# Duality in potential curve crossing: Application to quantum coherence

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A field-dependent su(2) gauge transformation connects between the adiabatic and diabatic pictures in the (Landau-Zener-Stueckelberg) potential curve crossing. It is pointed out that weak and strong potential curve crossing interactions are interchanged under this transformation, thus realizing a naive strong and weak duality. A reliable perturbation theory should thus be formulated in limits of both weak and strong interactions. In fact, the main characteristics of the potential crossing phenomena such as the Landau-Zener formula including its numerical coefficient are well described by simple (time-independent) perturbation theory without referring to Stokes phenomena. We also show that quantum coherence in a double-well potential is generally suppressed by the effect of a potential curve crossing, which is analogous to the effect of Ohmic dissipation on quantum coherence. [S1050-2947(97)09310-4]

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## I. INTRODUCTION

Potential curve crossing is related to a wide range of physical and chemical processes, and the celebrated Landau-Zener formula [1–3] correctly describes the qualitative features of those processes [4–8]. An effort to improve the Landau-Zener formula and to make it a more quantitative formula is actively going on [9,10]. The purpose of the present paper is to study this old problem on the basis of modern field-theoretical ideas, namely, duality and gauge transformation.

Adiabatic and diabatic pictures in a potential curve crossing problem are related to each other by a field-dependent su(2) gauge transformation [5,8], and we point out that this transformation leads to an interchange of strong and weak potential curve crossing interactions, which is analogous to the electric and magnetic duality in conventional gauge theory [11]. This strong and weak duality should allow a reliable perturbative treatment of potential curve crossing phenomena at the both limits of very weak (adiabatic picture) and very strong (diabatic picture) potential crossing interactions. In fact, it is shown that the main features of potential curve crossing phenomena are well described by straightforward time-independent perturbation theory combined with the zeroth order WKB wave functions [5,8,12], without referring to Stokes phenomena; perturbation theory thus becomes more flexible to cover a wide range of problems.

To illustrate duality, we first reexamine the old problem of the Landau-Zener formula, and show that simple time-independent perturbation theory gives an adequate description of the Landau-Zener formula including numerical coefficients in limits of both adiabatic and diabatic pictures. We encounter an interesting topological object in the adiabatic picture. We then apply our formulation to an analysis of the effect of a potential curve crossing on quantum coherence in a double-well potential. We show that a potential crossing generally suppresses quantum coherence, which is analogous to the effect of Ohmic dissipation on quantum coherence [13,14]. To our knowledge, this clear recognition of duality, and the precise criterion for naive perturbation theory including the analysis of quantum coherence, have not been discussed before.

## II. MODEL HAMILTONIAN OF POTENTIAL CURVE CROSSING AND DUALITY

To analyze the potential curve crossing, we start with a model Hamiltonian defined in the so-called diabatic picture [5,8]

$$H=\frac{1}{2m}\,\hat{p}^2+\frac{V_1(x)+V_2(x)}{2}+\frac{V_1(x)-V_2(x)}{2}\,\sigma_3+\frac{1}{g}\,\sigma_1, \tag{2.1}$$

where $\sigma_3$ and $\sigma_1$ stand for the Pauli matrices. We assume throughout this paper that the potential crossing occurs at the origin, $V_1(0)=V_2(0)=0$ (see Fig. 1). We also take the convention that the slope of the first potential at the crossing point is positive, $V_1'(0)>0$. The sign of $V_2'(0)$ may be either the same as that of $V_1'(0)$ (Sec. III) or opposite to it (Sec. IV).

If one neglects the last term in the above Hamiltonian, one obtains the unperturbed Hamiltonian in the diabatic picture

$$H_0\equiv\frac{1}{2m}\,\hat{p}^2+\frac{V_1(x)+V_2(x)}{2}+\frac{V_1(x)-V_2(x)}{2}\,\sigma_3. \tag{2.2}$$

This Hamiltonian $H_0$ describes two potentials, which are decoupled from each other. The last term in Eq. (2.1), $H_I\equiv\sigma_1/g$, with a constant $g$, causes the transition between

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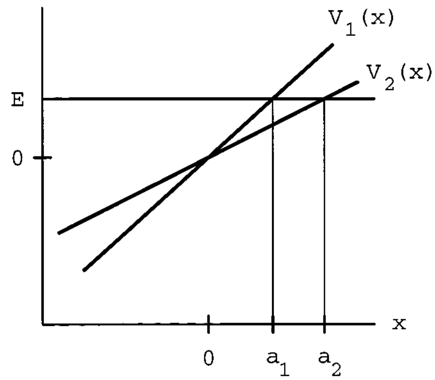


FIG. 1. Landau-Zener process in the diabatic picture.

these two otherwise independent potential curves. In other words, if one takes $g\to$large, this case physically corresponds to a *complete* potential crossing from a view point of an *adiabatic* two-potential crossing (Fig. 2). That is, $g$ stands for the strength of the potential crossing interaction, and $g\to$large corresponds to a very strong potential crossing interaction. On the other hand, if one lets $g$ become smaller, the effects of the last term in Eq. (2.1) become substantial and the Hamiltonian $H_0$, Eq. (2.2), does not present a sensible zeroth-order Hamiltonian.

To deal with the case of a small $g$, we perform the non-Abelian ''gauge transformation''

$$\Phi(x)=e^{i\theta(x)\sigma_2/2}\Psi(x),\quad H'=e^{i\theta(x)\sigma_2/2}He^{-i\theta(x)\sigma_2/2}, \tag{2.3}$$

where $\sigma_2$ is a Pauli matrix. The Hamiltonian in the new picture is given by

$$\begin{aligned}H'=&\frac{1}{2m}\left[\hat{p}-\frac{\hbar}{2}\,\partial_x\theta(x)\sigma_2\right]^2+\frac{V_1(x)+V_2(x)}{2}\\&+\left[\frac{V_1(x)-V_2(x)}{2}\cos\,\theta(x)+\frac{1}{g}\sin\,\theta(x)\right]\sigma_3\\&+\left[-\frac{V_1(x)-V_2(x)}{2}\sin\,\theta(x)+\frac{1}{g}\cos\,\theta(x)\right]\sigma_1.\end{aligned} \tag{2.4}$$

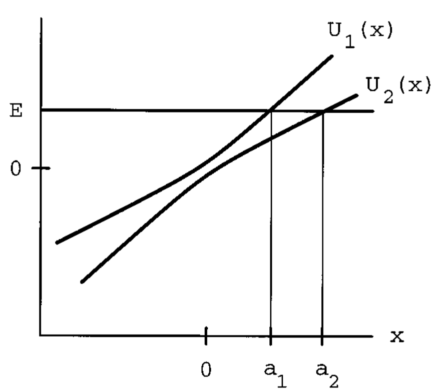


FIG. 2. Landau-Zener process in the adiabatic picture.

