^{-\Delta}}{1+e^{-\Delta}}, \tag{1.2}$$

and goes to 1/2 in the limit. Interestingly, in the exponential model (two exponential diabatic potentials coupled by an exponential potential) the corresponding probability contains two parameters and can cover both LZS and RZD cases mentioned above in the high-energy limit [1]. This suggests that it might be possible to formulate a unified theory based on the exponential model.

It was Nikitin who solved an exponential model for the first time within the framework of time-dependent semiclassical theory based on the linear trajectory approximation [1,10–12]. Recently, the exact quantum mechanical solution was obtained for a special case of the exponential model [13,14]. Based on these achievements we want to eventually formulate a unified theory that relies only on phase integrals along the adiabatic potentials and can be free from any exponential potential parameters. Our main concern is the following nonadiabatic transition matrix in the adiabatic representation:

$$\begin{pmatrix} \sqrt{1-p}\,e^{-\varphi} & \sqrt{p}\,e^{i\psi} \\ -\sqrt{p}\,e^{-i\psi} & \sqrt{1-p}\,e^{i\varphi} \end{pmatrix}, \tag{1.3}$$

where p is the nonadiabatic transition probability for one passage of the avoided crossing point, and φ and ψ represent the accompanying phases called dynamical phases. This matrix represents a transition at the crossing point in the incoming (from right to left) segment of the two-state scattering process. It should be noted that the adiabatic state 1 corresponds to the lower one [see Eq. (2.2)]. Once we obtain these quantities (p,φ,ψ), then not only the whole two-state process but also multichannel problems can be formulated [4–8]. In the present work we solve the time-independent two-state exponential potential problem with use of the Bessel transformation and the WKB (Wentzel-Kramers-Brillouin) type semiclassical approximation. The above three quantities are expressed in terms of two parameters, as is known, which are found to be expressed in terms of contour integrals in momentum space. They can be generalized to forms of the phase integral along adiabatic potentials. Accuracies of these expressions are confirmed by using quantum mechanically exact numerical solutions and analytical solutions for the special case.

This paper is organized as follows. Our model discussed in this paper is explained in Sec. II. In Sec. III the problem is transformed into the momentum space by the Bessel transformation and the WKB type wave functions are derived. In Sec. IV the nonadiabatic transition matrix is expressed in terms of the two parameters that are defined by contour integrals in the momentum space. Section V summarizes the semiclassical theory convenient for practical applications. Some numerical examinations are presented in Sec. VI. Concluding remarks and discussions for the final goal of the present project are provided in Sec. VII. Derivations of some formulas presented in the text are summarized in Appendixes.

II. BASIC MODEL

A. Model potential system

Model diabatic potentials considered in this paper are defined by

$$H_{11}(x)=u_1-V_1e^{-\alpha x},$$
$$H_{22}(x)=u_2-V_2e^{-\alpha x}, \tag{2.1}$$
$$H_{12}(x)=Ve^{-\alpha x},$$

where $H_{jj}(x)(j=1,2)$ are the diabatic potentials, $H_{12}(x)$ represents a coupling between them, and the parameters are assumed to satisfy the relations, $u_1>u_2$, $V_1>V_2>0$, and $V>0$. Adiabatic potentials and the diabatic-adiabatic transformation are given as usual by

$$u_j^a(x)=\frac{1}{2}[H_{11}(x)+H_{22}(x)]\pm\left[\left(\frac{H_{11}(x)-H_{22}(x)}{2}\right)^2+H_{12}^2(x)\right]^{1/2}\quad [j=1(2)\quad \text{for}\quad -(+)], \tag{2.2}$$

$$\begin{pmatrix}\varphi_1(x)\\ \varphi_2(x)\end{pmatrix}=T\begin{pmatrix}\psi_1(x)\\ \psi_2(x)\end{pmatrix}, \tag{2.3}$$

$$T=\begin{pmatrix}\cos g, & -\sin g\\ \sin g, & \cos g\end{pmatrix} \tag{2.4}$$

with

$$\sin 2g=2H_{12}(x)/[u_2^a(x)-u_1^a(x)], \tag{2.5}$$

where $\varphi_j(\psi_j)(j=1,2)$ represent adiabatic (diabatic) wave functions.

The diabatic potential crossing occurs at

$$x_c^d=-\frac{1}{\alpha}\ln\frac{u_1-u_2}{V_1-V_2} \tag{2.6}$$

and the corresponding complex crossing point is given by

$$x_*=-\frac{1}{\alpha}\ln\left[\frac{(u_1-u_2)/2V}{1+[(V_1-V_2)/2V]^2}\left(\frac{V_1-V_2}{2V}\pm i\right)\right]. \tag{2.7}$$

It should be noted that the potentials exponentially negatively diverge at $x\rightarrow-\infty$. The main purpose of the present work is to derive a general expression for the so-called nonadiabatic transition matrix [Eq. (1.3)] which provides transition amplitudes at the avoided crossing. If necessary, we can put repulsive potential walls at $x<0$ to describe a scattering process in radial coordinate.

B. Relation to the Nikitin's model

Nikitin solved an exponential model within the time-dependent framework in which the coordinate is a linear function of time t [1,10–12]. In this treatment only the difference between the two adiabatic potentials is important and it is given by

$$\Delta U(t)=\Delta\epsilon[1-2\cos 2\theta_0 e^{-\alpha vt}+e^{-2\alpha vt}]^{1/2}, \tag{2.8}$$

where v represents the velocity, and $\Delta\epsilon$ and θ_0 are the basic parameters.

In the present model we have

$$\Delta u^a(x)=(u_1-u_2)[1-2B\cos 2\theta_0 e^{-\alpha x}+B^2e^{-2\alpha x}]^{1/2} \tag{2.9}$$

with

$$B\cos 2\theta_0=(V_1-V_2)/(u_1-u_2)$$

and

$$B\sin 2\theta_0=2V/(u_1-u_2). \tag{2.10}$$

If we put $B=e^{\alpha x_0}$, then the coordinate x is shifted by x_0 and Eq. (2.9) is essentially the same as Eq. (2.8). It should be noted, however, that we deal with the time-independent quantum mechanical problem in this paper. Thus the basic parameters appearing in the nonadiabatic transition matrix are more general than those in the Nikitin's treatment.

III. BESSEL TRANSFORMATION AND SEMICLASSICAL WAVE FUNCTIONS

A. Bessel transformation

If we introduce the following variable and parameters,

$$\rho^2=\frac{8mV}{\hbar^2\alpha^2}e^{-\alpha x}, \tag{3.1a}$$

$$\nu^2=\frac{8m}{\hbar^2\alpha^2}(E-u_1),\quad \mu^2=\frac{8m}{\hbar^2\alpha^2}(E-u_2), \tag{3.1b}$$

and

$$\beta_j=V_j/V\quad (j=1,2), \tag{3.1c}$$

then the basic coupled Schrödinger equations are expressed as

$$\left[\rho^2 \frac{d^2}{d\rho^2}+\rho \frac{d}{d\rho}+\nu^2+\beta_1\rho^2\right]\psi_1=\rho^2\psi_2, \tag{3.2a}$$

$$\left[\rho^2 \frac{d^2}{d\rho^2}+\rho \frac{d}{d\rho}+\mu^2+\beta_2\rho^2\right]\psi_2=\rho^2\psi_1. \tag{3.2b}$$

Here m represents the reduced mass of the system.

