

Integral definition of transition time in the Landau-Zener model

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We give a general definition for the transition time in the Landau-Zener model. This definition allows us to compute numerically the Landau-Zener transition time at any sweeping rate without ambiguity in both diabatic and adiabatic bases. With this new definition, analytical results are obtained in both the adiabatic limit and the sudden limit.

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I. INTRODUCTION

Tunneling is one of many fundamental quantum processes that have no classical counterparts. It exists ubiquitously in quantum systems and is a key to understanding many quantum phenomena [1–12]. Discussions on tunneling can be found in all textbooks on quantum mechanics. However, these discussions are mainly focused on the probability of tunneling from one quantum state to another or from one side of a potential barrier to the other. In contrast, there are few extensive and in-depth discussions in the literature on another aspect of tunneling, the time of tunneling, that is, how long it takes a particle to tunnel through a potential barrier. [13–22]. This disparity is partly caused by the difficulty of properly defining tunneling times in many situations.

The difficulty of having a proper definition for tunneling time has its root in the wave or probabilistic nature of quantum mechanics and is best demonstrated in the example of a wave packet tunneling through a potential barrier. In this case, one would intuitively define the tunneling time as the time spent by the peak (or centroid) of the wave packet under the barrier. However, as pointed out by Landauer and Martin [19], if this definition is used, a packet could leave the barrier before entering it. To overcome this difficulty, many different definitions have been suggested [19–22], and no clear consensus has been reached so far [19]. As a result, due to this lack of a general definition for tunneling time, one usually has to define the tunneling time case by case.

The focus of this study is on the transition time in the Landau-Zener (LZ) model [23,24], which describes a transition between two quantum states under a linearly changing external field. In fact, for the LZ model, because there is no tunneling in space, the “tunneling time” is usually called transition time [25–27]. We shall follow this convention in this paper. The transition in the LZ model is much simpler than the wave packet and barrier system because there is no complication of the wave packet distortion by the barrier. Nevertheless, a proper definition of transition time in this model is still missing in spite of the studies in the past by many authors. Mullen *et al.* [25] discussed the LZ transition time in the diabatic basis for the two limiting cases, the adiabatic limit and the sudden limit. They found that, for large Δ (the adiabatic limit), the transition time scales with Δ/α and for small Δ (the sudden limit), the transition time is about $\sqrt{\hbar/\alpha}$, where Δ is the minimal energy gap between the two eigenstates in the LZ model and α is the sweeping rate. However, Mullen *et al.* did not give a general definition for the transition time.

Vitanov [26,27] has made a much more thorough study on the LZ transition time and gave a definition for the transition time in both the diabatic basis and the adiabatic basis. However, his definition fails generally in the adiabatic basis.

In this paper we give a general definition for the transition time in the LZ model. We show both analytically and numerically that this definition yields reasonable results at any sweeping rate in both adiabatic basis and diabatic basis. With this general definition, we are able to reproduce the previous results obtained by Mullen *et al.* [25] and Vitanov [26,27]. Furthermore, we are able to compute analytically the transition time in the adiabatic basis at the adiabatic limit, which is proportional to Δ/α . This, to our best knowledge, has not been obtained before.

Besides its theoretical significance, our work has also potential applications. In the Monte Carlo simulation of quantum flipping of spins in molecular magnets, the authors in Ref. [28] have used an empirical formula for the LZ transition time. This formula, given by $\sqrt{\Delta^2/\alpha^2 + 2\hbar/\alpha}$ and interpolating the two limiting results in Ref. [25], is not well founded. With this newly proposed definition, one no longer needs this empirical formula to do the Monte Carlo simulation.

We note here that it is important to study the transition time in both the diabatic basis and the adiabatic basis. For the case of the flipping of spin under a sweeping magnetic field [28], the diabatic basis is a better choice. For the transition between Bloch bands under a constant force, it is better to use the adiabatic basis [29].

Our paper is organized as follows. In Sec. II and Sec. III, we introduce our definition of the transition probability function and transition time in the LZ model and we analyze the effectiveness of our definition. In Sec. IV, we present our results of the transition times, which include the analytical results at the adiabatic limit and the sudden limit and the numerical results for the general case. Our results are given in both the diabatic basis and the adiabatic basis. In the last section, we discuss our results and conclude.

II. TWO DEFINITIONS OF THE TRANSITION PROBABILITY FUNCTION

A. Transition probability function in the diabatic picture

The LZ model is a two-level system and is described by [23,24]

$$i\hbar \frac{d}{dt} \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \mathcal{H}(\gamma) \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}, \quad (1)$$

where

$$\mathcal{H}(\gamma) = \begin{pmatrix} \gamma/2 & \Delta/2 \\ \Delta/2 & -\gamma/2 \end{pmatrix}, \quad (2)$$

with $\gamma = \alpha t$ changing with time linearly with sweeping rate α . We describe the transition probability in both the diabatic basis and the adiabatic basis [26,27]. Provided the system is initially in state $(1, 0)$, in the diabatic basis, the transition probability is

$$P_d(t) = |b(t)|^2. \quad (3)$$

This is the projection of the state vector $|\psi(t)\rangle = (a, b)$ to the base vector $(0, 1)$. Similarly, by projecting the state vector $|\psi(t)\rangle$ to the second instantaneous eigenstate $|e_2(t)\rangle$ of \mathcal{H} , we have the transition probability in the adiabatic basis,

$$P_a(t) = |\langle \psi(t) | e_2(t) \rangle|^2. \quad (4)$$

Note that in all of our discussion the initial state is always $a(-\infty) = 1, b(-\infty) = 0$.