To eliminate the potential curve mixing, the last term of Eq. (2.4), we choose the gauge parameter $\theta(x)$ as [8]

$$\cot\,\theta(x)=g\,\frac{V_1(x)-V_2(x)}{2}\equiv f(x). \tag{2.5}$$

We then obtain the Hamiltonian in the *adiabatic* picture,

$$H'=H_0'+H_I', \tag{2.6}$$

where

$$H_0'\equiv\frac{1}{2m}\,\hat{p}^2+\frac{U_1(x)+U_2(x)}{2}+\frac{U_1(x)-U_2(x)}{2}\,\sigma_3 \tag{2.7}$$

and

$$H_I'\equiv-\frac{\hbar}{4m}\,[\hat{p}\,\partial_x\theta(x)+\partial_x\theta(x)\hat{p}]\sigma_2+\frac{\hbar^2}{8m}\,[\partial_x\theta(x)]^2. \tag{2.8}$$

The potential energies in the adiabatic picture are related to those in the adiabatic picture as (Fig. 2)

$$U_{1,2}(x)\equiv\frac{V_1(x)+V_2(x)}{2}\pm\left(\left[\frac{V_1(x)-V_2(x)}{2}\right]^2+\frac{1}{g^2}\right)^{1/2}. \tag{2.9}$$

From the definition of the gauge parameter in Eq. (2.5), the ''gauge field'' $\partial_x\theta(x)$ is expressed as

$$\partial_x\theta(x)=-\frac{f'(x)}{1+f(x)^2}. \tag{2.10}$$

The transition from the diabatic picture to the adiabatic picture is a local gauge transformation, or, in the conventional field theoretical sense, is regarded as a field-dependent transformation. The transformation from one of these two pictures to the other is an $x$-dependent notion.

In the adiabatic picture, the $\sigma_2$-dependent term in the interaction $H_I'$, Eq. (2.8), causes the potential crossing. If one neglects $H_I'$, the two potentials characterized by $U_1(x)$ and $U_2(x)$ do not mix with each other: Physically, this means *no* potential crossing. This suggests that $H_I'$ is proportional to the coupling constant $g$, since a small $g$ corresponds to *weak* potential crossing by definition. This is in fact the case as is clear from Eqs. (2.10) and (2.5).

We thus conclude that the two extreme limits of potential crossing interaction should be reliably handled in perturbation theory; that is, the strong potential crossing interaction in the *diabatic* picture, and the weak potential crossing interaction in the gauge transformed *adiabatic* picture. This is analogous to the electric-magnetic duality in conventional gauge theory [11]: The diabatic picture may correspond to the electric picture with a coupling constant $e=1/g$, and the adiabatic picture to the magnetic picture with a coupling constant $g$.

A general criterion for the validity of perturbation theory in the adiabatic picture (2.6) is

$$\frac{\hbar}{2}\,|\partial_x\theta(x)|\ll|p(x)|, \tag{2.11}$$

which is expected to be satisfied when the coupling constant $g$ is small and the incident particle is sufficiently energetic.

### III. LANDAU-ZENER FORMULA

As an illustration of the duality discussed in Sec. II, we reexamine a perturbative derivation of the Landau-Zener formula in both of the adiabatic and diabatic pictures [1,5,8]. For definiteness, we shall assume $V_1'(0)>V_2'(0)$ as in Fig. 1.

Let us start with the adiabatic picture with weak potential crossing interaction. Since the gauge field generally vanishes, $\partial_x\theta(x)\to 0$ for $|x|\to\infty$, we can define the *asymptotic* states in terms of the eigenstates of $H_0'$, Eq. (2.7). We define the initial and final states $\Phi_i$ and $\Phi_f$ by

$$\Phi_i(x)=\begin{pmatrix}\varphi_1(x)\\0\end{pmatrix},\quad \Phi_f(x)=\begin{pmatrix}0\\\varphi_2(x)\end{pmatrix}, \tag{3.1}$$

which satisfy

$$\left[\frac{1}{2m}\,\hat{p}^2+U_1(x)\right]\varphi_1(x)=E\varphi_1(x),$$

$$\left[\frac{1}{2m}\,\hat{p}^2+U_2(x)\right]\varphi_2(x)=E\varphi_2(x). \tag{3.2}$$

We then obtain the potential curve transition probability due to the perturbation $H_I'$, Eq. (2.8):

$$w(i\to f)=\frac{2\pi}{\hbar}\,|\langle\Phi_f|H_I'|\Phi_i\rangle|^2. \tag{3.3}$$

The transition matrix element is given by

$$\langle\Phi_f|H_I'|\Phi_i\rangle=-\frac{\hbar^2}{4m}\int_{-\infty}^{\infty}dx\;\partial_x\theta(x)[-\varphi_2'(x)\varphi_1(x)+\varphi_2(x)\varphi_1'(x)]. \tag{3.4}$$