In the special case $\beta_1\beta_2=1$ or $V_1V_2=V^2$, we can solve Eqs. (3.2) exactly in terms of the Meijer's G functions [13]. In order to solve Eqs. (3.2) approximately, we first move into the momentum space by using the Bessel transformation,

$$\psi_j(\rho)=\int_C pF_j(p)Z_{i\nu}(\rho p)dp, \tag{3.3}$$

where $Z_{i\nu}(z)$ is a Bessel function, which satisfies

$$\left[z^2 \frac{d^2}{dz^2}+z \frac{d}{dz}+z^2+\nu^2\right]Z_{i\nu}(z)=0. \tag{3.4}$$

Putting

$$F_1(p)=\frac{f_1(p)}{p^{1/2}(p^2-a_1)(p^2-a_2)} \tag{3.5}$$

with

$$a_{1,2}=\frac{1}{2}(\beta_1+\beta_2)\mp\left[\left(\frac{\beta_1-\beta_2}{2}\right)^2+1\right]^{1/2}, \tag{3.6}$$

we obtain the following differential equation for $f_1(p)$:

$$\left[\frac{d^2}{dp^2}+\frac{1+4\mu^2}{4}\frac{p^4-4\epsilon p^2+\lambda}{p^2(p^2-a_1)(p^2-a_2)}\right]f_1(p)=0, \tag{3.7}$$

where

$$\epsilon=\frac{\frac{1}{4}(\beta_1+\beta_2)+(\beta_2\nu^2+\beta_1\mu^2)}{1+4\mu^2} \tag{3.8}$$

and

$$\lambda=\frac{(\beta_1\beta_2-1)(1+4\nu^2)}{1+4\mu^2}. \tag{3.9}$$

The function $F_2(p)$ is simply obtained from $F_1(p)$ by

$$F_2(p)=(\beta_1-p^2)F_1(p). \tag{3.10}$$

The integral contour C in Eq. (3.3) should be chosen so that the following conditions are satisfied:

$$F_j(p)\frac{dZ_{i\nu}}{dp}p^n\Big|_C=0 \quad (n=1,3),$$

$$\frac{d}{dp}(F_j(p)p^n)Z_{i\nu}\Big|_C=0 \quad (n=1,3), \tag{3.11}$$

$$F_j(p)p^nZ_{i\nu}\Big|_C=0 \quad (n=0,2).$$

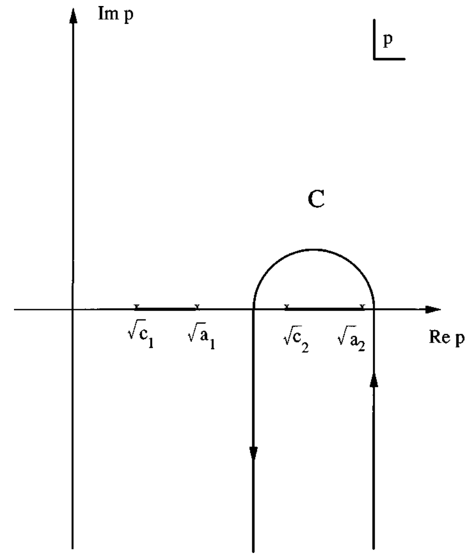

FIG. 1. The integral contour C to define the wave function ψ_1 [see Eq. (3.16)].

B. Semiclassical wave functions

In this subsection we derive general expressions of the wave functions ψ_1 and ψ_2 under the condition of $\mu^2,\nu^2\gg 1$. Under this condition Eq. (3.7) can be rewritten as

$$\left[\frac{d^2}{dp^2}+P_0(p)\right]f_1(p)=0 \tag{3.12}$$

with

$$P_0(p)=\mu^2\frac{(p^2-c_1)(p^2-c_2)}{p^2(p^2-a_1)(p^2-a_2)}, \tag{3.13}$$

$$c_{1,2}=\frac{1}{2}(\beta_1+\beta_2\nu^2/\mu^2)\mp\left[\left(\frac{\beta_1-\beta_2\nu^2/\mu^2}{2}\right)^2+\frac{\nu^2}{\mu^2}\right]^{1/2}. \tag{3.14}$$

Now, we apply the WKB approximation to Eq. (3.12) and use $H^{(2)}_{i\nu}(p\rho)$, the second kind of Hankel function, for $Z_{i\nu}(p\rho)$. Then we have

$$F_1(p)\simeq\frac{1}{p^{1/2}(p^2-a_1)(p^2-a_2)}\frac{\exp[i\int^p\sqrt{P_0}dp]}{P_0^{1/4}} \tag{3.15}$$

and

$$\psi_1(\rho)\simeq\int_C\frac{e^{iS(p,\rho)}p^{1/2}}{(p^2-a_1)(p^2-a_2)(p^2\rho^2+\nu^2)^{1/4}P_0^{1/4}}dp, \tag{3.16}$$

where

$$S(p,\rho)=\int^p\sqrt{P_0(p)}dp-\int^{p\rho}\sqrt{1+\nu^2/\xi^2}d\xi. \tag{3.17}$$

Here, the contour C is chosen as shown in Fig. 1. This satisfies Eq. (3.11), since $H^{(2)}_{i\nu}(z)$ exponentially decreases but $F_1(p)$ diverges only by power at $z\to-i\infty$. We evaluate Eq.

(3.16) by using the saddle-point method; and the jth saddle point gives the following contribution ($j=1,2$):

$$\psi_{1j}(\rho)\cong A_j(\rho)e^{iS_j(\rho)-i\pi/4}, \tag{3.18}$$

where

$$S_j(\rho)=\int^{p_j^\dagger(\rho)}\sqrt{P_0}dp-\int^{\rho p_j^\dagger(\rho)}[1+\nu^2/\xi^2]^{1/2}d\xi$$
$$=-\int^{\rho}[(p_j^\dagger(\rho))^2+\nu^2/\rho^2]^{1/2}dp$$
$$=\frac{1}{\hbar}\int^{x}\sqrt{2m[E-u_j^a(x)]}dx, \tag{3.19}$$

$$A_j(\rho)=\frac{(p_j^\dagger)^{1/2}|2\pi/S_j''(\rho)|^{1/2}}{[(p_j^\dagger)^2-a_1][(p_j^\dagger)^2-a_2][(p_j^\dagger\rho)^2+\nu^2]^{1/4}P_0^{1/4}(p_j^\dagger)} \tag{3.20a}$$

$$=\left(\frac{2\pi}{\mu^2-\nu^2}\right)^{1/2}\left[\frac{8m}{\hbar^2\alpha^2}[E-u_j^a(x)]\right]^{-1/4}\times\begin{cases}\cos g & \text{for } j=1\\ -\sin g & \text{for } j=2,\end{cases} \tag{3.20b}$$

and $p_j^\dagger(\rho)$ ($j=1,2$) are the saddle points given by

$$[p_j^\dagger(\rho)]^2=\frac{\beta_1+\beta_2}{2}-\frac{\nu^2-\mu^2}{2\rho^2}\pm\left[\left(\frac{\beta_1-\beta_2}{2}-\frac{\mu^2-\nu^2}{2\rho^2}\right)^2+1\right]^{1/2}. \tag{3.21}$$

It should be noted that the saddle point $p_j^\dagger$ corresponds to the one on the adiabatic state $u_j^a(x)$.