B. Transition probability function in the adiabatic picture

The LZ model in Eq. (8) is in fact written in the diabatic basis. It can be equivalently written in the adiabatic basis. To do so, we diagonalize $\mathcal{H}(t)$ in Eq. (2) [30],

$$S^+(t)\mathcal{H}(t)S(t) = H(t) = \begin{pmatrix} E_1(t) & 0 \\ 0 & E_2(t) \end{pmatrix}, \quad (5)$$

where the unitary transformation matrix is given by

$$S(t) = \begin{pmatrix} \cos \theta(t) & \sin \theta(t) \\ -\sin \theta(t) & \cos \theta(t) \end{pmatrix}, \quad (6)$$

and $E_{1,2}(t) = \mp \frac{1}{2} \sqrt{\alpha^2 t^2 + \Delta^2}$ are two instantaneous energy levels of the Hamiltonian $\mathcal{H}(t)$. In addition, $\tan 2\theta(t) = -\Delta/\alpha t$ ($0 \leq 2\theta < \pi$). For a state expressed in the adiabatic picture

$$|\psi(t)\rangle = \vartheta_1(t)|e_1(t)\rangle + \vartheta_2(t)|e_2(t)\rangle, \quad (7)$$

where $|e_1(t)\rangle$ and $|e_2(t)\rangle$ are two adiabatic instantaneous eigenstates of the Hamiltonian in Eq. (2) corresponding to energy levels $E_1(t)$ and $E_2(t)$, respectively. The time evolution is given by

$$i\hbar \frac{d}{dt} \begin{pmatrix} \vartheta_1(t) \\ \vartheta_2(t) \end{pmatrix} = \mathcal{H}_A(t) \begin{pmatrix} \vartheta_1(t) \\ \vartheta_2(t) \end{pmatrix}. \quad (8)$$

The Hamiltonian \mathcal{H}_A is given by [30,31]

$$\mathcal{H}_A(t) = H(t) - i\hbar S^+(t) \frac{dS(t)}{dt} = \begin{pmatrix} E_1(t) & m^*(t) \\ m(t) & E_2(t) \end{pmatrix}, \quad (9)$$

where

$$m(t) = i\hbar \frac{\Delta\alpha}{2(\Delta^2 + \alpha^2 t^2)}. \quad (10)$$

In the adiabatic picture, we can similarly define the transition probability. The transition probability function in the diabatic basis is defined as

$$\mathcal{P}_d(t) = |\langle \psi_2 | \psi(t) \rangle|^2, \quad (11)$$

where $|\psi_2\rangle = (0, 1)$. And the transition probability in the adiabatic basis is defined as

$$\mathcal{P}_a(t) = |\vartheta_2(t)|^2. \quad (12)$$

The diabatic and adiabatic pictures presented here are equivalent mathematically. In our following discussion, we shall use mostly the diabatic picture because the LZ model is commonly written in the diabatic basis. However, as we shall see, the adiabatic picture sometimes offers great insights into the results.

III. DEFINITION OF THE TRANSITION TIME

In our discussion, we use the subscripts d and a to indicate the diabatic basis and adiabatic basis, respectively. When our discussion is independent of the basis, we will remove the subscripts and simply use P for both P_d and P_a . Both analytical and numerical approaches will be used. The analytical approach is used for two limiting cases, the adiabatic limit and the sudden limit. We introduce a ‘‘quickness’’ parameter

$$\eta \equiv \frac{2\hbar\alpha}{\Delta^2}; \quad (13)$$

the adiabatic limit is $\eta \ll 1$ while $\eta \gg 1$ corresponds to the sudden limit.

The time evolution of the transition probability function $P(t)$ can be found by numerically solving Eq. (8). A typical result of $P(t)$ is shown in Fig. 1, where we see a sharp transition occurs around $t = 0$ and is followed by decaying oscillations. This observation suggests an intuitive (or natural) definition for the transition time. One may first fit the P curve with a smooth steplike function [dashed line in Fig. 1(a)], and then define the half-width of its time derivative [dashed line in Fig. 1(b)] as the transition time. However, like its counterpart in the wave packet and barrier system, this kind of intuitive definition of transition time fails because of its two shortcomings. First, there are numerous methods to find the fitting steplike function in Fig. 1(a); there is no obvious criterion by which one can judge which method is better than the other. Second, at the adiabatic limit, the P curve looks drastically different from the typical case in Fig. 1(a). As shown in Fig. 2, P is a

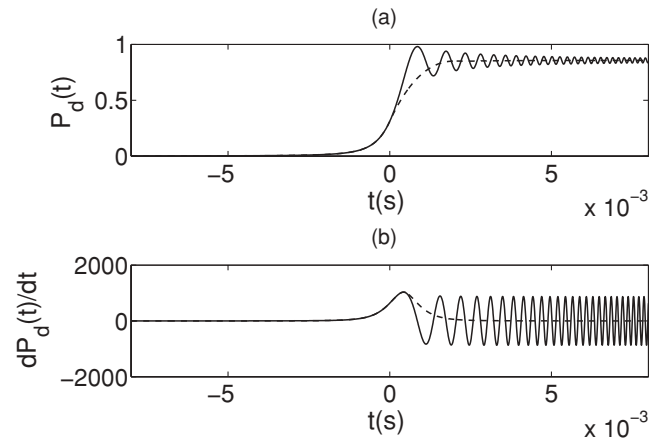


FIG. 1. (a) Time evolution of the transition probability function $P_d(t)$ (solid line) and its steplike function fit (dashed line). (b) The time derivative of the two functions in (a) and $\eta = 0.2565$. t is in units of seconds.

