BRIEF REPORTS

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Analytic solution of two-state time-independent coupled Schrödinger equations in an exponential model

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Quantum mechanically exact analytical solutions are obtained for a two-state exponential model, in which the exponent of diabatic coupling is one-half of that of the diabatic potential curve. A very simple and accurate semiclassical formula is found for the nonadiabatic transition probability. This gives a direct generalization of the Landau-Zener and Rosen-Zener formulas.
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Here, we report a quantum mechanically exact analytical solution of the following coupled Schrödinger equations:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\hat{V}(x)\right]\hat{\psi}(x)=E\hat{\psi}(x), \tag{1}$$

where

$$\hat{V}(x)=\begin{pmatrix} U_1 & Ve^{-\alpha x} \\ Ve^{-\alpha x} & U_2+V_2e^{-2\alpha x}\end{pmatrix} \tag{2}$$

with $U_1>U_2$ and $V_2>0$, and

$$\hat{\psi}(x)=\begin{pmatrix}\psi_1(x)\\ \psi_2(x)\end{pmatrix}. \tag{3}$$

This model is different from the ordinary exponential model, in which the exponents are the same for diagonal and off-diagonal potentials [1–3]. Since the latter exponential model is known to cover both the Landau-Zener formula and the Rosen-Zener formula in certain limits, we are working on a more general exponential model in attempt to formulate a unified theory which can cover both Landau-Zener-Stueckelberg and Rosen-Zener-Demkov cases. The present work presents one step forward to that aim, since the two exponents are different.

Introducing the new variables,

$$z=\frac{mV_2}{2\hbar^2\alpha^2}e^{-2\alpha x}, \tag{4}$$

$$\mu^2=\frac{8m}{\hbar^2\alpha^2}(E-U_1) \quad\text{and}\quad \nu^2=\frac{8m}{\hbar^2\alpha^2}(E-U_2), \tag{5}$$

we can transform Eq. (1) into

$$\left\{z\prod_{p=1}^{2}\left(z\frac{d}{dz}-a_p+1\right)-\prod_{p=1}^{4}\left(z\frac{d}{dz}-b_p\right)\right\}\psi_1=0, \tag{6}$$

where

$$a_{1,2}=1\pm i\eta/4,$$

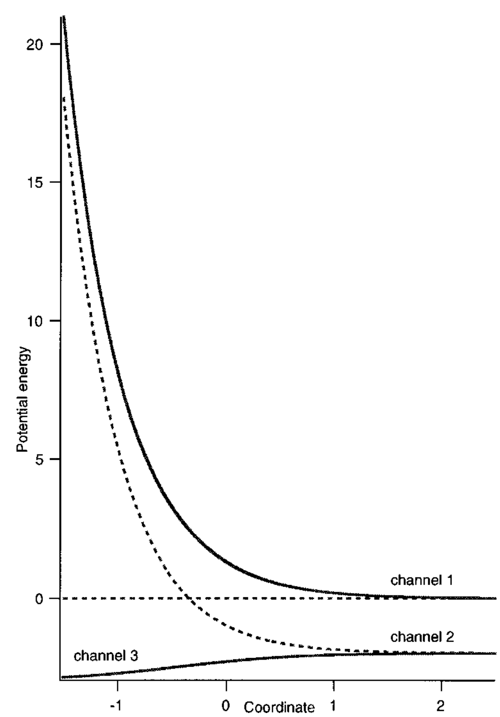

FIG. 1. Diabatic (dash line) and adiabatic (solid line) potentials. The potential energies and coordinate are scaled as $\epsilon=2mE/(\hbar^2\alpha^2)$ and $X=\alpha x$ [see Eq. (18) also], i.e., dimensionless. The dimensionless energy parameters are $\epsilon_1=0.0$, $\epsilon_2=-2.0$, and $\epsilon_3=-3.0$ [see Eq. (18)], and $2mV/(\hbar^2\alpha^2)=\sqrt{3}$.