To evaluate the matrix element, we use the WKB wave functions [4]

$$\varphi_1(x)=\begin{cases}\dfrac{C_1}{2\sqrt{|p_1(x)|}}\exp\left[-\dfrac{1}{\hbar}\displaystyle\int_{a_1}^{x}dx|p_1(x)|\right] & \text{for } x>a_1\\[2ex] \dfrac{C_1}{\sqrt{p_1(x)}}\cos\left[\dfrac{1}{\hbar}\displaystyle\int_{x}^{a_1}dx\;p_1(x)-\dfrac{\pi}{4}\right] & \text{for } x<a_1\end{cases} \tag{3.5}$$

and

$$\varphi_2(x)=\begin{cases}\dfrac{C_2}{2\sqrt{|p_2(x)|}}\exp\left[-\dfrac{1}{\hbar}\displaystyle\int_{a_2}^{x}dx|p_2(x)|\right] & \text{for } x>a_2\\[2ex] \dfrac{C_2}{\sqrt{p_2(x)}}\cos\left[\dfrac{1}{\hbar}\displaystyle\int_{x}^{a_2}dx\;p_2(x)-\dfrac{\pi}{4}\right] & \text{for } x<a_2\end{cases} \tag{3.6}$$

where the semiclassical momenta in the adiabatic picture are defined by

$$p_{1,2}(x)\equiv\sqrt{2m[E-U_{1,2}(x)]} \tag{3.7}$$

and $a_1$ and $a_2$ denote the classical turning points (Fig. 2). Within the WKB approximation, we also have

$$\varphi_1'(x)\simeq\begin{cases}-\dfrac{C_1}{2\hbar}\sqrt{|p_1(x)|}\exp\left[-\dfrac{1}{\hbar}\displaystyle\int_{a_1}^{x}dx|p_1(x)|\right] & \text{for } x>a_1\\[2ex] \dfrac{C_1}{\hbar}\sqrt{p_1(x)}\sin\left[\dfrac{1}{\hbar}\displaystyle\int_{x}^{a_1}dx\;p_1(x)-\dfrac{\pi}{4}\right] & \text{for } x<a_1\end{cases} \tag{3.8}$$

and a similar relation for $\varphi_2'(x)$. The normalization of $\varphi_1(x)$ is chosen as $C_1=2\sqrt{m}$ to make the probability flux of the incident wave unity. On the other hand, the final-state wave function in Eq. (3.3) has to be normalized by the $\delta$ function with respect to the energy, $\langle\Phi_2'|\Phi_2\rangle=\delta(E_2'-E_2)$, and this specifies $C_2=2\sqrt{m}/\sqrt{2\pi\hbar}$.

We estimate the matrix element (3.4) by using the oscillating parts of the wave functions (3.5) and (3.6). This treatment is justified if the following conditions are satisfied: (i) $|p(0)|\to$large and $m\to$large with $v=|p(0)|/m$ kept fixed such that nonrelativistic treatment is valid in the physically relevant region and (ii) $g\to$small, but with

$$\frac{1}{g}\ll\frac{1}{2m}\,|p(0)|^2 \tag{3.9}$$

to ensure Eq. (2.11) and the condition

$$\beta\ll a, \tag{3.10}$$

where $a$ is an average turning point and $\beta$ is a typical geometrical extension of $\partial_x\theta(x)$. If Eq. (3.10) is satisfied, we can estimate the matrix element by using the oscillating parts of wave functions only since $\partial_x\theta(x)$ rapidly goes to zero for $|x|\gg\beta$ on the real axis.

The integral (3.4) is then written as

$$\langle\Phi_f|H_I'|\Phi_i\rangle\simeq-\frac{i\hbar C_1C_2}{8m}\int dx\;\partial_x\theta(x)\times\left\{\exp\left[\frac{i}{\hbar}\int_{a_1}^{x}dx\;p_1(x)-\frac{i}{\hbar}\int_{a_2}^{x}dx\;p_2(x)\right]-\exp\left[-\frac{i}{\hbar}\int_{a_1}^{x}dx\;p_1(x)+\frac{i}{\hbar}\int_{a_2}^{x}dx\;p_2(x)\right]\right\}, \tag{3.11}$$

where we have set $p_1(x)/p_2(x)=1$ in the prefactors. This is justified within the saddle-point approximation for $\hbar\to 0$; this is also justified if $\hbar/|p(0)|\ll\beta$, the characteristic length scale of the present problem, by setting $p(0)$ large, as specified in (i). Therefore we need to evaluate an integral of the form

$$I\equiv\int_{-\infty}^{\infty}dx\ \partial_x\theta(x)\exp\left[\frac{i}{\hbar}\int_{a_1}^{x}dx\ p_1(x)-\frac{i}{\hbar}\int_{a_2}^{x}dx\ p_2(x)\right]. \tag{3.12}$$

Here we present an explicit evaluation of Eq. (3.12) for the linear potential crossing problem, $V_1(x)=V_1'(0)x$ and $V_2(x)=V_2'(0)x$, on the basis of local data without referring to Stokes phenomena. For sufficiently large energy, $E-(U_1+U_2)/2\gg(U_1-U_2)/2$, the difference of momenta can be approximated as [see Eq. (2.9)]

$$\int_0^x dx[p_1(x)-p_2(x)]\simeq-\int_0^x dx\ \frac{2}{v(x)g\beta}\ \sqrt{x^2+\beta^2}, \tag{3.13}$$

where we used

$$f(x)=g\ \frac{V_1'(0)-V_2'(0)}{2}\ x\equiv\frac{x}{\beta},$$

$$v(x)\equiv\frac{1}{m}\left(2m\left[E-\frac{U_1(x)+U_2(x)}{2}\right]\right)^{1/2}, \tag{3.14}$$

and $v(x)$ is approximated to be a constant $v=v(0)$ in the following. From Eq. (2.10), we also have

$$\partial_x\theta(x)=-\frac{\beta}{x^2+\beta^2}, \tag{3.15}$$

and thus

$$\begin{aligned}I\simeq&-\exp\left[\frac{i}{\hbar}\int_{a_1}^{0}dx\ p_1(x)-\frac{i}{\hbar}\int_{a_2}^{0}dx\ p_2(x)\right]\\&\times\int_{-\infty}^{\infty}dx\ \frac{\beta}{x^2+\beta^2}\ \exp\left(-\frac{2i}{\hbar vg\beta}\int_0^x dx\sqrt{x^2+\beta^2}\right)\\=&-\exp\left[\frac{i}{\hbar}\int_{a_1}^{0}dx\ p_1(x)-\frac{i}{\hbar}\int_{a_2}^{0}dx\ p_2(x)\right]\\&\times\int_{-\infty}^{\infty}dx\ \frac{1}{x^2+1}\ \exp\left(-i\alpha\int_0^x dx\sqrt{x^2+1}\right)\\=&-\exp\left[\frac{i}{\hbar}\int_{a_1}^{0}dx\ p_1(x)-\frac{i}{\hbar}\int_{a_2}^{0}dx\ p_2(x)\right]\\&\times\int_{-\infty}^{\infty}dx\ \exp[-i\alpha F(x)],\end{aligned} \tag{3.16}$$

where

$$F(x)\equiv\int_0^x dx\sqrt{x^2+1}+\frac{1}{i\alpha}\ \ln(x^2+1),$$

$$\alpha\equiv\frac{2\beta}{\hbar vg}=\frac{4}{\hbar vg^2[V_1'(0)-V_2'(0)]}>0. \tag{3.17}$$

