It is pointed out that there exists an interesting strong and weak duality in the Landau-Zener-Stueckelberg potential curve crossing. A reliable perturbation theory can thus be formulated in the both limits of weak and strong interactions. It is shown that 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. A kink-like topological object appears in the “magnetic” picture, which is responsible for the absence of the coupling constant in the prefactor of the Landau-Zener formula. It is also shown that quantum coherence in a double well potential is generally suppressed by the effect of potential curve crossing, which is analogous to the effect of Ohmic dissipation on quantum coherence.

1. Introduction

The potential curve crossing is related to a wide range of physical and chemical processes, and the celebrated Landau-Zener formula correctly describes the qualitative features of those processes. It has been recently shown that the potential crossing problem contains interesting modern field theoretical ideas, namely, the duality and gauge transformation.

The adiabatic and diabatic pictures in potential curve crossing problem are related to each other by a field dependent $su(2)$ gauge transformation, 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. This strong and weak duality allows a reliable perturbative treatment of potential curve crossing phenomena at the both limits of very weak (adiabatic picture) and very strong (diabatic picture) potential curve crossing interactions.

2. A 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:

$$ H = \frac{1}{2m} \dot{\vec{r}}^2 + \frac{V_1(x) + V_2(x)}{2} + \frac{V_1(x) - V_2(x)}{2} \sigma_3 + \frac{1}{g} \sigma_1 $$

where $\sigma_3$ and $\sigma_1$ stand for the Pauli matrices. We assume throughout this article that the potential crossing occurs at the origin, $V_1(0) = V_2(0) = 0$ (see Fig. 1).

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

$$ H_0 = \frac{1}{2m} \dot{\vec{r}}^2 + \frac{V_1(x) + V_2(x)}{2} + \frac{V_1(x) - V_2(x)}{2} \sigma_3. $$

This Hamiltonian $H_0$ describes two potentials, which are decoupled from each other. The last term in $H$, $H_I \equiv \sigma_1/g$ with a constant $g$, causes the transition between 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 viewpoint of adiabatic two-potential crossing in Fig. 2. Namely, $g$ stands for the strength of potential crossing interaction, and $g \to \text{large}$ corresponds to a very strong potential crossing interaction. On the other hand, if one lets $g \to \text{small}$, the effects of the last term in (1) become substantial and the Hamiltonian $H_0$ (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,”

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

(3)

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

$$H' = \frac{1}{2m} \left[ \frac{\hat{p}^2}{2} + \frac{U_1(x)}{2} \right] + \frac{V_1(x) + V_2(x)}{2} \cos \theta(x) + \frac{1}{g} \sin \theta(x) \sigma_3,$$

(4)

To eliminate the potential curve mixing, the last term of (5), we choose the gauge parameter $\theta(x)$ as

$$\cot \theta(x) = \frac{V_1(x) - V_2(x)}{2} = f(x).$$

(5)

We then obtain the Hamiltonian in the adiabatic picture

$$H' = H'_0 + H'_I,$$

(6)

where

$$H'_0 = \frac{1}{2m} \hat{p}^2 + \frac{U_1(x) + U_2(x)}{2} + \frac{U_1(x) - U_2(x)}{2} \sigma_3,$$

(7)

and

$$H'_I = \frac{\hbar}{4m} [\hat{p} \partial_x \theta(x) + \partial_x \theta(x) \hat{p}] \sigma_2 \quad \text{and} \quad \frac{\hbar^2}{8m} [\partial_x \theta(x)]^2.$$
The potential energies in the adiabatic picture are related to those in the diabatic picture as (Fig. 2)

\[
U_{1,2}(x) = \frac{V_1(x) + V_2(x)}{2} \pm \sqrt{\left[\frac{V_1(x) - V_2(x)}{2}\right]^2 + \frac{1}{g^2}}. \quad (9)
\]

From the definition of the gauge parameter in (5), the “gauge field” \( \partial_x \theta(x) \) is expressed as

\[
\partial_x \theta(x) = -\frac{f'(x)}{1 + f(x)^2}. \quad (10)
\]

The transition from the diabatic picture to the adiabatic picture is a field dependent transformation.

In the adiabatic picture, the \( \sigma_2 \) dependent term in the interaction \( H'_i \) 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 (10) and (5).