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$$b_{1,2}=\tfrac{1}{2}\pm i\nu/4 \quad\text{and}\quad b_{3,4}=\pm i\mu/4 \tag{7}$$

with

$$\eta^2=\frac{8m}{\hbar^2\alpha^2}\left\{E-\left(U_1-\frac{V^2}{V_2}\right)\right\}. \tag{8}$$

Equation (6) can be solved in terms of the Meijer's G functions [4] and asymptotic expressions of the adiabatic wave functions $\varphi_j(x)(j=1,2)$ are explicitly obtained in the same way as before [2],

$$\varphi_j(x)\xrightarrow{x\to+\infty}A_j j_+ + B_j j_-(j=1,2),$$
$$\varphi_1(x)\xrightarrow{x\to-\infty}0 \tag{9}$$

and

$$\varphi_2(x)\xrightarrow{x\to-\infty}A_j j_- + B_j j_+(j=3),$$

where

$$j_\pm=\frac{1}{\sqrt{p_j}}\exp\left[\pm i\frac{p_j}{\hbar}x\right] \tag{10}$$

with $p_j=\sqrt{2m(E-U_j)}$ and $U_3=U_1-V^2/V_2$. The adiabatic potential 1 is the upper one and repulsive at $x\to-\infty$, but the adiabatic potential 2 converges to the constant U_3 in the limit, which is called channel 3 (see Fig. 1). The 3×3 nonadiabatic transition matrix N defined by $A_i=\Sigma_j N_{ij}B_j$ are finally obtained as

$$N_{11}=A^{b_4-b_3}\frac{\Gamma(b_1-b_4)\Gamma(b_2-b_4)\Gamma(b_3-b_4)\Gamma(a_2-b_3)\Gamma(a_1-b_3)}{\Gamma(b_1-b_3)\Gamma(b_2-b_3)\Gamma(b_4-b_3)\Gamma(a_2-b_4)\Gamma(a_1-b_4)}\frac{\sin[\pi(b_4-b_1)]\sin[\pi(b_3-b_1)]}{\sin[\pi(b_4-a_1)]\sin[\pi(b_3-a_1)]}, \tag{11a}$$

$$N_{12}=\sqrt{\frac{p_1}{p_2}}A^{b_4-b_1+1/2}\frac{1}{4\lambda^{1/2}(b_1^2-b_3^2)}\frac{\Gamma(b_1-b_4)\Gamma(b_2-b_4)\Gamma(b_3-b_4)\Gamma(a_2-b_1)\Gamma(a_1-b_1)}{\Gamma(b_2-b_1)\Gamma(b_3-b_1)\Gamma(b_4-b_1)\Gamma(a_2-b_4)\Gamma(a_1-b_4)}$$
$$\times\frac{\sin[\pi(b_3-b_4)]\sin[\pi(b_1-a_1)]}{\sin[\pi(b_3-b_1)]\sin[\pi(b_4-a_1)]}, \tag{11b}$$

$$N_{13}=\sqrt{\frac{p_3}{p_1}}A^{a_1-b_3-1}\frac{\Gamma(1+b_1-a_1)\Gamma(1+b_2-a_1)\Gamma(1+b_3-a_1)\Gamma(1+b_4-a_1)\Gamma(a_2-b_3)\Gamma(a_1-b_3)}{\Gamma(1+a_2-a_1)\Gamma(b_1-b_3)\Gamma(b_2-b_3)\Gamma(b_4-b_3)}$$
$$\times\frac{\sin[\pi(b_3-a_1)]\sin[\pi(b_1-a_1)]}{\pi\sin[\pi(b_3-b_1)]}, \tag{11c}$$

$$N_{22}=A^{b_2-b_1}\frac{b_2^2-b_4^2}{b_1^2-b_3^2}\frac{\Gamma(b_1-b_2)\Gamma(b_3-b_2)\Gamma(b_4-b_2)\Gamma(a_2-b_1)\Gamma(a_1-b_1)}{\Gamma(b_2-a_1)\Gamma(b_3-b_1)\Gamma(b_4-b_1)\Gamma(a_2-b_2)\Gamma(a_1-b_2)}\frac{\sin[\pi(b_3-b_2)]\sin[\pi(b_1-a_1)]}{\sin[\pi(b_2-a_1)]\sin[\pi(b_3-b_1)]}, \tag{11d}$$