We evaluate integral (3.16) by a saddle-point approximation with respect to $\alpha$. We thus seek the saddle point

$$F'(x)=\sqrt{x^2+1}+\frac{1}{i\alpha}\ \frac{2x}{x^2+1}=0, \tag{3.18}$$

which is located between the real axis and the pole positions $x=\pm i$ of $\partial_x\theta(\beta x)$ so that we can smoothly deform the integration contour; these poles also coincide with the complex potential crossing points. If one sets $x=iy$ in Eq. (3.18) for $-1<y<1$, one has

$$\sqrt{1-y^2}=-\frac{1}{\alpha}\ \frac{2y}{1-y^2}, \tag{3.19}$$

which has a *unique* solution

$$x_s=iy_s\simeq-i+\frac{i}{2}\left(\frac{2}{\alpha}\right)^{2/3} \tag{3.20}$$

for large $\alpha$. (The complex conjugate of $x_s$ is located in the second Riemann sheet.) For this value of the saddle point

$$\begin{aligned}F(x_s)=&\int_0^{x_s}dx\sqrt{x^2+1}+\frac{1}{i\alpha}\ \ln\left(\frac{2}{\alpha}\right)^{2/3}\\\simeq&-\frac{\pi i}{4}+\frac{2}{3}\ \frac{i}{\alpha}+\frac{1}{i\alpha}\ \ln\left(\frac{2}{\alpha}\right)^{2/3},\\F''(x_s)\simeq&-3i\left(\frac{\alpha}{2}\right)^{1/3}.\end{aligned} \tag{3.21}$$

We thus have a Gaussian integral which decreases in the direction parallel to the real axis

$$\begin{aligned}I\simeq&-\left(\frac{\alpha}{2}\right)^{2/3}e^{2/3}\ \exp\left[\frac{i}{\hbar}\int_{a_1}^{0}dx\ p_1(x)-\frac{i}{\hbar}\int_{a_2}^{0}dx\ p_2(x)\right]\\&\times\int_{-\infty}^{\infty}dx\ \exp\left[-3\left(\frac{\alpha}{2}\right)^{4/3}(x-x_s)^2\right]\exp\left(-\frac{\pi\alpha}{4}\right)\\=&-\left(\frac{\pi}{3}\right)^{1/2}e^{2/3}\\&\times\exp\left[\frac{i}{\hbar}\int_{a_1}^{0}dx\ p_1(x)-\frac{i}{\hbar}\int_{a_2}^{0}dx\ p_2(x)\right]\exp\left(-\frac{\pi\alpha}{4}\right).\end{aligned} \tag{3.22}$$

From Eq. (3.11), we obtain

$$\begin{aligned}\langle\Phi_f|H_I'|\Phi_i\rangle\simeq&-\left(\frac{\pi}{3}\right)^{1/2}e^{2/3}\left(\frac{\hbar}{2\pi}\right)^{1/2}\\&\times\sin\left\{\frac{1}{\hbar}\left[\int_{a_1}^{0}dx\ p_1(x)-\int_{a_2}^{0}dx\ p_2(x)\right]\right\}\\&\times\exp\left\{-\frac{\pi}{\hbar vg^2[V_1'(0)-V_2'(0)]}\right\}.\end{aligned} \tag{3.23}$$

It is interesting that the numerical value of the coefficient of the above expression, $\sqrt{\pi}e^{2/3}/\sqrt{3}=1.993\,17$, is very close to the canonical value 2 [4], and we replace it by 2 in the following. For a past analysis of the prefactor in the timedependent perturbation theory, see Refs. [15]. We thus have the transition probability from Eq. (3.3),

$$w(i\to f)\simeq 4\sin^2\left\{\frac{1}{\hbar}\left[\int_{a_1}^{0}dx\ p_1(x)-\int_{a_2}^{0}dx\ p_2(x)\right]\right\}$$
$$\times\times\exp\left\{-\frac{2\pi}{\hbar v g^2[V_1'(0)-V_2'(0)]}\right\}$$
$$\simeq 2\exp\left\{-\frac{2\pi}{\hbar v g^2[V_1'(0)-V_2'(0)]}\right\}, \qquad (3.24)$$

where we replaced the square of sine function by its average $\frac{1}{2}$ in the final expression. We emphasize that the numerical coefficient of $w(i\to f)$ is fixed by time-independent perturbation theory and the local data without referring to global Stokes phenomena; this is satisfactory, since linear potential crossing is a locally valid idealization.

We interpret that $w(i\to f)$ in Eq. (3.24) expresses *twice* the nonadiabatic transition probability. Notice that our initial-state wave function contains the reflection wave as well as the incident wave. Therefore the transition probability per *one* crossing is given by half of Eq. (3.24),

$$P(1\to 2)\simeq\exp\left\{-\frac{2\pi}{\hbar v g^2[V_1'(0)-V_2'(0)]}\right\}, \qquad (3.25)$$

which is the celebrated Landau-Zener formula [4,5]. Our perturbative derivation presented here is conceptually much simpler than the past works [1,4,5,8,12], and it should also be useful for a pedagogical purpose also.