The second and third equations in Eq. (3.19) are derived by noting the following relations:

$$\frac{dS_j}{d\rho}=\frac{\partial p_j^\dagger}{\partial\rho}\frac{\partial S_j}{\partial p_j^\dagger}+\frac{\partial S_j}{\partial\rho}=-\frac{\partial p_j^\dagger\rho}{\partial\rho}\left[1+\frac{\nu^2}{(\rho p_j^\dagger)^2}\right]^{1/2}$$
$$=-[(p_j^\dagger)^2+\nu^2/\rho^2]^{1/2} \tag{3.22}$$

and

$$2m[E-u_j^a(x)]=\frac{\hbar^2\alpha^2}{4}\rho^2\left\{\frac{\nu^2+\mu^2}{2\rho^2}+\frac{\beta_1+\beta_2}{2}\pm\left[\left(\frac{\mu^2-\nu^2}{2\rho^2}-\frac{\beta_1-\beta_2}{2}\right)^2+1\right]^{1/2}\right\}$$
$$=\frac{\hbar^2\alpha^2}{4}\rho^2\{[p_j^\dagger(\rho)]^2+\nu^2/\rho^2\}. \tag{3.23}$$

The saddle points in the p space defined by Eq. (3.21) are functions of the coordinate ρ, and give dominant contributions to the integral in Eq. (3.16) in the sense of semiclassical approximation.

The second equation in Eq. (3.20) can be obtained from the following relations:

$$\frac{\nu^2}{(p_j^\dagger)^2}-\frac{\mu^2}{(p_j^\dagger)^2}\frac{[(p_j^\dagger)^2-c_1][(p_j^\dagger)^2-c_2]}{[(p_j^\dagger)^2-a_1][(p_j^\dagger)^2-a_2]}$$
$$\equiv\frac{(\nu^2-\mu^2)[(p_j^\dagger)^2-\beta_1]}{[(p_j^\dagger)^2-a_1][(p_j^\dagger)^2-a_2]}=-\rho^2, \tag{3.24}$$

$$(p_j^\dagger)^2-\beta_1=-\left\{\frac{\beta_1-\beta_2}{2}-\frac{\mu^2-\nu^2}{2\rho^2}\mp\left[\left(\frac{\beta_1-\beta_2}{2}-\frac{\mu^2-\nu^2}{2\rho^2}\right)^2+1\right]^{1/2}\right\} \tag{3.25a}$$

$$=\pm\begin{cases}\sin g/\cos g & \text{for } j=1\\ \cos g/\sin g & \text{for } j=2,\end{cases} \tag{3.25b}$$

and

$$S_j''(\rho)=\frac{p_j^\dagger}{\sqrt{P_0(p_j^\dagger)}}\frac{\rho^4}{\nu^2-\mu^2}\begin{cases}1/\sin^2 g & \text{for } j=1\\ 1/\cos^2 g & \text{for } j=2.\end{cases} \tag{3.26}$$

The saddle points $p_j^\dagger$ ($j=1,2$) are monotonic functions of ρ:

$$p_1^\dagger\xrightarrow[\rho\to\infty]{}\sqrt{a_2},\quad p_1^\dagger\xrightarrow[\rho\to0]{}\infty,$$
$$p_2^\dagger\xrightarrow[\rho\to\infty]{}\sqrt{a_1},\quad p_2^\dagger\xrightarrow[\rho\to0]{}\sqrt{\beta_1}, \tag{3.27}$$

where $a_1<\beta_1<a_2$. It is interesting to note that the turning points in ρ and p space correspond to each other. The former (ρ_0) are given by [see Eqs. (3.23) and (3.21)]

$$\rho_0^{-2}=\frac{1}{2\nu^2\mu^2}\{-(\beta_1\mu^2+\beta_2\nu^2)\pm\sqrt{(\beta_1\mu^2+\beta_2\nu^2)^2-4\nu^2\mu^2(\beta_1\beta_2-1)}\}$$
$$=-c_{1,2}/\nu^2, \tag{3.28}$$

and the latter are equal to $c_{1,2}$ [see Eq. (3.13)]. There holds the following correspondence

$$(p_1^\dagger)^2=c_2\leftrightarrow\rho_0\quad\text{with the lower sign,}$$
$$(p_2^\dagger)^2=c_1\leftrightarrow\rho_0\quad\text{with the upper sign.} \tag{3.29}$$

The jth saddle point contribution to the wave function $\psi_2(\rho)$ can be easily obtained from Eq. (3.18) as [see Eq. (3.10) and Eqs. (3.25)]

$$\psi_{2j}(\rho)\simeq B_j(\rho)e^{iS_j(\rho)-i\pi/4} \tag{3.30}$$

with

$$B_j(\rho)=-[(p_j^\dagger)^2-\beta_1]A_j(\rho)$$
$$=-\left(\frac{2\pi}{\mu^2-\nu^2}\right)^{1/2}\left[\frac{8m}{\hbar^2\alpha^2}\,[E-u_j^a(x)]\right]^{-1/4}$$
$$\times\begin{cases}\sin g & \text{for}\quad j=1\\ \cos g & \text{for}\quad j=2.\end{cases} \qquad (3.31)$$

Since $\cos g\to 0$ $(\sin g\to 1)$ for $\rho\to 0$ or $x\to\infty$, only $p_2^\dagger$ contributes in Eq. (3.18) and we have

$$\varphi_2(x)\xrightarrow[x\to\infty]{} A\,\frac{e^{iS_2}}{\{2m[E-u_2^a(x)]\}^{1/4}} \qquad (3.32)$$

with

$$A=\left(\frac{\pi\hbar^3\alpha^3}{8m(u_1-u_2)}\right)^{1/2}e^{-\pi i/4}. \qquad (3.33)$$

On the other hand, at $\rho\to\infty$ or $x\to-\infty$ the contour C (see Fig. 1) cannot go through $p_2^\dagger$ and we obtain

$$\varphi_1(x)=\cos g\,\psi_1(x)$$
$$-\sin g\,\psi_2(x)\xrightarrow[x\to-\infty]{} A\,\frac{e^{iS_1}}{\{2m[E-u_1^a(x)]\}^{1/4}}. \qquad (3.34)$$

Equations (3.32) and (3.34) suggest that the transition matrix element N_{12} for the transition $\varphi_1(x=-\infty)\to\varphi_2(x=\infty)$ (see Ref. [13]) is given by

$$N_{12}=e^{i\Delta S} \qquad (3.35)$$

with

$$\Delta S=S_2-S_1=\frac{1}{\hbar}\oint\sqrt{2m[E-u^a(x)]}\,dx, \qquad (3.36)$$

where the contour integral is taken from the real axis to go around the complex crossing point, then back to the real axis on the different adiabatic potential. Explicit expressions of p, φ, and ψ in the nonadiabatic transition matrix Eq. (1.3) are provided in the next section.