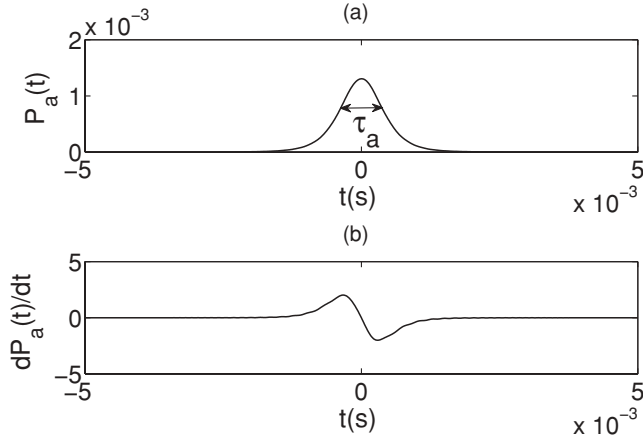


FIG. 2. (a) Time evolution of transition probability $P_a(t)$ and (b) its time derivative $dP_a(t)/dt$ at the adiabatic limit for $\eta = 0.1425$. t is in units of seconds in both figures and $dP_a(t)/dt$ is in units of inverse seconds.

single-peaked function, which would be difficult to fit it with a steplike function. These two drawbacks show that this intuitive definition of the transition time based on curve-fitting is not a good choice. One has to find an alternative.

In Ref. [27], Vitanov introduced a definition for the LZ transition time in both bases, which he called jump time. His definition is

$$\tau = \frac{P(\infty)}{P'(0)}, \quad (14)$$

where the time derivative value $P'(0)$ at $t = 0$ is used to represent the rate of the transition around $t = 0$. For the typical time evolution of the transition probability function $P(t)$ shown in Fig. 1, this definition works well. However, Vitanov's definition does not work in the adiabatic basis in general because the jump time defined in Eq. (14) tends to over-represent the transition time. We explain this point in detail in the following.

For clarity, we consider the transition in the adiabatic limit. In the diabatic basis, as seen in Fig. 3(a), almost nothing happens before the transition region around $t = 0$. This is

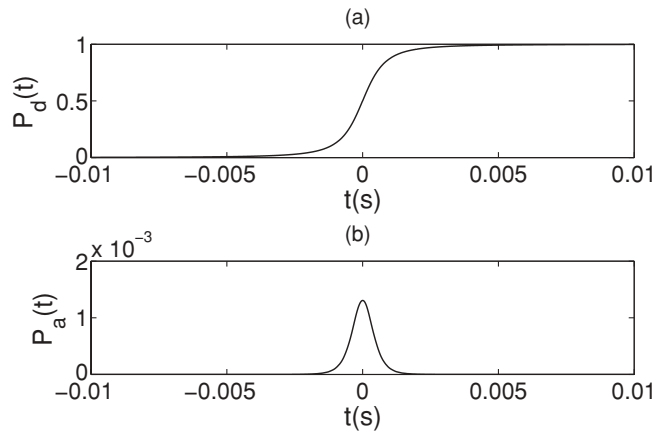


FIG. 3. Time evolution of the transition probability $P(t)$ in the adiabatic limit in (a) the diabatic basis and (b) the adiabatic basis for $\eta = 0.1425$. t is in units of seconds.

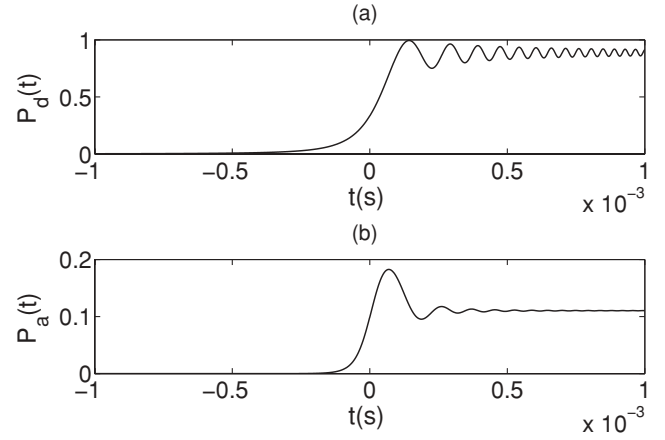


FIG. 4. Time evolution of the transition probability in (a) the diabatic basis and (b) the adiabatic basis respectively. $\eta = 1.425$. t is in units of seconds.

followed by a sharp increase around $t = 0$, which indicates that the spin flips with a slowly changing magnetic field. The transition probability function $P_d(t)$ immediately reaches its saturation value, signaling the end of the transition. With this in mind, we now look at the transition process in the adiabatic basis. As shown in Fig. 3(b), before $t = 0$ the transition function $P_a(t)$ looks very similar to what occurs in the diabatic basis: Nothing happens at first then a sharp increase follows. However, after $t = 0$, the function $P_a(t)$ starts to drop sharply and relax to a small value. The reason is simple. Before $t = 0$ the adiabatic basis is similar to the diabatic basis; in contrast, after $t = 0$ the two bases becomes very different, representing almost opposite spin states.

This evolution of a sharp increase followed by a drop persists for all the sweeping rates for the transition process $P_a(t)$ in the adiabatic basis. One example for nonadiabatic evolution is shown in Fig. 4. Because of this feature, the transition rate at $t = 0$ in the adiabatic basis tends to over-represent the overall transition.