$$N_{23}=-\sqrt{\frac{p_3}{p_2}}A^{a_1-b_1-1/2}\frac{1}{4\lambda^{1/2}(b_1^2-b_3^2)}\frac{\Gamma(1+b_1-a_1)\Gamma(1+b_2-a_1)\Gamma(1+b_3-a_1)\Gamma(1+b_4-a_1)\Gamma(a_2-b_1)\Gamma(a_1-b_1)}{\Gamma(1+a_2-a_1)\Gamma(b_2-b_1)\Gamma(b_3-b_1)\Gamma(b_4-b_1)}$$
$$\times\frac{\sin[\pi(b_3-a_1)]\sin[\pi(b_1-a_1)]}{\pi\sin[\pi(b_3-b_1)]}, \tag{11e}$$

and

$$N_{33}=-A^{a_1-a_2}\frac{\Gamma(1+b_1-a_1)\Gamma(1+b_2-a_1)\Gamma(1+b_3-a_1)\Gamma(1+b_4-a_1)\Gamma(1+a_1-a_2)}{\Gamma(1+b_1-a_2)\Gamma(1+b_2-a_2)\Gamma(1+b_3-a_2)\Gamma(1+b_4-a_2)\Gamma(1+a_2-a_1)}\frac{\sin[\pi(b_3-b_1)]\sin[\pi(b_1-a_1)]}{\sin[\pi(a_2-b_3)]\sin[\pi(a_2-b_1)]}, \tag{11f}$$

where $A=mV_2/(2h^2\alpha^2)$, $\lambda=\hbar^2\alpha^2V_2/(8mV^2)$ and $\Gamma(x)$ is the gamma function. From these expressions we can obtain the following simple expressions for transition probabilities:

$$|N_{11}|^2=\frac{\cosh^2\left[\frac{\pi}{2}(q_1+q_2)\right]\sinh^2\left[\frac{\pi}{2}(q_3-q_1)\right]}{\sinh^2\left[\frac{\pi}{2}(q_1+q_3)\right]\cosh^2\left[\frac{\pi}{2}(q_2-q_1)\right]}, \tag{12a}$$

$$|N_{12}|^2=\frac{\sinh(\pi q_1)\sinh(\pi q_2)\sinh\left[\frac{\pi}{2}(q_3-q_1)\right]\cosh\left[\frac{\pi}{2}(q_2-q_3)\right]}{\cosh^2\left[\frac{\pi}{2}(q_2-q_1)\right]\cosh\left[\frac{\pi}{2}(q_2+q_3)\right]\sinh\left[\frac{\pi}{2}(q_1+q_3)\right]}, \tag{12b}$$

$$|N_{13}|^2=\frac{\sinh(\pi q_1)\sinh(\pi q_3)\cosh\left[\frac{\pi}{2}(q_2-q_3)\right]\cosh\left[\frac{\pi}{2}(q_1+q_2)\right]}{\cosh\left[\frac{\pi}{2}(q_2+q_3)\right]\sinh^2\left[\frac{\pi}{2}(q_1+q_3)\right]\cosh\left[\frac{\pi}{2}(q_2-q_1)\right]}, \quad (12c)$$

$$|N_{22}|^2=\frac{\cosh^2\left[\frac{\pi}{2}(q_1+q_2)\right]\cosh^2\left[\frac{\pi}{2}(q_2-q_3)\right]}{\cosh^2\left[\frac{\pi}{2}(q_2+q_3)\right]\cosh^2\left[\frac{\pi}{2}(q_2-q_1)\right]}, \quad (12d)$$