IV. NONADIABATIC TRANSITION MATRIX

A. High-energy approximation

Before employing the high-energy approximation we introduce the following parameters:

$$\delta_j=\frac{1}{2\pi i}\oint_{\mathcal{L}_j}\sqrt{P_0(p)}\,dp \quad (j=1,2) \qquad (4.1)$$

and

$$\delta=\delta_1+\delta_2, \qquad (4.2)$$

where $P_0(p)$ is given by Eq. (3.13) and the contours $\mathcal{L}_j$ are defined in Fig. 2. It can be easily shown that δ of Eq. (4.2) is given by

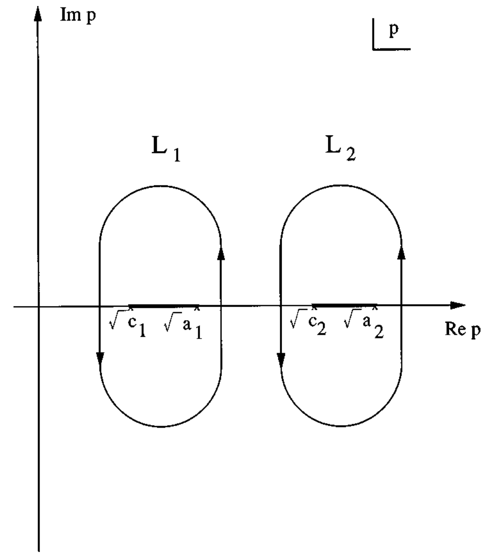

FIG. 2. The integral contours $\mathcal{L}_1$ and $\mathcal{L}_2$ to define δ_1 and δ_2 [see Eq. (4.1)].

$$\delta=\frac{1}{4\pi i}\left\{\oint_{\mathcal{L}'}+\oint_{\mathcal{L}''}\right\}\frac{\mu}{t}\left(\frac{(t-c_1)(t-c_2)}{(t-a_1)(t-a_2)}\right)^{1/2}dt$$
$$=\frac{1}{2}(\mu-\nu), \qquad (4.3)$$

where the contour $\mathcal{L}'$ and $\mathcal{L}''$ are shown in Fig. 3. As will be seen later, these parameters play crucial roles in determining the nonadiabatic transition amplitudes.

Now, we introduce the high-energy approximation,

$$\nu^2/\mu^2\to 1. \qquad (4.4)$$

Then we have

$$a_1-c_1=\frac{(\mu^2-\nu^2)a_1(a_1-\beta_1)}{\mu^2(a_1-c_2)}\equiv 2\epsilon_1\to 0 \quad (E\to\infty), \qquad (4.5a)$$

$$a_2-c_2=\frac{(\mu^2-\nu^2)a_2(a_2-\beta_1)}{\mu^2(a_2-c_1)}\equiv 2\epsilon_2\to 0 \quad (E\to\infty), \qquad (4.5b)$$

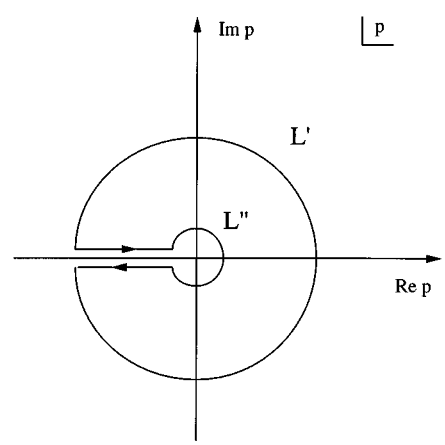

FIG. 3. The deformed integral contours $\mathcal{L}'$ and $\mathcal{L}''$ to define δ [see Eq. (4.3)].

and

$$\sqrt{P_0(p)} \simeq \frac{\nu}{p} + \frac{\mu\epsilon_1}{2a_1}\frac{2p}{p^2-a_1} + \frac{\mu\epsilon_2}{2a_2}\frac{2p}{p^2-a_2} + o(\epsilon^2). \tag{4.6}$$

According to the definition of Eq. (4.1), δ_1 and δ_2 are explicitly given by the following expressions in the present approximation:

$$\delta_1 \simeq \frac{\mu\epsilon_1}{2a_1} \simeq \frac{\mu-\nu}{4}\left(1+\frac{(\beta_1-\beta_2)/2}{\sqrt{1+[(\beta_1-\beta_2)/2]^2}}\right)$$

$$= \frac{\mu-\nu}{4}(1+\cos 2g_0) \tag{4.7a}$$

and

$$\delta_2 \simeq \frac{\mu\epsilon_2}{2a_2} \simeq \frac{\mu-\nu}{4}\left(1-\frac{(\beta_1-\beta_2)/2}{\sqrt{1+[(\beta_1-\beta_2)/2]^2}}\right)$$

$$= \frac{\mu-\nu}{4}(1-\cos 2g_0), \tag{4.7b}$$

where $\cos 2g_0$ is the value of $\cos 2g$ in the $\rho \to \infty (x \to -\infty)$ limit.

The diabatic wave functions $\psi_1(x)$ in the limits $x \to \infty$, $-\infty (\rho \to 0,\infty)$ are shown to be given by

$$\psi_1(x) \xrightarrow[x\to\infty]{} A_1 \frac{1}{\sqrt{\nu}} \rho^{-i\nu} \tag{4.8a}$$

with

$$A_1 = \frac{\pi i}{\sqrt{\nu}} e^{-i\varphi_0}(a_2-a_1)^{i\delta-1} e^{-\pi\delta_2} \frac{\Gamma(1-i\delta)}{\Gamma(1-i\delta_1)\Gamma(1-i\delta_2)}, \tag{4.8b}$$

and

$$\psi_1(x) \xrightarrow[x\to-\infty]{} B_1 \frac{1}{a_2^{1/4}\rho^{1/2}} e^{-i\sqrt{a_2}\rho} \tag{4.9a}$$

with

$$B_1 = \frac{\pi i}{\sqrt{\mu}} \left(\frac{\delta}{\sqrt{\delta_1\delta_2}}\right)^{i\delta_1-1} a_2^{i\nu/2} \left(\frac{a}{\mu}\right)^{i\delta_2} \frac{e^{-\pi\delta_2/2}}{\Gamma(1-i\delta_2)}, \tag{4.9b}$$

where

$$\varphi_0 = \nu - \nu \ln(2\nu). \tag{4.10}$$

Derivation of these expressions is given in Appendix A. On the other hand, the diabatic wave function $\psi_2(x)$ at $x \to \infty (\rho \to 0)$ is obtained as

$$\psi_2(x) \xrightarrow[x\to\infty]{} A_2 \frac{1}{\sqrt{\mu}} \rho^{-i\mu} \tag{4.11a}$$

with

$$A_2 = \frac{1}{\sqrt{\nu}} e^{-\pi\delta_2+\pi\delta/2} \sinh(\pi\delta_2)\Gamma(i\delta) e^{-i\varphi_0+i\delta\ln(4\nu)}. \tag{4.11b}$$

Derivation of Eqs. (4.11) is provided in Appendix B.