It is interesting to study the same problem in the diabatic picture in Fig. 1 with $H_I=\sigma_1/g$ for large $g$. We first note that the initial state in the adiabatic picture asymptotically corresponds to the eigenfunction of $V_2(x)$ and the final state corresponds to $V_1(x)$, under the present setup $V_1'(0)>V_2'(0)$. Therefore the initial and final zeroth-order wave functions in the diabatic picture are taken as

$$\Psi_i(x)=\begin{pmatrix}0\\ \psi_2(x)\end{pmatrix},\qquad \Psi_f(x)=\begin{pmatrix}\psi_1(x)\\ 0\end{pmatrix}. \qquad (3.26)$$

In the WKB approximation,

$$\psi_1(x)=\begin{cases}\dfrac{C_1}{2\sqrt{|p_1(x)|}}\exp\left[-\dfrac{1}{\hbar}\displaystyle\int_{a_1}^{x}dx|p_1(x)|\right] & \text{for } x>a_1\\[2ex] \dfrac{C_1}{\sqrt{p_1(x)}}\cos\left[\dfrac{1}{\hbar}\displaystyle\int_{x}^{a_1}dx\ p_1(x)-\dfrac{\pi}{4}\right] & \text{for } x<a_1\end{cases} \qquad (3.27)$$

and

$$\psi_2(x)=\begin{cases}\dfrac{C_2}{2\sqrt{|p_2(x)|}}\exp\left[-\dfrac{1}{\hbar}\displaystyle\int_{a_2}^{x}dx|p_2(x)|\right] & \text{for } x>a_2\\[2ex] \dfrac{C_2}{\sqrt{p_2(x)}}\cos\left[\dfrac{1}{\hbar}\displaystyle\int_{x}^{a_2}dx\ p_2(x)-\dfrac{\pi}{4}\right] & \text{for } x<a_2.\end{cases} \qquad (3.28)$$

In the above expressions, semiclassical momenta are defined by

$$p_{1,2}(x)\equiv\sqrt{2m[E-V_{1,2}(x)]}. \qquad (3.29)$$

The transition probability in the diabatic picture is then given by

$$w(i\to f)=\frac{2\pi}{\hbar}\,|\langle\Psi_f|H_I|\Psi_i\rangle|^2. \qquad (3.30)$$

The evaluation of the matrix element in Eq. (3.30) is the standard one described in the textbook by Landau and Lifshitz [4], for example. The saddle point for $\hbar\ll 1$ is located at the origin $x_s=0$ and we have an integral, for example,

$$\int_{-\infty}^{\infty}dx\ \frac{1}{\sqrt{p_1(x)p_2(x)}}$$
$$\times\exp\left[\frac{i}{\hbar}\int_{a_1}^{x}dx\ p_1(x)-\frac{i}{\hbar}\int_{a_2}^{x}dx\ p_2(x)\right]$$
$$\simeq\frac{\sqrt{2\pi\hbar}}{\sqrt{m[V_1'(0)-V_2'(0)]}(2mE)^{1/4}}$$
$$\times\exp\left[\frac{i}{\hbar}\int_{a_1}^{0}dx\ p_1(x)-\frac{i}{\hbar}\int_{a_2}^{0}dx\ p_2(x)-\frac{\pi i}{4}\right]. \qquad (3.31)$$

Under this approximation, we have, for $E>0$,

$$w(i\to f)\simeq\frac{8\pi}{\hbar v(0)g^2[V_1'(0)-V_2'(0)]}$$
$$\times\cos^2\left[\frac{1}{\hbar}\int_{0}^{a_2}dx\ p_2(x)-\frac{1}{\hbar}\int_{0}^{a_1}dx\ p_1(x)-\frac{\pi}{4}\right]$$
$$\simeq\frac{4\pi}{\hbar v g^2[V_1'(0)-V_2'(0)]}. \qquad (3.32)$$

[$v(0)$ is the velocity at the crossing point, and $v(0)=\sqrt{2E/m}$.] For $E<0$, one can verify that there is no saddle point and, therefore,

$$w(i\to f)\simeq 0. \qquad (3.33)$$

We again interpret Eq. (3.32) as twice the potential crossing probability, because our initial-state wave function contains the reflection wave as well as the incident wave. The transition probability per one potential crossing is given by half of Eq. (3.32).

A simple *interpolating* formula, which reproduces Eq. (3.24) in the weak-coupling limit and Eq. (3.32) in the strong-coupling limit, is given by

$$w(i\rightarrow f)\simeq 2\exp\left\{-\frac{2\pi}{\hbar v g^2[V_1'(0)-V_2'(0)]}\right\}\times\left(1-\exp\left\{-\frac{2\pi}{\hbar v g^2[V_1'(0)-V_2'(0)]}\right\}\right). \tag{3.34}$$

This expression is also consistent with the (semiclassical) conservation of probability [4]. A justification of Eq. (3.34) is facilitated by combining the analysis of Stokes phenomena and the conservation of probability [6].

Motivated by duality, we reexamined a perturbative derivation of the Landau-Zener formula, and we rederived formula (3.24) including its numerical coefficient on the basis of perturbation theory. However, our final result (3.24) in the adiabatic picture does not contain the coupling constant as a prefactor. This is related to an interesting topological object in the present formulation. From the definition of Eq. (2.10), the ''gauge field'' satisfies the relation

$$\int_{-\infty}^{\infty}dx\ \partial_x\theta(x)=\theta(\infty)-\theta(-\infty)=-\pi, \tag{3.35}$$

which is *independent* of the coupling constant $g$; we assume $f(x)\rightarrow\pm\infty$ for $x\rightarrow\pm\infty$, respectively. Because of this kinklike topological behavior of $\theta(x)$, the coupling constant does not appear as a prefactor of the matrix element in perturbation theory if the wave functions spread over the range which covers the geometrical size of $\partial_x\theta(x)$ well. The precise criterion of the validity of perturbation theory is thus given by Eq. (2.11): This condition is in fact satisfied if conditions (3.9)–(3.10) are satisfied. For small values of $x$, the small coupling $g$ helps to satisfy Eq. (2.11). Even for the values of $x$ near the average turning point $a$, we have

$$\frac{\hbar}{2}\,|\partial_x\theta(a)|\simeq\frac{1}{2}\left(\frac{\beta}{a}\right)\frac{\hbar}{a}\ll\frac{\hbar}{a}\simeq|p(a)|, \tag{3.36}$$

where $\beta$ stands for the typical geometrical size of $\partial_x\theta(x)$. The estimate on the left-hand side is based on linear potentials (3.15), but we expect that the condition is satisfied for more general potentials as well. To conclude this section, we clarified the basic mechanism why the prefactor of the Landau-Zener formula (3.25) should come out to be very close to unity in time-independent perturbation theory.