We overcome these difficulties and find a general definition of the transition time. In the definition, we first find a $t' < 0$ such that

$$P(t') = \frac{1}{2} P_{\max}, \quad (15)$$

where P_{\max} is the maximum value of P when $t \leq 0$. Usually, $P_{\max} = P(t = 0)$. This condition will be called the half-width condition from now on for ease of reference. We then introduce two more variables

$$S_1 = \int_{-\infty}^0 \frac{d}{dt} P(t) dt = P(0), \quad (16)$$

$$S_2 = \int_0^{\infty} \frac{d}{dt} P(t) dt = P(\infty) - P(0), \quad (17)$$

which are the left ($t < 0$) area and right ($t > 0$) area of the dP/dt curve, respectively. With these defined variables, we define the transition time as

$$\tau = |t'| \left(1 + \left| \frac{S_2}{S_1} \right| \right). \quad (18)$$

Three quick remarks are in order. (i) The three variables in the definition can be computed without any ambiguity.

(ii) For the typical case shown in Fig. 1, we have $S_1 \approx S_2$ and, therefore, $\tau = 2|t'|$, which is in agreement of the “intuitive” definition that we discussed before. (iii) The absolute value is used because S_2 can be negative in certain cases, for example, the case in Fig. 2. The reason for the appearance of negative S_2 is that the transition around $t = 0$ overshoots the overall transition $P(\infty) - P(-\infty)$ and the system needs some time to relax.

For a general case, we have to resort to the numerical method. We first solve numerically the equation of motion Eq. (8), then compute the transition probability function $P(t)$, and finally find the transition time with our definition in Eq. (18). In our computation, we use $\Delta = 1.2 \times 10^{-7} k_b$, where k_b is Boltzmann’s constant, which is a typical value in a molecular magnet [12].

The transition time will be computed in both the adiabatic basis and the diabatic basis. For clarity, we shall use τ_d for the transition time in the diabatic basis and τ_a for the transition time in the adiabatic basis.

The typical transition probability functions $P(t)$ in both the adiabatic basis and diabatic basis are shown in Fig. 4. Obviously, the transition includes two different processes: (1) the time it takes the system to “jump” around $t = 0$; (2) the time it takes the system to relax and finally reach its asymptotic value $P(\infty)$. A proper definition of the transition time should include both the jump time and the relaxation time. This is particularly important in the adiabatic basis where the relaxation process is very prominent. In Refs. [26,27], Vitanov treated the two processes separately. By contrast, our definition integrates them together.

IV. TRANSITION TIMES IN THE DIABATIC BASIS

We first consider the diabatic basis and follow it with a discussion on the adiabatic basis in the next section.

A. Analytical results

At the adiabatic limit ($\eta \ll 1$), according to Vitanov [26,27]

$$P_d(t) \approx \frac{1}{2} + \frac{\alpha t}{2\sqrt{\alpha^2 t^2 + \Delta^2}}, \quad (19)$$

and the variable t' can be obtained from the half-width condition

$$P_d(t)|_{t=t'} = \frac{1}{2} [P_d(t \leq 0)]_{\max} = \frac{1}{4}. \quad (20)$$

The result is

$$t' = -\frac{\sqrt{3}}{3} \frac{\Delta}{\alpha}. \quad (21)$$

Since we have $S_1 = S_2$ for the transition curve Eq. (19), the transition time with our definition of Eq. (18) is

$$\tau_d^a = \frac{2\sqrt{3}}{3} \frac{\Delta}{\alpha}, \quad (22)$$

which agrees well with the result of Mullen *et al.* [25].

At the sudden limit $\eta \gg 1$, it is beneficial to take a transformation

$$a(t) = \tilde{a}(t) \exp\left(-i \frac{\alpha t^2}{4\hbar}\right), \quad (23)$$

$$b(t) = \tilde{b}(t) \exp\left(i \frac{\alpha t^2}{4\hbar}\right). \quad (24)$$

As a result, the diagonal terms in the Hamiltonian are transformed away and we can expand $\tilde{a}(t)$ and $\tilde{b}(t)$ in powers of η (effectively, Δ) [25]. For the initial condition $a(-\infty) = 1$ and $b(-\infty) = 0$, we obtain

$$a(t) = \left[1 + \sum_{k=1}^{\infty} (-1)^k \frac{1}{(2\eta)^k} a_{2k}(y)\right] \exp\left(-i \frac{y^2}{4}\right), \quad (25)$$

$$b(t) = \left[\sum_{k=1}^{\infty} (-1)^{k+1} \frac{1}{i(2\eta)^{k/2}} b_{2k-1}(y)\right] \exp\left(i \frac{y^2}{4}\right), \quad (26)$$

where

$$a_n(y) = \int_{-\infty}^y \exp(ix_1^2/2) \int_{-\infty}^{x_1} \exp(-ix_2^2/2) \cdots \int_{-\infty}^{x_{n-1}} \exp[(-1)^{n+1} ix_n^2/2] dx_1 dx_2 \cdots dx_{n-1} dx_n, \quad (27)$$

$$b_n(y) = \int_{-\infty}^y \exp(-ix_1^2/2) \int_{-\infty}^{x_1} \exp(ix_2^2/2) \cdots \int_{-\infty}^{x_{n-1}} \exp[(-1)^n ix_n^2/2] dx_1 dx_2 \cdots dx_{n-1} dx_n, \quad (28)$$

with $y = t/(\hbar/\alpha)^{1/2}$. At the sudden limit, it is sufficient to keep Eq. (26) to the lowest order of $1/\eta$. Consequently, we obtain