Since

$$\varphi_2(x=\infty) = \psi_1(\infty) \tag{4.12a}$$

and

$$\varphi_1(x=-\infty) = \cos g_0 \psi_1(-\infty) - \sin g_0 \psi_2(-\infty)$$

$$= \psi_1(-\infty)/\cos g_0, \tag{4.12b}$$

the transition matrix element N_{12} is given by

$$N_{12} = \frac{A_1}{B_1}\cos g_0. \tag{4.13}$$

Inserting Eqs. (4.8b) and (4.9b) into this equation, we obtain

$$p \equiv |N_{12}|^2 = e^{-\pi\delta_2}\frac{\sinh(\pi\delta_1)}{\sinh(\pi\delta)} \tag{4.14}$$

and

$$\arg N_{12} = -\varphi_0 + \delta_2 \ln \frac{\mu(a_2-a_1)}{a_2} - \frac{\nu}{2}\ln a_2 + \arg\Gamma(i\delta_1)$$

$$-\arg\Gamma(i\delta). \tag{4.15}$$

This p should not be confused with the momentum used before. This result clearly indicates that the nonadiabatic transition probability given by Eq. (4.14) is equivalent to the one derived by Nikitin [Eq. (9.15a) of Ref. [1]] and the approximate expression obtained from the exact solution in the special case [Eq. (3.23) of Ref. [13]] within the following correspondences of the parameters δ_1 and δ_2:

$$\delta_1 \leftrightarrow \xi - \xi_p \text{ in Ref. [1]} \leftrightarrow q_3 - q_1 \text{ in Ref. [13]}$$

$$\delta_2 \leftrightarrow \xi_p \text{ in Ref. [1]} \leftrightarrow q_2 - q_3 \text{ in Ref. [13].} \tag{4.16}$$

In the present treatment, δ_1 and δ_2, which are given by Eqs. (4.7) in the high-energy approximation, are more generally defined by Eq. (4.1). The phase given by Eq. (4.15), on the other hand, is just a high-energy approximation, and its improvement will be discussed in the next subsection. Since $\varphi_1(x=\infty) = \psi_2(\infty)$, the transition matrix element N_{11} is given by

$$N_{11} = -\frac{A_2}{B_1}\cos g_0. \tag{4.17}$$

From Eqs. (4.9b) and (4.11b) we have

$$|N_{11}|^2 = e^{\pi\delta_1}\frac{\sinh(\pi\delta_2)}{\sinh(\pi\delta)} = 1 - p \tag{4.18}$$

and

$$\arg N_{11} = -\varphi_0 + \delta \ln(4\nu) - \delta_1 \ln(a_2 - a_1) - \nu/2 \ln a_2 - \delta_2 \ln(a_2/\mu) + \pi/2 + \arg\Gamma(i\delta) + \arg\Gamma(1 - i\delta_2). \quad (4.19)$$

B. Dynamical phases

First, we try to derive accurate expressions for the dynamical phase φ in Eq. (1.3) based on the quantum mechanically exact solutions in the special case [13]. In general, the semiclassical phase along the adiabatic potential $u_2^a(x)$ at $x \to \infty$ is given by

$$\xi_i(x) = \frac{-1}{\hbar} \int_{x_0}^{x} \sqrt{2m[E - u_2^a(x)]} dx = -\frac{\sqrt{2m}}{\hbar} \left\{ \int_{x_0}^{x} \frac{u_1 - u_2^a(x)}{\sqrt{E - u_2^a(x)} + \sqrt{E - u_1}} dx + \int_{x_0}^{x} \sqrt{E - u_1} dx \right\}, \quad (4.20)$$

where x_0 is an appropriate real position. Similarly, the phase along $u_2^a(x)$ at $x \to -\infty$ is given by

$$\xi_f(x) = -\frac{1}{\hbar} \int_{x_0}^{x} \sqrt{2m[E - u_2^a(x)]} dx = -\frac{\sqrt{2m}}{\hbar} \left\{ \int_{x_0}^{x} \frac{u_3 - u_2^a(x)}{\sqrt{E - u_2^a(x)} + \sqrt{E - u_3}} dx + \int_{x_0}^{x} \sqrt{E - u_3} dx \right\}, \quad (4.21)$$

where u_3 represents the asymptotic value of $u_2^a(x)$ at $x \to -\infty$ in the special case ($V_1 V_2 = V^2$) and is given by

$$u_3 = \frac{u_1 V_2 + u_2 V_1}{V_1 + V_2}. \quad (4.22)$$

On the other hand, quantum mechanical wave functions are expressed in each asymptotic region by

$$\varphi_2(x \to \infty) = [(2m/\hbar^2)(E - u_1)]^{-1/4} \times \exp[-(i/\hbar)\sqrt{2m(E - u_1)} x]$$

$$\varphi_2(x \to -\infty) = N_{41}^{(4)} [(2m/\hbar^2)(E - u_3)]^{-1/4} \times \exp[-(i/\hbar)\sqrt{2m(E - u_3)} x], \quad (4.23)$$

where $N_{41}^{(4)}$ is the 4-channel transition matrix element given by Eq. (3.4) of Ref. [13]. Thus the dynamical phase φ is given by

$$\varphi = \left[\xi_f(x) + \frac{1}{\hbar} \sqrt{2m(E - u_3)} x \right]_{x \to -\infty} - \arg N_{41}^{(4)} - \left[\xi_i(x) + \frac{1}{\hbar} \sqrt{2m(E - u_1)} x \right]_{x \to +\infty}. \quad (4.24)$$