We thus conclude that the two extreme limits of potential crossing interaction should be reliably handled in perturbation theory; namely, 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. 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 is

\[
\frac{\hbar}{2} |\partial_x \theta(x)| \ll |p(x)|, \quad (11)
\]

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

3. Landau-Zener formula

As an illustration of the duality discussed in Section 3, we re-examine a perturbative derivation of the Landau-Zener formula in both of the adiabatic and diabatic pictures. 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 \( H'_1 \). We define the initial and final states \( \Phi_i \) and \( \Phi_f \) by

\[
\Phi_i(x) = \begin{pmatrix} \varphi_1(x) \\ 0 \end{pmatrix}, \quad \Phi_f(x) = \begin{pmatrix} 0 \\ \varphi_2(x) \end{pmatrix}, \quad (12)
\]

which satisfy

\[
\begin{aligned}
\left[ \frac{1}{2m} \dot{p}^2 + U_1(x) \right] \varphi_1(x) &= E \varphi_1(x), \\
\left[ \frac{1}{2m} \dot{p}^2 + U_2(x) \right] \varphi_2(x) &= E \varphi_2(x).
\end{aligned} \quad (13)
\]

We then obtain the potential curve crossing probability due to the perturbation \( H'_i \)

\[
w(i \to f) = \frac{2\pi}{\hbar} |\langle \Phi_f | H'_i | \Phi_i \rangle|^2. \quad (14)
\]

The transition matrix element is given by

\[
\langle \Phi_f | H'_i | \Phi_i \rangle = -\frac{\hbar^2}{4m} \int_{-\infty}^{\infty} dx \partial_x \theta(x) \quad (15)
\]

\[
\times \left[ -\varphi_2(x) \varphi_2'(x) + \varphi_2(x) \varphi_1'(x) \right].
\]

To evaluate the matrix element, we use the WKB wave functions:

\[
\varphi_1(x) = \begin{cases} 
\frac{C_1}{2\sqrt{|p_1(x)|}} \exp \left[ -\frac{1}{\hbar} \int_{a_1}^{x} dx |p_1(x)| \right], \\
\frac{C_1}{\sqrt{|p_1(x)|}} \cos \left[ \frac{1}{\hbar} \int_{a_1}^{x} dx p_1(x) - \frac{\pi}{4} \right],
\end{cases} \quad (16)
\]

for \( x > a_1 \) and \( x < a_1 \), respectively, and

\[
\varphi_2(x) = \begin{cases} 
\frac{C_2}{2\sqrt{|p_2(x)|}} \exp \left[ -\frac{1}{\hbar} \int_{a_2}^{x} dx |p_2(x)| \right], \\
\frac{C_2}{\sqrt{|p_2(x)|}} \cos \left[ \frac{1}{\hbar} \int_{a_2}^{x} dx p_2(x) - \frac{\pi}{4} \right],
\end{cases} \quad (17)
\]
for $x > a_2$ and $x < a_2$, respectively. The semi-classical momenta in the adiabatic picture are defined by

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

and $a_1$ and $a_2$ denote the classical turning points (see Fig. 2). 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 (14) 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 (15) 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 (15) is then written as

$$\langle \Phi_f | H_f | \Phi_i \rangle \simeq -\frac{i\hbar C_1 C_2}{8m} \int dx \partial_x \theta(x) \quad (21)$$

$$\times \left\{ \exp \left[ i \int_{x_1}^{x} dx p_1(x) - i \int_{a_2}^{x} dx p_2(x) \right] - \exp \left[ - i \int_{a_1}^{x} dx p_1(x) + i \int_{a_2}^{x} dx p_2(x) \right] \right\},$$

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

$$I \equiv \int_{-\infty}^{\infty} dx \partial_x \theta(x) \quad (22)$$

$$\times \exp \left[ \frac{i}{\hbar} \int_{a_1}^{x} dx p_1(x) - \frac{i}{\hbar} \int_{a_2}^{x} dx p_2(x) \right].$$

We here present an explicit evaluation of (22) 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 (11)],

$$\int_{0}^{x} dx [p_1(x) - p_2(x)] \quad (23)$$

$$\simeq -\int_{0}^{x} dx \frac{2}{v(x)g \beta} \sqrt{x^2 + \beta^2}$$

where we used

$$f(x) = g \frac{V_1'(0) - V_2'(0)}{2} x = \frac{x}{\beta^2}, \quad (24)$$

$$v(x) = \frac{1}{m} \sqrt{2m \left[ E - \frac{U_1(x) + U_2(x)}{2} \right]}$$

and $v(x)$ is approximated to be a constant $v = v(0)$ in the following. We also have from (14)

$$\partial_x \theta(x) = -\frac{\beta}{x^2 + \beta^2} \quad (25)$$

and thus

$$I \simeq -\exp \left[ \frac{i}{\hbar} \int_{a_1}^{0} dx p_1(x) - \frac{i}{\hbar} \int_{0}^{a_2} dx p_2(x) \right]$$