$$\begin{aligned} P_d(t) &= |b(t)|^2 \approx \left| \frac{1}{\sqrt{2\eta}} \int_{-\infty}^y \exp\left(-i \frac{x^2}{2}\right) dx \right|^2 \\ &= \frac{1}{2\eta} \left| -\frac{\sqrt{2\pi}}{2} \exp\left(i \frac{3\pi}{4}\right) + \int_0^y \exp\left(-i \frac{x^2}{2}\right) dx \right|^2 \\ &= \frac{\pi}{2\eta} \left\{ \left[\frac{1}{2} + C\left(\frac{y}{\sqrt{\pi}}\right) \right]^2 + \left[\frac{1}{2} + S\left(\frac{y}{\sqrt{\pi}}\right) \right]^2 \right\}, \end{aligned} \quad (29)$$

where $C(y/\sqrt{\pi})$ and $S(y/\sqrt{\pi})$ are the Fresnel integrals [32]. It is very interesting to see that the evolution of the transition probability $P_d(t)$ in the sudden limit is quite similar to the transient current function $J(x, t)$ in the particle shutter problem [33]. Interestingly, the time evolution of the probability function $P_d(t)$ and the transient current function $J(x, t)$ are identical in the space region where $x \gg \lambda$, where λ is the wavelength of the particle, given the dimensionless parameter $u \rightarrow y/\sqrt{\pi}$ and the phenomenon of time diffraction, which has been verified by a recent experiment [34].

One can prove that the maximum value of P_d for $t \leq 0$ is at $t = 0$, where $P_d = \pi/(4\eta)$. Thus with the half-width condition

$$P_d(t') = \frac{1}{2} P_d(0) = \frac{\pi}{8\eta}, \quad (30)$$

we find numerically that $t' \approx -0.6241 \sqrt{\frac{\hbar}{\alpha}}$. According to Refs. [23,24], we have

$$P_d(\infty) = 1 - \exp\left(-\frac{\pi}{\eta}\right). \quad (31)$$

Therefore, at the sudden limit ($\eta \gg 1$), we have

$$\left| \frac{S_2}{S_1} \right| = \frac{P_d(\infty) - P_d(0)}{P_d(0)} \approx 3. \quad (32)$$

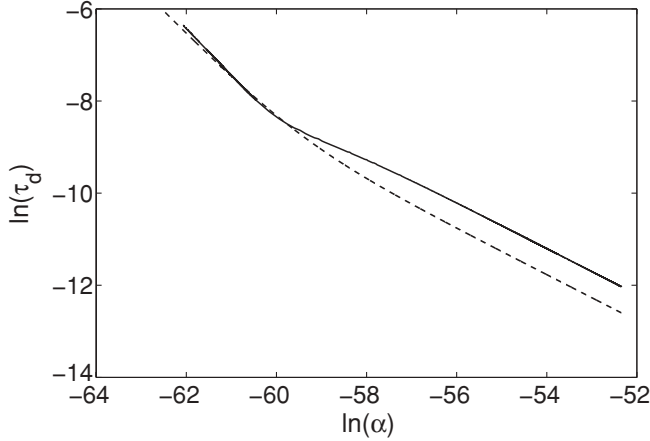


FIG. 5. Transition times τ_d in the diabatic basis. The solid line is our numerical result and the dashed line is the empirical formula $\tau_d = \sqrt{\Delta^2/\alpha^2 + 2\hbar/\alpha}$ used in Ref. [28]. α is in units of $\frac{\Delta^2}{2\hbar}$ and τ_d is in units of seconds.

Based on our definition in Eq. (18), the transition time is

$$\tau_d^s \approx 4|t'| = 2.4964\sqrt{\frac{\hbar}{\alpha}}. \quad (33)$$

The fact that τ_d^s scales as $\sqrt{\hbar/\alpha}$ can be seen clearly in Eqs. (23)–(26) as having been pointed out by Mullen *et al.* [25].

B. Numerical results

Our numerical results for the transition time τ_d in the diabatic basis are plotted on a log-log scale in Fig. 5. In the figure, we see that the results for the two limiting cases are connected by a smooth kink. We have also compared these results with the empirical relation $\tau_d = \sqrt{\Delta^2/\alpha^2 + 2\hbar/\alpha}$ that was used in Ref. [28]; the agreement is quite good.

We have amplified the results at the adiabatic and the sudden limits and plotted them in Fig. 6 and Fig. 7, respectively. In these two figures, we have also compared them to the analytical results and the agreement is excellent.

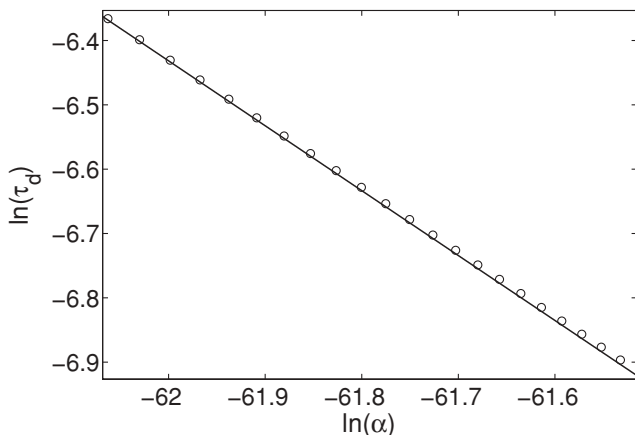


FIG. 6. Transition time τ_d at the adiabatic limit in the diabatic basis. The circles are the theoretical results given in Eq. (22) and the solid line is the numerical results. α is in units of $\frac{\Delta^2}{2\hbar}$ and τ_d is in units of seconds.