At relatively high energies $\arg N_{41}^{(4)}$ can be replaced by the following expression with good accuracy,

$$\arg N_{41}^{(4)} \simeq \delta_1 \ln \frac{V_1 + V_2}{\hbar v \alpha} - \arg\Gamma(i\delta) + \arg\Gamma(i\delta_2) \quad (4.25)$$

with

$$\delta_1 = \frac{u_1 - u_2}{\hbar v \alpha} \frac{V_1}{V_1 + V_2} \quad \text{and} \quad \delta_2 = \frac{u_1 - u_2}{\hbar v \alpha} \frac{V_2}{V_1 + V_2}, \quad (4.26)$$

where v is the velocity. The expressions of δ_1 and δ_2 of Eq. (4.26) can be obtained from Eqs. (4.7) under the condition $V_1 V_2 = V^2$ [see also the correspondence (4.16)]. Since φ should not depend on x_0, we can put $x_0 = 0$, and obtain

$$\varphi = \frac{\sqrt{2m}}{\hbar} \left\{ \int_{-\infty}^{0} \frac{u_3 - u_2^a(x)}{\sqrt{E - u_2^a(x)} + \sqrt{E - u_3}} dx + \int_{0}^{\infty} \frac{u_1 - u_2^a(x)}{\sqrt{E - u_2^a(x)} + \sqrt{E - u_1}} dx \right\} - \delta_1 \ln \frac{V_1 + V_2}{\hbar v \alpha} + \arg\Gamma(i\delta) - \arg\Gamma(i\delta_2). \quad (4.27)$$

A simpler semiclassical expression of φ can be obtained if we use the high-energy expansion

$$\sqrt{2m[E - u^a(x)]} \simeq \sqrt{2mE} - \frac{1}{\hbar v} u^a(x), \quad (4.28)$$

and the asymptotic forms of the semiclassical wave function $\varphi_1(x)$ at $x \to \pm\infty$ derived in the previous subsection. Using the similar procedure as above, we can finally obtain

$$\varphi = \gamma(\delta_2) - \gamma(\delta) \quad (4.29)$$

with $\delta = \delta_1 + \delta_2$ and

$$\gamma(X) = X \ln X - X - \arg\Gamma(iX), \quad (4.30)$$

where δ_1 and δ_2 are given by Eq. (4.26).

The same analysis can be carried out for the dynamical phase ψ, and we finally obtain the following compact semiclassical expression:

$$\psi = \gamma(\delta_1) - \gamma(\delta) - 2\left[\sqrt{\delta\delta_2} + \frac{\delta_1}{2} \ln \frac{\sqrt{\delta} - \sqrt{\delta_2}}{\sqrt{\delta} + \sqrt{\delta_2}} \right]. \quad (4.31)$$

This phase depends on the choice of reference point (x_0), and the present one is the same as that of Nikitin [$x_0 = \mathrm{Re}(x_*)$]. It should be noted that

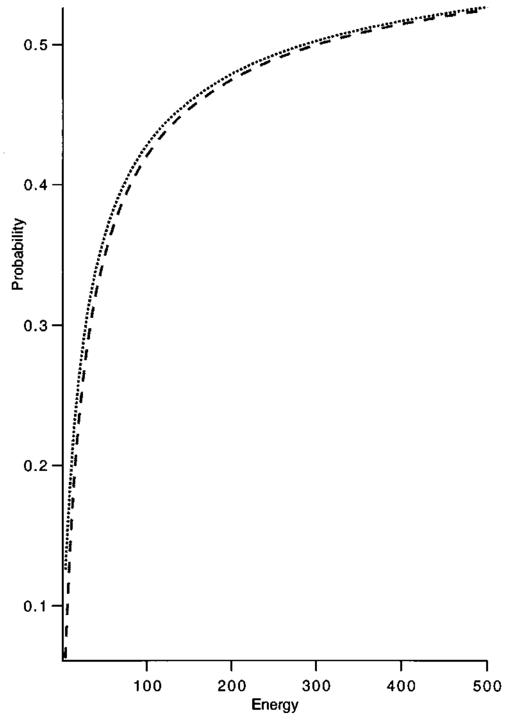

FIG. 4. The nonadiabatic transition probability p as a function of dimensionless energy. The potentials used are defined by Eqs. (2.1) and (5.1). Dotted line: exact numerical solution of the coupled equations. Dashed line: Asymptotic semiclassical approximation [Eq. (4.14)] with δ and δ_2 given by Eqs. (5.2) and (5.3), respectively.

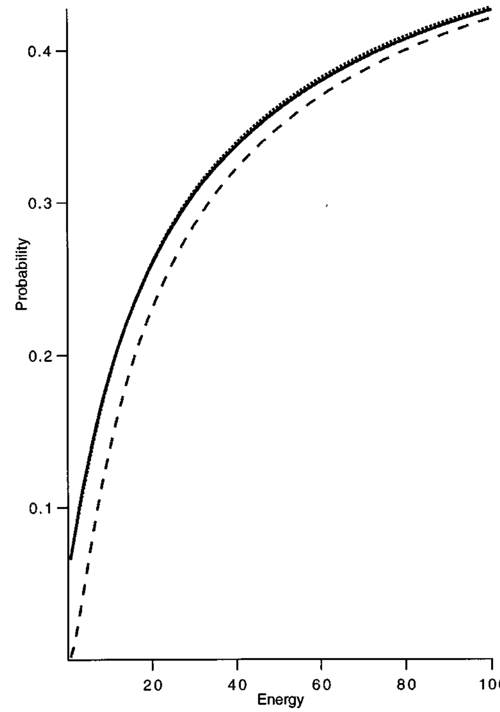

FIG. 5. The same as Fig. 4 in the narrower energy range. Dotted and dashed lines are the same as those in Fig. 4. Solid line: Semiclassical approximation [Eq. (4.14)] with δ and δ_2 given by Eqs. (4.3) and (4.33b).

$$\mathrm{Re}\left\{\frac{1}{\hbar}\int_{\mathrm{Re}(x_*)}^{x_*}\{\sqrt{2m[E-u_1^a(x)]}-\sqrt{2m[E-u_2^a(x)]}\}\right\}dx \simeq \frac{1}{\hbar v}\,\mathrm{Re}\left\{\int_{\mathrm{Re}(x_*)}^{x_*}[u_2^a(x)-u_1^a(x)]dx\right\} =2\sqrt{\delta\delta_2}+\delta_1\ln\frac{\sqrt{\delta}-\sqrt{\delta_2}}{\sqrt{\delta}+\sqrt{\delta_2}}, \quad (4.32)$$

where x_* is the complex crossing point given by Eq. (2.7).