$$\times \int_{-\infty}^{\infty} dx \frac{\beta}{x^2 + \beta^2} \exp \left( -\frac{2i}{\hbar vg \beta} \int_{0}^{x} dx \sqrt{x^2 + \beta^2} \right)$$

$$= \exp \left[ \frac{i}{\hbar} \int_{a_1}^{0} dx p_1(x) - \frac{i}{\hbar} \int_{0}^{a_2} dx p_2(x) \right]$$

$$\times \int_{-\infty}^{\infty} dx \exp [\mp i\alpha F(x)] \quad (26)$$

where

$$F(x) \equiv \int_{0}^{x} dx \sqrt{x^2 + 1 + \frac{1}{i\alpha} \ln(x^2 + 1)},$$

$$\alpha \equiv \frac{2\beta}{\hbar vg} = \frac{4}{\hbar vg^2[V_1'(0) - V_2'(0)]} > 0. \quad (27)$$
We evaluate the integral \( I \) by a saddle point approximation with respect to \( \alpha \). We thus seek the saddle point
\[
F'(x) = \sqrt{x^2 + 1} + \frac{1}{i\alpha} x^2 + \frac{2x}{i\alpha} = 0,
\]
which is located between the real axis and the pole positions \( x = \pm i \) of \( \partial_x \theta(3x) \) 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 (28) for \(-1 < y < 1\), one has
\[
\sqrt{1-y^2} = -\frac{1}{2\alpha} \frac{2y}{1-y^2} \quad \text{(29)}
\]
which has a unique solution
\[
x_s = iy_s \simeq -i + \frac{i}{2} \left( \frac{2}{\alpha} \right)^{2/3} \quad \text{(30)}
\]
for large \( \alpha \). (The complex conjugate of \( x_s \) is located in the second Riemann sheet.) For this value of the saddle point
\[
F(x_s) = \int_0^{x_s} dx \sqrt{x^2 + 1} + \frac{1}{i\alpha} \ln \left( \frac{2}{\alpha} \right)^{2/3} \simeq -\frac{\pi i}{4} + \frac{2i}{3\alpha} + \frac{1}{i\alpha} \ln \left( \frac{2}{\alpha} \right)^{2/3},
\]
\[
F''(x_s) \simeq -3i \left( \frac{\alpha}{2} \right)^{1/3}. \quad \text{(31)}
\]
We thus have a Gaussian integral which decreases in the direction parallel to the real axis
\[
I \simeq -\left( \frac{\alpha}{2} \right)^{2/3} e^{2/3} \exp \left( -\frac{\pi \alpha}{4} \right) \quad \text{(32)}
\]
\[
\times \exp \left[ \frac{i}{\hbar} \int_{a_1}^{0} dx \, p_1(x) - \frac{i}{\hbar} \int_{a_2}^{0} dx \, p_2(x) \right] \times \int_{-\infty}^{\infty} dx \exp \left[ -3 \left( \frac{\alpha}{2} \right)^{4/3} (x-x_s)^2 \right] \times \exp \left[ \frac{i}{\hbar} \int_{a_1}^{0} dx \, p_1(x) - \frac{i}{\hbar} \int_{a_2}^{0} dx \, p_2(x) \right]
\]
From (29) we obtain
\[
\langle \Phi_f | H_f | \Phi_i \rangle \simeq -\sqrt{\frac{\pi}{3}} \times \left( \frac{3}{2} \right)^{2/3} \sqrt{\frac{\hbar}{2\pi}} \times \sin \left\{ \frac{1}{\hbar} \left[ \int_{a_1}^{0} dx \, p_1(x) - \int_{a_2}^{0} dx \, p_2(x) \right] \right\} \times \exp \left\{ -\frac{\pi}{\hbar g^2 |V_1(0) - V_2(0)|} \right\} \quad \text{(33)}
\]
It is interesting that the numerical value of the coefficient of the above expression, \( \sqrt{\pi e^{2/3}}/\sqrt{3} = 1.99317 \), is very close to the canonical value 2, and we replace it by 2 in the following. As for the past analysis of the prefactor in the time-dependent perturbation theory, see papers in [1]. We thus have the transition probability from (34)
\[
w(i \to f) \simeq 4 \sin^2 \left\{ \frac{1}{\hbar} \left[ \int_{a_1}^{0} dx \, p_1(x) - \int_{a_2}^{0} dx \, p_2(x) \right] \right\} \times \exp \left\{ -\frac{2\pi}{\hbar g^2 |V_1(0) - V_2(0)|} \right\} \quad \text{(34)}
\]
where we replaced the square of sine function by its average 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 (34) expresses twice the non-adiabatic 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 the half of (34).
\[
P(1 \to 2) \simeq \exp \left\{ -\frac{2\pi}{\hbar g^2 |V_1(0) - V_2(0)|} \right\}, \quad \text{(35)}
\]
which is the celebrated Landau-Zener formula [4]. Our perturbative derivation presented here is conceptually much simpler than the past works [1, 5], and it should 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 \( g \). The evaluation of the matrix element is the standard one described in the textbook of Landau and Lifshitz [4], for example. We have
for \( E > 0 \),
\[
w(i \to f) \simeq \frac{8\pi}{h v(0) g^2 [V'_1(0) - V'_2(0)]} \\
\times \cos^2 \left[ \frac{1}{\hbar} \int_0^{a_2} dx p_2(x) - \frac{1}{\hbar} \int_0^{a_1} dx p_1(x) - \frac{\pi}{4} \right] \\
\simeq \frac{8\pi}{h v(0) g^2 [V'_1(0) - V'_2(0)]}.
\]