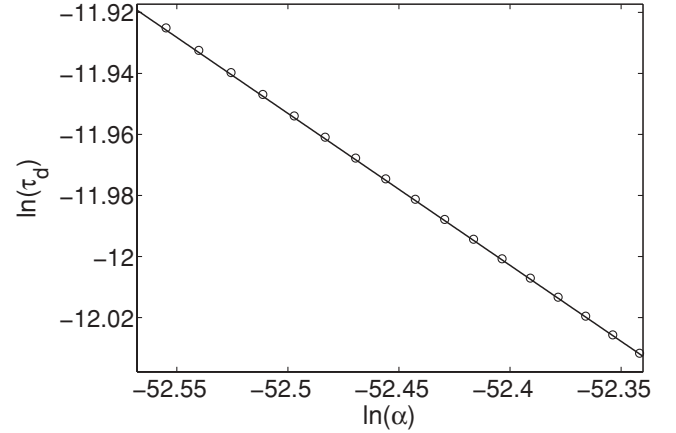


FIG. 7. Transition time τ_d at the sudden limit in the diabatic basis. The circles are the theoretical results given in Eq. (33) and the solid line is the numerical results. α is in units of $\frac{\Delta^2}{2\hbar}$ and τ_d is in units of seconds.

V. TRANSITION TIMES IN THE ADIABATIC BASIS

As mentioned already, when one applies the LZ model to describe the transition between Bloch bands, it is more convenient to use the adiabatic basis. It turns out that the results in the adiabatic basis are quite different from the ones in the diabatic basis.

A. Analytical results

As in the case of the diabatic basis, at the adiabatic limit ($\eta \ll 1$), the transition probability function P_a in the adiabatic basis has been found by Vitanov [26,27],

$$P_a(t) \approx \frac{\alpha^2 \hbar^2 \Delta^2}{4(\alpha^2 t^2 + \Delta^2)^3}. \quad (34)$$

With the half-width condition

$$P_a(t)|_{t=t'} = \frac{1}{2}[P_a(t \leq 0)]_{\max} = \frac{\alpha^2 \hbar^2}{8\Delta^4}, \quad (35)$$

we find that

$$t' = -\sqrt{2^{1/3} - 1} \frac{\Delta}{\alpha}. \quad (36)$$

Thus, based on our definition in Eq. (18), the transition time is

$$\tau_a^a = 2\sqrt{2^{1/3} - 1} \frac{\Delta}{\alpha} \approx \frac{\Delta}{\alpha}, \quad (37)$$

which is very similar to the transition time of Eq. (22) in the diabatic basis. Our result in Eq. (37) can be viewed as the first successful attempt to find the transition time at the adiabatic limit in the adiabatic basis because Vitanov's definition Eq. (14) may fail in this case.

We next consider the sudden limit ($\eta \gg 1$). In terms of $y = t/\sqrt{\hbar/\alpha}$, the instantaneous eigenstates of the Hamiltonian (2) are

$$|e_2(t)\rangle = \begin{pmatrix} \Theta_1(y) \\ \Theta_2(y) \end{pmatrix} = \begin{pmatrix} \left[\frac{1}{2} \left(1 + \frac{y}{\sqrt{y^2 + 2/\eta}} \right) \right]^{1/2} \\ \left[\frac{1}{2} \left(1 - \frac{y}{\sqrt{y^2 + 2/\eta}} \right) \right]^{1/2} \end{pmatrix}. \quad (38)$$

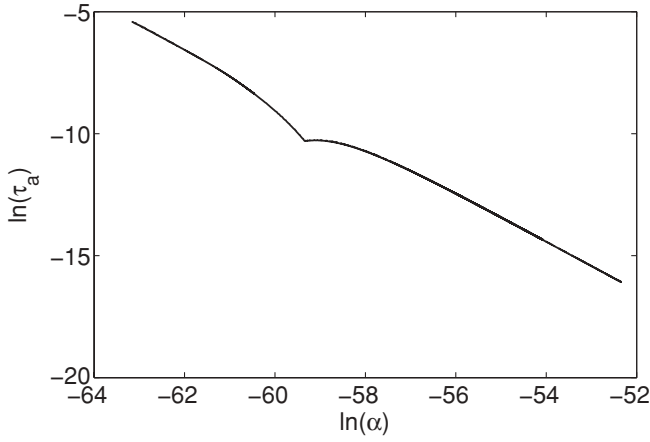


FIG. 8. Transition time τ_a in the adiabatic basis. α is in units of $\frac{\Delta^2}{2\hbar}$ and τ_a is in units of seconds.

According to Eq. (25) and Eq. (26), we can obtain the transition probability up to first order of $1/\eta$ as

$$P_a(y) \approx \left| (\Theta_1(y)\Theta_2(y)) \begin{pmatrix} \exp\left(-i\frac{y^2}{4}\right) \\ b_1(y)\exp\left(i\frac{y^2}{4}\right) \end{pmatrix} \right|^2. \quad (39)$$

With Eq. (28), we arrive at

$$P_a(y) \approx \frac{1}{2} + \frac{1}{2} \frac{y}{\sqrt{y^2 + \frac{2}{\eta}}} - \frac{1}{\sqrt{\eta(\eta y^2 + 2)}} \cos \frac{y^2}{2} \times \int_{-\infty}^y \sin \frac{x^2}{2} dx + \frac{1}{2\eta} \left(\frac{1}{2} - \frac{1}{2} \frac{y}{\sqrt{y^2 + \frac{2}{\eta}}} \right). \quad (40)$$