$$|N_{23}|^2=\frac{\sinh(\pi q_2)\sinh(\pi q_3)\sinh\left[\frac{\pi}{2}(q_3-q_1)\right]\cosh\left[\frac{\pi}{2}(q_1+q_2)\right]}{\cosh^2\left[\frac{\pi}{2}(q_2+q_3)\right]\sinh\left[\frac{\pi}{2}(q_1+q_3)\right]\cosh\left[\frac{\pi}{2}(q_2-q_1)\right]}, \quad (12e)$$

and

$$|N_{33}|^2=\frac{\sinh^2\left[\frac{\pi}{2}(q_3-q_1)\right]\cosh^2\left[\frac{\pi}{2}(q_2-q_3)\right]}{\sinh^2\left[\frac{\pi}{2}(q_1+q_3)\right]\cosh^2\left[\frac{\pi}{2}(q_2+q_3)\right]}, \quad (12f)$$

with

$$q_j=p_j/\hbar\alpha(j=1-3). \quad (13)$$

It should be noted that these are quantum mechanically exact expressions.

$|N_{13}|^2$ is the most interesting quantity, because this represents the nonadiabatic transition probability for one passage of the transition region. In the special case of $V_2=0$, this becomes

$$|N_{13}|^2 \xrightarrow{V_2\to 0} 2\exp[-\pi(q_1+q_2)] \times \frac{\sinh(\pi q_1)\cosh\left[\frac{\pi}{2}(q_1+q_2)\right]}{\cosh\left[\frac{\pi}{2}(q_2-q_1)\right]}. \quad (14)$$

This case corresponds to the Rosen-Zener case [1,2] and Eq. (14) coincides with the exact solution obtained by Osherov and Voronin [5]. It can be easily seen that

$$\text{Eq. (14)}=[1+e^{\pi(q_2-q_1)}]^{-1}(1-e^{-2\pi q_2})(1+e^{-\pi(q_1+q_2)})$$
$$\equiv p_{RZ}(1-e^{-2\pi q_2})(1+e^{-\pi(q_1+q_2)}), \quad (15)$$

where p_{RZ} is the Rosen-Zener probability and the residual two factors represent the threshold effect.

At high energies the following approximate formulas (semiclassical approximation) hold

$$|N_{13}|^2\simeq\exp\left[\frac{\pi}{2}(q_1-q_3)\right]\frac{\cosh\left[\frac{\pi}{2}(q_2-q_3)\right]}{\cosh\left[\frac{\pi}{2}(q_2-q_1)\right]}\equiv p, \quad (16)$$

$$|N_{11}|^2\simeq(1-p)^2, \quad |N_{12}|^2=(1-p)p, \quad |N_{22}|^2=p^2,$$
$$|N_{23}|^2\simeq 1-p, \text{ and } |N_{33}|^2\simeq 0. \quad (17)$$

Figures 2 and 3 show $|N_{13}|^2$ of Eq. (12c) and its approximation (p) given by Eq. (16) for certain parameter values, where ϵ and $\epsilon_j(j=1-3)$ are dimensionless quantities defined as

$$\epsilon=2mE/\hbar^2\alpha^2, \quad \epsilon_j=2mU_j/\hbar^2\alpha^2,$$
$$\text{and } q_j=\sqrt{\epsilon-\epsilon_j}. \quad (18)$$

Except at very low energies near threshold, the semiclassical approximation [Eq. (16)] works very well. It is interesting to note that the Landau-Zener and the Rosen-Zener parameters are given by