\([v(0)]\) is the velocity at the crossing point, \( v(0) = \sqrt{2E/m} \). We again interpret \((33)\) 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 the half of \((36)\).

A simple interpolating formula, which reproduces \((33)\) in the weak coupling limit and \((36)\) in the strong coupling limit, is given by
\[
w(i \to f) \simeq 2 \exp \left\{ - \frac{2\pi}{h v g^2 [V'_1(0) - V'_2(0)]} \right\} \\
\times \left( 1 - \exp \left\{ - \frac{2\pi}{h v g^2 [V'_1(0) - V'_2(0)]} \right\} \right)
\]

This expression is also consistent with the (semiclassical) conservation of probability \([1]\).

Motivated by duality, we re-examined a perturbative derivation of the Landau-Zener formula, and we re-derived the formula \((33)\) including its numerical coefficient on the basis of perturbation theory. However, our final result \((33)\) 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 \([1]\), the “gauge field” satisfies the relation
\[
\int_{-\infty}^{\infty} dx \partial_x \theta(x) = \theta(\infty) - \theta(-\infty) = -\pi,
\]
which is independent of the coupling constant \( g \); we assume \( f(x) \to \pm \infty \) for \( x \to \pm \infty \), respectively. Because of this kink-like 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 well covers the geometrical size of \( \partial_x \theta(x) \). The precise criterion of the validity of perturbation theory is thus given by \([1]\).

This condition is in fact satisfied if the conditions \([14]\)–\((20)\) are satisfied. For small values of \( x \), the small coupling \( g \) helps to satisfy \([11]\). Even for the values of \( x \) near the average turning point \( a \), we have
\[
\frac{\hbar}{2} |\partial_x \theta(a)| \simeq \frac{1}{2} \left( \frac{\beta}{a} \right) \frac{\hbar}{a} \ll \frac{\hbar}{a} \simeq |p(a)|, \tag{39}
\]
where \( \beta \) stands for the typical geometrical size of \( \partial_x \theta(x) \). The estimate in the left hand side is based on linear potentials \((25)\), but we expect that the condition is satisfied for more general potentials as well. We thus clarified the basic mechanism why the prefactor of the Landau-Zener formula \((33)\) should come out to be very close to unity in time-independent perturbation theory.

4. Discussions

Motivated by the presence of interesting weak and strong duality in the model Hamiltonian \([1]\) of potential curve crossing, we re-examined a perturbative approach to potential crossing phenomena. We have shown that straightforward time-independent perturbation theory combined with the 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. Formulated in this manner, perturbation theory becomes more flexible to cover a wide range of problems.

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

It is plausible that the effects of potential curve crossing with nearby potentials influence the quantum coherence of the two degenerate ground states. One can in fact confirm that the potential curve crossing generally suppress the quantum coherence by using the perturbation
theory for both limits of strong and weak curve crossing interactions \cite{11}. From a viewpoint of symmetry, the lowest order perturbation in the present problem and the dissipative interaction in the Caldeira-Leggett model \cite{14} both correspond to a dipole approximation. However, a perturbative analysis of basically non-perturbative tunneling phenomena requires a great care. In Ref. \cite{11}, an explicit calculation of rather limited configurations has been performed, which in fact indicates the general suppression of quantum coherence by potential curve crossing. 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 processes.

From a 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 the so-called moduli space \cite{12}. We hope that our work may turn out to be relevant from this viewpoint also.

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