It is quite obvious that the last two terms of this equation are much smaller than the first two terms. Finally, we obtain

$$P_a(t) \approx \frac{1}{2} + \frac{1}{2} \frac{\alpha t}{\sqrt{\alpha^2 t^2 + \Delta^2}}, \quad (41)$$

which is surprisingly identical to the result at the adiabatic limit in the diabatic basis [see Eq. (19)]. As a result, we can

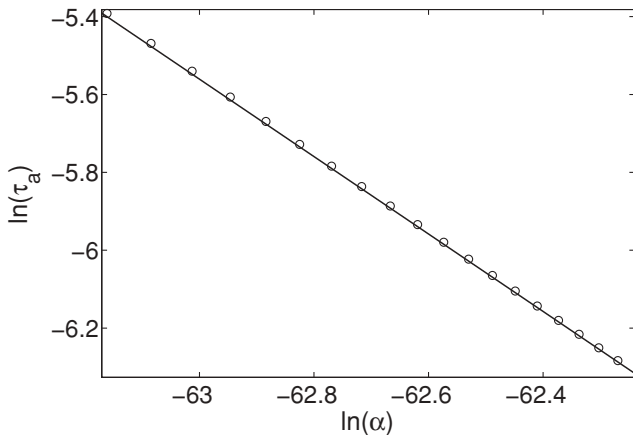


FIG. 9. Transition time τ_a at the adiabatic limit in the adiabatic basis. The circles are the theoretical results given by Eq. (37); the solid line is the numerical results. α is in units of $\frac{\Delta^2}{2\hbar}$ and τ_a is in units of seconds.

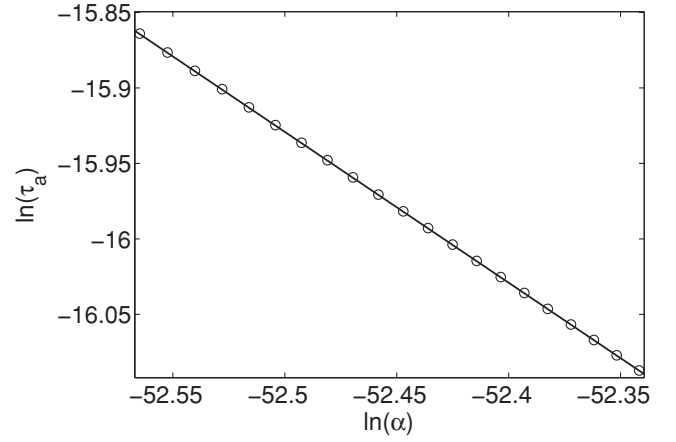


FIG. 10. Transition time τ_a at the sudden limit in the adiabatic basis. The circles are the theoretical results given by Eq. (42); the solid line is the numerical results. α is in units of $\frac{\Delta^2}{2\hbar}$ and τ_a is in units of seconds.

similarly obtain the transition time

$$\tau_a^s = \frac{2\sqrt{3}}{3} \frac{\Delta}{\alpha}, \quad (42)$$

which agrees very well with Vitanov's result [26,27].

B. Numerical results

In the adiabatic basis, the numerical results of the transition time are shown in Fig. 8. We see that the results in the two limiting cases are also connected by a kink. However, this kink is not as smooth as the kink in the diabatic basis; the first derivative of the transition time with respect to α is not continuous. The numerical results for the two limits, the adiabatic limit and the sudden limit, are plotted and compared to the theoretical results in Fig. 9 and Fig. 10, respectively. Again, we find excellent agreement.

VI. DISCUSSION AND CONCLUSION

We have obtained analytical results for the transition times in the LZ model at two different limits and in two different bases. They are, respectively, τ_d^a , τ_d^s , τ_a^a , and τ_a^s , which are listed in Table I. We have found that only τ_d^s is proportional to $\sqrt{\hbar/\alpha}$ while the rest of the three transition times all scale as Δ/α . It is not hard to understand why τ_d^s , the transition time at the sudden limit and in the diabatic basis, does not scale as Δ/α . The effect of Δ is to couple the two bare states, (1, 0) and (0, 1), which serve as the base vectors in the diabatic basis. At the sudden limit, the system changes very fast and its wave function remains almost unchanged. As a result, the system does not feel the effect of Δ . It is also not hard to

TABLE I. Transition time in the LZ model.

Basis	Adiabatic limit	Sudden limit
Diabatic	$\tau_d^a = \frac{2\sqrt{3}}{3} \Delta/\alpha$	$\tau_d^s = 2.4964\sqrt{\frac{\hbar}{\alpha}}$
Adiabatic	$\tau_a^a = \Delta/\alpha$	$\tau_a^s = \frac{2\sqrt{3}}{3} \Delta/\alpha$

understand that the two transition times at the adiabatic limit, τ_a^a and τ_d^a , scale as Δ/α . At the adiabatic limit, the effect of Δ is fully felt by the system and gets reflected in the transition time.