With the replacement of δ_1 and δ_2 by $\xi-\xi_p$ and ξ_p, respectively, Eqs. (4.29) and (4.31) coincide with the expressions obtained by Nikitin [1,10–12], where $\xi=\Delta\xi/\alpha v$ and $\xi_p=\xi(1-\cos 2\theta_0)/2$ [see Eq. (2.8)]. In the present treatment δ_1 and δ_2 can be more generally expressed in terms of contour integrals. Both δ_1 and δ_2 are defined by Eq. (4.1) and δ is given by Eq. (4.3) within the exponential model. Both parameters δ_1 and δ_2 can further be generalized as

$$\delta_1=\frac{1}{\pi}\,\mathrm{Im}\left\{\int_{x_1}^{x_*}k_1(x)dx-\int_{x_2}^{x_*}k_2(x)dx\right\} \quad (4.33a)$$

and

$$\delta_2=\frac{1}{\pi}\,\mathrm{Im}\left\{\int_{\mathrm{Re}(x_*)}^{x_*}[k_1(x)-k_2(x)]dx\right\}, \quad (4.33b)$$

where $x_j (j=1,2)$ are the complex turning points and

$$k_j(x)=\frac{1}{\hbar}\sqrt{2m[E-u_j^a(x)]}. \quad (4.34)$$

These can be free from the exponential potential model and be utilized for general curved potentials. This generalization is not only quite natural from the long history of the semiclassical theory of nonadiabatic transitions for the LZS and RZD problems [1–6], but also confirmed in the present treatment by Eq. (3.36). This could provide us with a possibility to formulate a unified theory that works for general potentials and can cover both LZS and RZD cases.

V. NUMERICAL EXAMINATIONS

A simple numerical confirmation of the present semiclassical theory has been carried for the nonadiabatic transition probability p and the dynamical phase φ by using the following model potential:

$$u_1=0 \quad u_2/(\hbar^2\alpha^2/2m)=-5, \quad V_1/(\hbar^2\alpha^2/2m)=3,$$

$$V_2/(\hbar^2\alpha^2/2m)=2, \quad V/(\hbar^2\alpha^2/2m)=\sqrt{5}. \quad (5.1)$$

The probability p and the phase φ are defined by Eq. (1.3), and are given by Eqs. (4.14) and (4.29), respectively, in the present semiclassical approximation.

Figures 4 and 5 show the probability p against the dimensionless energy $E/(\hbar^2\alpha^2/2m)$. The dotted line represents the exact numerical solution of coupled equations, and the dashed lines in Fig. 4 and Fig. 5 are the results of Eq. (4.14) with δ and δ_2 given by

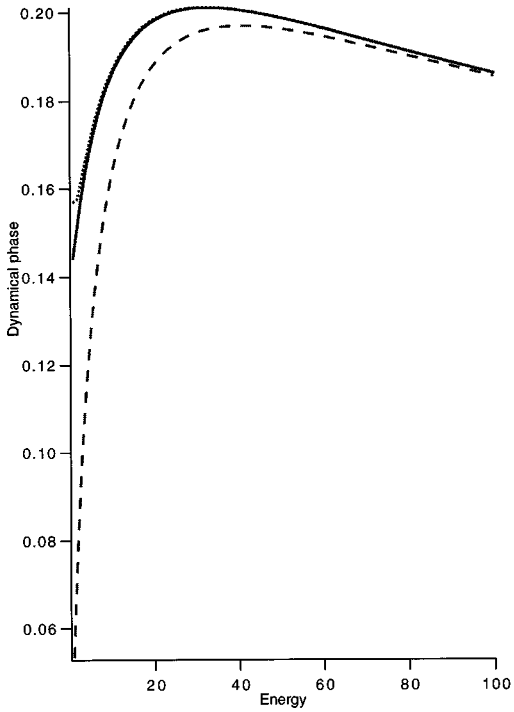

FIG. 6. Dynamical phase φ (in radian) as a function of dimensionless energy. The potentials are given by Eqs. (2.1) and (5.1) except that $V/(\hbar^2\alpha^2/2m)=\sqrt{6}$. Dotted line: quantum mechanical result given by Eq. (4.24). Dashed line: asymptotic semiclassical approximation [Eq. (4.29)] with δ and δ_2 given by Eqs. (5.2) and (5.3). Solid line: semiclassical approximation [Eq. (4.29)] with δ and δ_2 given by Eqs. (4.3) and (4.33b).

$$\delta=\frac{u_1-u_2}{\hbar v\alpha} \tag{5.2}$$

and

$$\delta_2=\frac{u_1-u_2}{2\hbar v\alpha}\left[1-\frac{(\beta_1-\beta_2)/2}{\sqrt{1+[(\beta_1-\beta_2)/2]^2}}\right]. \tag{5.3}$$

These are the high-energy limits of Eq. (4.7). This asymptotic semiclassical approximation deviates from the exact one at low energies. In Fig. 5 the solid line represents the result of Eq. (4.14) with δ and δ_2 given by Eq. (4.3) and Eq. (4.33b), respectively. This semiclassical theory works almost perfectly. Figure 6 shows the results for the dynamical phase φ in the special case $V/(\hbar^2\alpha^2/2m)=\sqrt{6}$ [see Eq. (5.1)]. The dotted line is the most accurate result of Eq. (4.24) with arg $N_{41}^{(4)}$ given by the exact solution in Ref. [13]. The solid and dashed lines represent the semiclassical results of Eq. (4.29) with δ and δ_2 evaluated by Eqs. (4.3) and (4.33b) (solid line) or by the asymptotic expressions of Eqs. (5.2) and (5.3) (dashed line). The accurate semiclassical approximation (solid line) works very well.

These numerical results clearly indicate that the present semiclassical theory is a very good approximation, if we use δ and δ_2 given by Eq. (4.3) and Eq. (4.33), respectively.

VI. CONCLUDING REMARKS

With use of the Bessel transformation and the WKB type approximation, we have developed an accurate semiclassical theory for the general exponential model defined by Eq. (2.1). We have discussed only the nonadiabatic transition matrix defined by Eq. (1.3) in this paper; but, as is well known, this suffices to solve not only all kinds of two-state problems but also even multichannel problems [4–8]. The nonadiabatic transition probability p is expressed by Eq. (4.14), and the dynamical phases φ and ψ are given by Eqs. (4.29) and (4.31), respectively. These expressions are actually the same as those obtained by Nikitin [1,10–12] the pioneer of the exponential model. A development made in the present work is that the important basic parameters δ and δ_2 are generalized and expressed by Eqs. (4.3) [or (4.33a)] and (4.33b), respectively. These were confirmed to be very accurate and useful.

One nice thing about the exponential model is that, as was noticed before by Nikitin [1,10–12] this model can cover both Landau-Zener-Stueckelberg and Rosen-Zener-Demkov problems. Actually, the nonadiabatic transition probability p defined by Eq. (4.14) gives the Landau-Zener probability $p=e^{-\delta_2}$ in the limit $\delta\to\infty$ or $\delta_2\to 0$, and covers the Rosen-Zener probability for one passage of the transition point $p=(1+e^{2\pi\delta_2})^{-1}$ in the limit $\delta\to 2\delta_2$. This suggests, as mentioned in the Introduction, that we should be able to formulate a unified theory that works for general potentials and can cover both LZS and RZD cases. Zhu pursued a similar idea in the diabatic representation [15]. We want to do this within the adiabatic representation in such a way that no nonunique diabatization is required and the two basic parameters δ_1 and δ_2 (or δ and δ_2) are expressed in terms of complex phase integrals along the adiabatic potentials. Equations (4.33) meet this requirement. With use of Eqs. (4.33) we should be able to treat the general cases. An investigation on this line is under way, and is planned to be reported in the future.