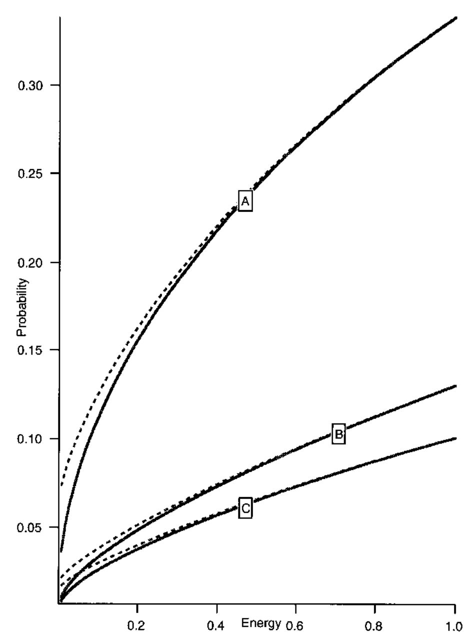

FIG. 2. Nonadiabatic transition probability $|N_{13}|^2$. The exact one (solid line) is given by Eq. (12c) and the approximate one (dashed line) is given by Eq. (16). The energy is scaled, i.e., dimensionless, as in Fig. 1. The dimensionless parameters are $\epsilon_1=0.0$, $\epsilon_2=-2.0$, $\epsilon_3=-1.0(A)$, $-3.0(B)$, and $-5.0(C)$ [see Eq. (18)].

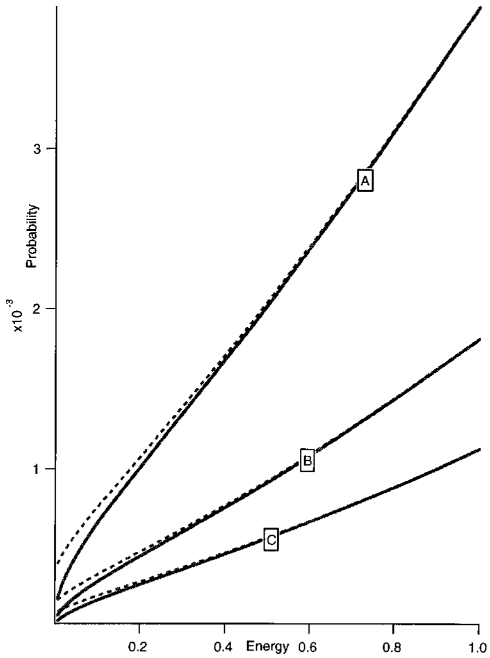

FIG. 3. The same as Fig. 2 except for the parameters $\epsilon_2 = -10.0$, and $\epsilon_3 = -7.0(A)$, $-9.0(B)$, and $-11.0(C)$.

$$\delta_{\rm LZ} = \frac{\pi(\text{adiabatic coupl.})^2}{\hbar v|\text{slope differ.}|}\bigg|_{\text{diab. cross.}} = \frac{\pi}{2}(q_3 - q_1) \quad (19)$$

and

$$\delta_{\rm RZ} = \frac{\pi|\text{asymp. pot. diff.}|}{\hbar v|\text{expon. of coupl.}|} = \pi(q_2 - q_1).$$

Thus, in the limit $V_2 \to 0$ or $q_3 \to \infty$ Eq. (16) agrees with the Rosen-Zener formula, $p_{\rm RZ} = [1 + \exp(\delta_{\rm RZ})]^{-1}$ and in the limit $(q_2 - q_1) \to \infty$ Eq. (16) covers the Landau-Zener formula, $p_{\rm LZ} = \exp(-2\delta_{\rm LZ})$. Since both parameters are explicitly contained in the formula (16), this makes a direct generalization of the two LZ and RZ formulas.

In this Report we have discussed the case $V_2 > 0$. In the case of $V_2 < 0$ the system becomes a four-channel problem, but could be solved exactly with use of the method similar to the present one. Furthermore, a bit more general case that the channel 1 contains also the function $\propto e^{-2\alpha x}$ can be treated by the semiclassical (Eikonal) approximation. These will be discussed in a future publication. These works including our previous ones [2,3], however, just present one step towards our ambitious goal of formulating a unified theory which should work for general potentials and could cover both Landau-Zener-Stueckelberg and Rosen-Zener-Demkov cases. Recently, the former (LZS) case has been solved completely by Zhu and Nakamura to cover practically whole ranges of energy and coupling strength [6,7]. It would be a very challenging task to formulate a unified theory to include even this one.

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