## IV. POTENTIAL CURVE CROSSING AND QUANTUM COHERENCE

The effects of dissipative interactions on macroscopic quantum tunneling have been extensively analyzed in the path-integral formalism [13] and also in the canonical (field theoretical) formalism [14]. It is generally accepted that Ohmic dissipation suppresses the macroscopic quantum coherence; in fact, an attractive idea of a dissipative phase transition has been suggested [13].

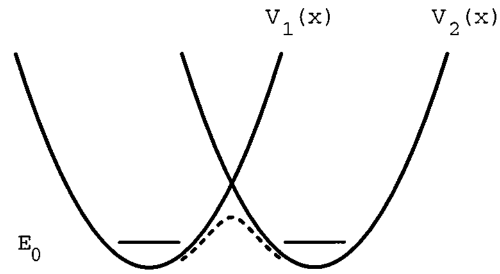


FIG. 3. Quantum coherence in the diabatic picture.

It is plausible that the effects of a potential curve crossing with nearby potentials influence the quantum coherence of the two degenerate ground states. Here we analyze the general features of the effects of potential crossing on quantum coherence on the basis of time-independent perturbation theory, which was confirmed in Sec. III to be reliable in limits of both weak and strong potential curve crossing interaction. We assume $V_2(x)=V_1(-x)$ and $V_2'(0)<0$. We thus analyze this problem from two different view points.

### A. Strong potential curve crossing interaction $g\gg 1$ (diabatic picture)

We start with the diabatic picture in Fig. 3, and incorporate the effects of the potential crossing interaction $\sigma_1/g$. That is, we (approximately) diagonalize the total Hamiltonian in the diabatic picture. By treating the last term of Eq. (2.1) as a perturbation for $g\gg 1$, we obtain the energy eigenvalues of the two lowest-lying states as (with $E_0$ the zeroth order degenerate energy eigenvalue)

$$E_{\pm}^{(1)}=E_0\mp\frac{1}{g}\int_{-\infty}^{\infty}dx\ \psi_L(x)\psi_R(x), \tag{4.1}$$

with the corresponding eigenfunctions

$$\Psi_+(x)\simeq\frac{1}{\sqrt{2}}\begin{pmatrix}\psi_L(x)\\ -\psi_R(x)\end{pmatrix}\equiv\frac{1}{\sqrt{2}}[e_+\psi_L(x)-e_-\psi_R(x)],$$

$$\Psi_-(x)\simeq\frac{1}{\sqrt{2}}\begin{pmatrix}\psi_L(x)\\ \psi_R(x)\end{pmatrix}\equiv\frac{1}{\sqrt{2}}[e_+\psi_L(x)+e_-\psi_R(x)]. \tag{4.2}$$

That is, both of these two states $\Psi_\pm(x)$ choose

$$e_+\psi_L(x)\quad\text{in the region of left valley,}$$

$$e_-\psi_R(x)\quad\text{in the region of right valley.} \tag{4.3}$$

The ''spin'' eigenstates $e_\pm$ and the ''space'' eigenstates $\psi_L(x)$ or $\psi_R(x)$ are strongly correlated. Note that one can conveniently think of the two potentials as spin-up and spin-down states. Originally, before we incorporate the perturbation $\sigma_1/g$ in Eq. (4.1), we have two energetically degenerate states with energy $E_0$ defined by

$$\Psi_L(x)=\begin{pmatrix}\psi_L(x)\\0\end{pmatrix}\equiv e_+\psi_L(x), \tag{4.4}$$

which is always a spin-up state, and

$$\Psi_R(x)=\begin{pmatrix}0\\\psi_R(x)\end{pmatrix}\equiv e_-\psi_R(x), \tag{4.5}$$

which is always a spin-down state.

In the strong potential crossing limit, $g\to\infty$, we have *no effect* of the conventional quantum tunneling in addition to the mixing in Eq. (4.2), since the conventional tunneling goes through the interaction $\sigma_1/g$ in Eq. (2.1), and thus higher-order effects in $1/g$.

We can find the $O(1/g)$ energy splitting in the WKB approximation. The left wave function $\psi_L(x)$ is given by Eq. (3.27) with $C_1=\sqrt{2m\omega/\pi}$. (For a sufficiently low-energy state such as the ground state, $\omega$ can be regarded as the curvature of the potential energy at the minimum.) The right wave function $\psi_R(x)$ is given by

$$\psi_R(x)=\begin{cases}\dfrac{C_2}{2\sqrt{|p_2(x)|}}\exp\left[-\dfrac{1}{\hbar}\displaystyle\int_x^{a_2}dx|p_2(x)|\right] & \text{for } x<a_2\\ \dfrac{C_2}{\sqrt{p_2(x)}}\cos\left[\dfrac{1}{\hbar}\displaystyle\int_{a_2}^{x}dx p_2(x)-\dfrac{\pi}{4}\right] & \text{for } x>a_2,\end{cases} \tag{4.6}$$

with $C_2=\sqrt{2m\omega/\pi}$. In the saddle-point approximation, we have the overlap integral

$$\begin{aligned}\int dx\,&\frac{1}{\sqrt{|p_1(x)||p_2(x)|}}\\&\times\exp\left[-\frac{1}{\hbar}\int_{a_1}^{x}dx|p_1(x)|+\frac{1}{\hbar}\int_{a_2}^{x}dx|p_2(x)|\right]\\&\simeq\frac{\sqrt{2\pi\hbar}}{\sqrt{m[V_1'(0)-V_2'(0)]}(-2mE)^{1/4}}\\&\times\exp\left[-\frac{1}{\hbar}\int_{a_1}^{0}dx|p_1(x)|+\frac{1}{\hbar}\int_{a_2}^{0}dx|p_2(x)|\right],\end{aligned} \tag{4.7}$$

which yields the energy splitting

$$\begin{aligned}E_-^{(1)}-E_+^{(1)}\simeq&\frac{\sqrt{2\hbar}}{g\sqrt{\pi[V_1'(0)-V_2'(0)]}}\left(\frac{m}{-2E_0}\right)^{1/4}\\&\times\exp\left\{-\frac{1}{\hbar}\int_{a_1}^{a_2}dx\sqrt{2m[\overline{V}(x)-E_0]}\right\}.\end{aligned} \tag{4.8}$$