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APPENDIX A: DERIVATION OF EQS. (4.8) AND (4.9)

From the asymptotic expression of $H_{i\nu}^{(2)}(p\rho)$ for $\nu^2\gg 1$,

$$H_{i\nu}^{(2)}(p\rho)\simeq\frac{1}{(p^2\rho^2+\nu^2)^{1/4}}\exp\left[-i\int^{p\rho}\sqrt{1+\nu^2/\xi^2}\,d\xi\right], \tag{A1}$$

we have at $\rho\to 0(x\to\infty)$

$$H_{i\nu}^{(2)}(p\rho)\simeq\frac{1}{\sqrt{\nu}}(p\rho)^{-i\nu}e^{-i\varphi_0} \tag{A2}$$

with

$$\varphi_0=\nu-\nu\ln(2\nu), \tag{A3}$$

since

$$\int^{p\rho}(1+\nu^2/\xi^2)^{1/2}d\xi \xrightarrow[\rho\to 0]{} \nu\ln(p\rho)+\varphi_0+o(\rho^2). \tag{A4}$$

Then from Eqs. (3.16), (3.17), (4.6), and (4.7) we obtain

$$\begin{aligned}\psi_1(x\to\infty)&\simeq\frac{\rho^{-i\nu}}{2\nu}e^{-i\varphi_0}(a_2-a_1)^{i\delta-1}\\&\times\int_{C_Z}(1+z)^{i\delta_1-1}z^{i\delta_2-1}dz\\&=\frac{\pi i e^{-\pi\delta_2}\rho^{-i\nu}}{\nu\Gamma(1-i\delta_2)}e^{-i\varphi_0}(a_2-a_1)^{i\delta-1}\Psi(i\delta_2,i\delta;0),\end{aligned} \tag{A5}$$

where $z=(p^2-a_2)/(a_2-a_1)$ and $\Psi(a,c;\zeta)$ is the confluent hypergeometric function defined by [16]

$$\Psi(a,c;\zeta)=\frac{\Gamma(c-1)}{\Gamma(a-c+1)}\Phi(a,c;\zeta)+\frac{\Gamma(c-1)}{\Gamma(a)}\zeta^{1-c}\times\Phi(a-c+1,2-c;\zeta) \tag{A6}$$

with

$$\Phi(a,c;\zeta)=1+\frac{a}{c}\frac{\zeta}{1!}+\frac{a(a+1)}{c(c+1)}\frac{\zeta^2}{2!}+\cdots. \tag{A7}$$

This leads to Eqs. (4.8).

Next, let us consider the wave function $\psi_1(x)$ at $\rho\to\infty(x\to-\infty)$. Because of the exponential behavior of $H^{(2)}_{i\nu}(\rho p)$ [see Eq. (A12) below] we take into consideration only a contribution from the vicinity of $p\sim\sqrt{a_2}$. Equation (3.12) is rewritten as

$$\frac{d^2f_1}{d\eta^2}+\left(-\frac{1}{4}+\frac{i\delta_2}{\eta}\right)f_1=0 \tag{A8}$$

with

$$\eta=-2i\mu(p-\sqrt{a_2})/\sqrt{a_2}, \tag{A9}$$

since P_0 at $p\sim\sqrt{a_2}$ is given by

$$P_0(p)\simeq\frac{\nu^2}{a_2}+\frac{\nu^2\epsilon_2}{a_2\sqrt{a_2}}\frac{1}{p-\sqrt{a_2}}. \tag{A10}$$

The general solution of Eq. (A8) should be matched to the semiclassical one given by Eq. (3.15). As a result we have

$$\begin{aligned}F_1(p)&=a_2^{i\nu/2}(a_2-a_1)^{i\delta_1-1}(2\sqrt{a_2})^{i\delta_2-1}\\&\times\frac{1}{\sqrt{\mu}}e^{-\eta/2}\frac{(p-\sqrt{a_2})^{i\delta_2-1}}{\eta^{i\delta_2}}\Psi(1-i\delta_2,0,\eta).\end{aligned} \tag{A11}$$

Since $H^{(2)}_{i\nu}(p\rho)$ at $p\sim\sqrt{a_2}$ and $\rho\to\infty$ is given by

$$H^{(2)}_{i\nu}(p\rho)\simeq\frac{e^{-i\sqrt{a_2}\rho}}{a_2^{1/4}\rho^{1/2}}, \tag{A12}$$

we finally obtain Eqs. (4.9).

APPENDIX B: DERIVATION OF EQS. (4.11)

Because of Eq. (3.10), the wave function $\psi_2(x)$ is given by

$$\psi_2(x)=\int_C(\beta_1-p^2)F_1(p)H^{(2)}_{i\nu}(p\rho)p\,dp. \tag{B1}$$

Using Eq. (4.6) and

$$H^{(2)}_{i\nu}(p\rho)\simeq\frac{1}{\sqrt{\nu}}e^{-i\varphi_0}(p\rho)^{-i\nu}e^{-i\rho^2p^2/4\nu}, \tag{B2}$$

we have the following expression from Eq. (B1),

$$\begin{aligned}\psi_2(x\to\infty)&\simeq-\frac{e^{-i\varphi_0}}{2\nu}\rho^{-i\nu}(a_2-a_1)^{i\delta}\\&\times\int_{C_z}e^{-i\zeta z}(1+z)^{i\delta_1-1}z^{i\delta_2-1}\left(z+\frac{\delta_2}{\delta}\right)dz\\&=\frac{-\pi i e^{-i\varphi_0}}{\nu}\rho^{-i\nu}(a_2-a_1)^{i\delta}e^{-\pi\delta_2}\\&\times\left\{\frac{e^{\pi i}}{\Gamma(-i\delta_2)}\Psi(i\delta_2+1,i\delta+1;i\zeta)\right.\\&\left.+\frac{\delta_2}{\delta}\frac{1}{\Gamma(1-i\delta_2)}\Psi(i\delta_2,i\delta;i\zeta)\right\},\end{aligned} \tag{B3}$$

where the term $\rho^2p^2/4\nu$ is retained in Eq. (B2) [see Eq. (A4)] and the following relations are used:

$$z=(p^2-a_2)/(a_2-a_1),$$

$$p^2-a_1=(a_2-a_1)(1+z),$$

$$\xi=\frac{(a_2-a_1)}{4\nu}\rho^2,$$

$$\begin{aligned}\beta_1-p^2&=-(a_2-a_1)[z+(a_2-\beta_1)/(a_2-a_1)]\\&\simeq-(a_2-a_1)(z+\delta_2/\delta).\end{aligned} \tag{B4}$$

From the behavior of the confluent hypergeometric function $\Psi(a,c;i\zeta)$ at $\zeta\to 0$ we finally obtain Eqs. (4.11).

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