The transition time τ_a^s at the sudden limit in the adiabatic basis, unlike the other transition time τ_d^s at the sudden limit, is proportional to Δ/α . This can be clearly explained by Eq. (9), in which the width of the coupling function between the two instantaneous eigenstates is Δ/α . Moreover, its corresponding probability function $P_a(t)$ described by Eq. (41) is surprisingly identical to the probability function $P_d(t)$ in Eq. (19), which is at the adiabatic limit in the diabatic basis. To understand this, we have to look into the details of the evolution. At the adiabatic limit, the system follows its instantaneous eigenstate as demanded by the quantum adiabatic theorem [35]. $P_d(t)$ in Eq. (19) is obtained by projecting this instantaneous eigenstate to the bare state (0, 1). At the sudden limit, the wave function of the system changes little and remains in the bare state (1, 0). However, in the adiabatic basis, this wave function needs to be projected to the instantaneous eigenstate to obtain $P_a(t)$ described by Eq. (41). As we know, projecting a bare state to

an instantaneous eigenstate is identical to projecting the same instantaneous eigenstate to the same bare state. This explains why the probability function $P_a(t)$ in Eq. (41) is the same as $P_d(t)$ in Eq. (19). Consequently, this also explains why τ_a^s scales as Δ/α .

In sum, we have presented a general definition of the transition time for the Landau-Zener model. We have shown that this definition works for any sweeping rate and can be used for the numerical computation of the transition time without any ambiguity. In particular, we have obtained analytical results for the two limiting cases, the adiabatic limit and the sudden limit. We have not only reproduced known results but also found the transition time at the adiabatic limit in the adiabatic basis, which has not been found before to our knowledge.

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- [1] H. Frauenfelder and P. G. Wolynes, *Science* **229**, 337 (1985).
 [2] A. Garg, J. N. Onuchi, and V. Ambegaokar, *J. Chem. Phys.* **83**, 4491 (1985).
 [3] J. J. Hopfield, *Proc. Natl. Acad. Sci. USA* **71**, 3640 (1974).
 [4] See, for example, E. E. Nikitin and S. Ya. Umanskii, *Theory of Slow Atomic Collisions* (Spring-Verlag, Berlin 1984); A. Yoshimori and K. Makoshi, *Prog. Surf. Sci.* **21**, 251 (1986).
 [5] C. R. Leavens and G. C. Aers, in *Scanning Tunneling Microscopy III*, edited by R. Wiesendanger and H.-J. Güntherodt (Springer, New York, 1993).
 [6] D. Sokolovski and L. M. Baskin, *Phys. Rev. A* **36**, 4604 (1987).
 [7] K. L. Jensen and F. A. Buot, *Appl. Phys. Lett.* **55**, 669 (1989).
 [8] J. Liu, L. Fu, B. Y. Ou, and S. G. Chen, D. I. Choi, B. Wu, and Q. Niu, *Phys. Rev. A* **66**, 023404 (2002).
 [9] J. Liu, B. Wu, and Q. Niu, *Phys. Rev. Lett.* **90**, 170404 (2003).
 [10] D. F. Ye, L. B. Fu, and J. Liu, *Phys. Rev. A* **77**, 013402 (2008).
 [11] G. F. Wang, D. F. Ye, L. B. Fu, X. Z. Chen, and J. Liu, *Phys. Rev. A* **74**, 033414 (2006).
 [12] W. Wernsdorfer, R. Sessoli, A. Caneschi, D. Gatteschi, A. Cornia, and D. Mailly, *J. Appl. Phys.* **87**, 5481 (2000).
 [13] R. Landauer, *Nature (London)* **341**, 567 (1989).
 [14] Th. Martin and R. Landauer, *Phys. Rev. A* **47**, 2023 (1993).
 [15] A. Peres, *Am. J. Physiol.* **48**, 552 (1980).
 [16] M. Büttiker and R. Landauer, *Phys. Rev. Lett.* **49**, 1739 (1982).
 [17] D. Sokolovski and L. M. Baskin, *Phys. Rev. A* **36**, 4604 (1987).
 [18] Q. Niu and M. G. Raizen, *Phys. Rev. Lett.* **80**, 3491 (1998).
 [19] R. Landauer and Th. Martin, *Solid State Commun.* **84**, 115 (1992).
 [20] R. Landauer and Th. Martin, *Rev. Mod. Phys.* **66**, 217 (1994).
 [21] E. H. Hauge and J. A. Støveng, *Rev. Mod. Phys.* **61**, 917 (1989).
 [22] N. Yamada, *Phys. Rev. Lett.* **93**, 170401 (2004).
 [23] L. Landau, *Phys. Z. Sowjetunion* **2**, 46 (1932).
 [24] C. Zener, *Proc. R. Soc. London, Ser. A* **137**, 696 (1932).
 [25] K. Mullen, E. Ben-Jacob, Y. Gefen, and Z. Schuss, *Phys. Rev. Lett.* **62**, 2543 (1989).
 [26] N. V. Vitanov and B. M. Garraway, *Phys. Rev. A* **53**, 4288 (1996).
 [27] N. V. Vitanov, *Phys. Rev. A* **59**, 988 (1999).
 [28] J. Liu, B. Wu, L. Fu, R. B. Diener, and Q. Niu, *Phys. Rev. B* **65**, 224401 (2002).
 [29] B. Wu and Q. Niu, *Phys. Rev. A* **61**, 023402 (2000).
 [30] J. C. D'Olivo, *Phys. Rev. D* **45**, 924 (1992).
 [31] A. D. Bandrauk and M. S. Child, *Mol. Phys.* **19**, 95 (1970).
 [32] M. Abramowitz and T. A. Stegun, *Handbook of Mathematical Functions—With Formulas, Graphs, and Mathematical Tables* (Dover, New York, 1970).
 [33] M. Moshinsky, *Phys. Rev.* **88**, 625 (1952).
 [34] A. del Campo, G. García-Calderón, and J. G. Muga, *Phys. Rep.* **476**, 1 (2009).
 [35] A. Messiah, *Quantum Mechanics* (Dover, New York, 1999).