In the above expression, we have defined $\overline{V}(x)$ as the following "$\Lambda$-shape" potential:

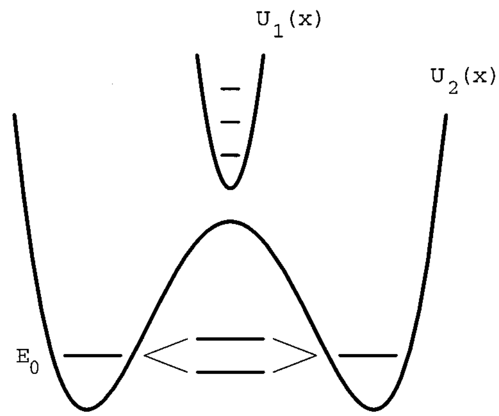


FIG. 4. Quantum coherence in the adiabatic picture.

$$\overline{V}(x)=\begin{cases}V_1(x) & \text{for } x<0\\V_2(x) & \text{for } x>0.\end{cases} \tag{4.9}$$

We recall that, when the upper adiabatic potential $U_1(x)$ is absent, the standard WKB formula gives the energy splitting of lowest levels [4],

$$E_--E_+\simeq\frac{\hbar\omega}{\pi}\exp\left\{-\frac{1}{\hbar}\int_{-a}^{a}dx\sqrt{2m[U_2(x)-E_0]}\right\}. \tag{4.10}$$

Comparing this with Eq. (4.8), we find that the quantum coherence is actually suppressed by two elements; the overall small coefficient $1/g\ll1$ and the exponential suppression factor; $\overline{V}(x)$ is always larger than the lower potential, $\overline{V}(x)>U_2(x)$.

### B. Weak potential curve crossing interaction $g\ll1$ (adiabatic picture)

In this case, we can use the gauge transformed adiabatic picture defined by Eq. (2.6). In this scheme, the low-lying eigenstates for $H_0'$ are described by the nearly degenerate two states in the lower potential curve $U_2(x)$; see Fig. 4. For a small $g$, the two potential curves $U_1(x)$ and $U_2(x)$ are widely separated. We thus take the ground states of the spin-down sector (i.e., the nearly degenerate two ground states of the lower potential curve),

$$\Phi_+(x)=\begin{pmatrix}0\\\varphi_{2+}(x)\end{pmatrix},\quad \Phi_-(x)=\begin{pmatrix}0\\\varphi_{2-}(x)\end{pmatrix}, \tag{4.11}$$

as the zeroth-order approximation of the lowest-lying states. These two states correspond to the conventional symmetric and antisymmetric tunneling eigenstates of the double-well potential $U_2(x)$, whose energy splitting gives the *order parameter* of the quantum coherence [13]. To the second order of the gauge field $\partial_x\theta(x)$, the energy eigenvalue is perturbed to

$$E_{\pm}^{(2)}=E_{\pm}+\langle\Phi_{\pm}|H_I'|\Phi_{\pm}\rangle-\sum_n \frac{|\langle\Phi_{1,n}|H_I'|\Phi_{\pm}\rangle|^2}{E_{1,n}-E_{\pm}}$$
$$=E_{\pm}+\frac{\hbar^2}{8m}\int dx[\partial_x\theta(x)]^2\varphi_{2\pm}(x)^2$$
$$-\frac{\hbar^2}{16m^2}\sum_n \frac{1}{E_{1,n}-E_{\pm}}$$
$$\times\left|\int dx\,\varphi_{1,n}(x)[\hat{p}\partial_x\theta(x)+\partial_x\theta(x)\hat{p}]\varphi_{2\pm}(x)\right|^2, \tag{4.12}$$

where $\Phi_{1,n}(x)$ [and $\varphi_{1,n}(x)$] is the $n$th energy eigenstate of the upper potential $U_1(x)$.

It is generally difficult to conclude the suppression or enhancement of the quantum coherence solely from the perturbation formula (4.12). The reason is that the effect of intermediate state sum can depend on the details of the upper potential curve. Nevertheless, when the well of the upper potential is narrow enough, we can show that the quantum coherence is always suppressed.

We first assume that the lowest-lying parity even- and odd-parity states are given, respectively, by a linear combination of the ground states in left and right wells:

$$\sigma_{2\pm}(x)=\frac{1}{\sqrt{2}}[\varphi_{2L}(x)\pm\varphi_{2R}(x)], \tag{4.13}$$

where in the WKB approximation in the classically forbidden region,

$$\varphi_{2L}(x)=\varphi_{2R}(-x)=\frac{C_2}{2\sqrt{|p_2(x)|}}\exp\left[-\frac{1}{\hbar}\int^x dx|p_2(x)|\right]. \tag{4.14}$$

The normalization constant is given by $C_2=\sqrt{2m\omega/\pi}$.

We next assume that the upper potential $U_1(x)$ is narrow enough and can be well approximated by a square well potential with the width $a$. The eigenfunctions in the upper potential are therefore given by

$$\varphi_{1,n}(x)=\left(\frac{2}{a}\right)^{1/2}\sin\left[\frac{n\pi}{a}\left(x+\frac{a}{2}\right)\right],\quad n=1,2,\ldots . \tag{4.15}$$

Moreover, since the gauge field $\partial_x\theta(x)$ defined in Eq. (2.10) is nonzero only within this narrow region, we may make the following replacements in integral (4.12):

$$\varphi_{2+}(x)\to\varphi_{2+}(0),\quad \varphi_{2-}(x)\to 0,$$
$$\hat{p}\varphi_{2+}(x)\to 0,\quad \hat{p}\varphi_{2-}(x)\to i|p_2(0)|\sigma_{2+}(0) \tag{4.16}$$

and

$$\hat{p}\varphi_{1,n}(x)\to -i|p_{1,n}|\left(\frac{2}{a}\right)^{1/2}\cos\left[\frac{n\pi}{a}\left(x+\frac{a}{2}\right)\right],$$
$$|p_{1,n}|\equiv\hbar\frac{n\pi}{a}. \tag{4.17}$$

Under these assumptions, the energy shift (4.12) is estimated for the even-parity state

$$E_{+}^{(2)}=E_{+}+\frac{\hbar^2}{8m}\int dx[\partial_x\theta(x)]^2\varphi_{2+}(0)^2$$
$$-\frac{\hbar^2}{16m^2}\sum_{n=1}^{\infty}\frac{|p_{1,n}|^2}{E_{1,n}-E_{+}}$$
$$\times\left|\int dx\left(\frac{2}{a}\right)^{1/2}\cos\left[\frac{n\pi}{a}\left(x+\frac{a}{2}\right)\right]\partial_x\theta(x)\right|^2\varphi_{2+}(0)^2. \tag{4.18}$$

By noting $|p_{1,n}|^2=2m[E_{1,n}-U_1(0)]$ and $U_1(0)>E_{+}$, we see that

$$\frac{\hbar^2}{16m^2}\frac{|p_{1,n}|^2}{E_{1,n}-E_{+}}=\frac{\hbar^2}{8m}\frac{E_{1,n}-U_1(0)}{E_{1,n}-E_{+}}<\frac{\hbar^2}{8m} \tag{4.19}$$

and thus

$$E_{+}^{(2)}>E_{+}+\frac{\hbar^2}{8m}\int dx[\partial_x\theta(x)]^2\varphi_{2+}(0)^2-\frac{\hbar^2}{8m}\sum_{n=0}^{\infty}$$
$$\times\left|\int dx\sqrt{\frac{2}{a}}\cos\left[\frac{n\pi}{a}\left(x+\frac{a}{2}\right)\right]\partial_x\theta(x)\right|^2\varphi_{2+}(0)^2$$
$$=E_{+}, \tag{4.20}$$

where we have added the $n=0$ mode to make the cosine functions a complete set. Therefore the perturbation always increases the ground-state energy.

On the other hand, Eq. (4.12) gives, for the odd-parity state,

$$E_{-}^{(2)}=E_{-}-\frac{\hbar^2}{16m^2}\sum_{n=1}^{\infty}\frac{|p_2(0)|^2}{E_{1,n}-E_{-}}$$
$$\times\left|\int dx\;\varphi_{1,n}(x)\partial_x\theta(x)\right|^2\varphi_{2+}(0)^2. \tag{4.21}$$

Since the second term of Eq. (4.21) is negative definite, we see that the perturbation always lowers the odd state energy,

$$E_{-}^{(2)}<E_{-}. \tag{4.22}$$

The perturbative corrections in Eqs. (4.18) and (4.21) are proportional to the wave function at the origin, which satisfies $\varphi_{2+}(0)^2\simeq m(E_{-}-E_{+})/[\hbar|p_2(0)|]$ [4], and therefore the correction to the energy splitting itself is proportional to the zeroth-order energy splitting $E_{-}-E_{+}$. Since the correction cannot excess the zeroth-order value in a reliable region of perturbation theory, we should have $E_-^{(2)} - E_+^{(2)} > 0$. By combining Eqs. (4.20) and (4.22), therefore, we find

$$0 < E_-^{(2)} - E_+^{(2)} < E_- - E_+, \tag{4.23}$$

which shows that the quantum coherence is suppressed.

Although we derived the suppression of quantum coherence for a very special configuration in the weak-coupling adiabatic picture, we expect that this suppression of quantum coherence is more general at least for small $g$. This is based on the following physical picture: When a particle tunnels the barrier in the lower potential curve, it has a small probability of crossing to the upper potential curve. This potential curve crossing means that the particle enters deep inside the tunneling region of the upper potential curve, and is repelled back by the upper potential (as is expected in the diabatic picture), which in turn leads to the suppression of quantum tunneling of the particle. This argument leads to the general suppression of quantum coherence by potential crossing. This is also consistent with the suppression of barrier transmission in the scattering process by nonadiabatic coupling in linear potential curve crossing [8].

Our explicit analyses both in weak and strong potential crossing interactions suggest the general suppression of quantum coherence by potential crossing, which is analogous to the effect of Ohmic dissipation on quantum coherence [13,14]. In this connection, we note that formula (4.12) and the Ohmic dissipation in the Caldeira-Leggett model [13] both correspond to a dipole approximation with the same selection rules. However, an analysis of the basically nonperturbative tunneling effect in second-order perturbation theory requires great care; for this reason, we were able to analyze explicitly only the very specific case in Eqs. (4.15)–(4.17). This suppression phenomenon of quantum coherence may become important in the future when one takes the effects of the environment into account in the analysis of potential curve crossing in physical and chemical processes.

## V. DISCUSSION AND CONCLUSION

Motivated by the presence of interesting weak and strong duality in the model Hamiltonian (2.1) of potential curve crossing, we reexamined a perturbative approach to potential crossing phenomena. We have shown that straightforward *time-independent* perturbation theory combined with zeroth-order WKB wave functions provides a reliable description of general potential crossing phenomena. Our analysis is based on the local data as much as possible without referring to global Stokes phenomena [12]. Formulated in this manner, perturbation theory becomes more flexible to cover a wide range of problems. From a perturbative view point, the treatment of the Landau-Zener formula in the adiabatic picture is most complicated, since it does not contain the coupling constant in the prefactor. We pointed out that this absence of a coupling constant in the prefactor is related to the presence of an interesting kinklike topological object in the present formulation of adiabatic picture. (The appearance of a topological object in the ''magnetic'' picture is reminiscent of gauge theory [11].) The absence of a coupling constant in the prefactor is thus perfectly consistent with perturbation theory, provided that a more precise criterion of the perturbation theory (2.11) is satisfied. In effect, we have explained why the prefactor of the Landau-Zener formula should come out to be very close to unity in perturbation theory.

The suppression of quantum coherence by potential curve crossing, which to our knowledge has not been discussed before in this context, has also been neatly formulated in our treatment, in the limits of both very strong and very weak potential crossing interactions. From the viewpoint of general gauge theory, it is not unlikely that the electric-magnetic duality in conventional gauge theory is also related to some generalized form of potential crossing in so-called moduli space [11]. We hope that our work may also turn out to be relevant from this viewpoint.

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