Effect of Landau–Zener tunneling by the varying sweeping rate of external field*

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We study the effect of Landau–Zener (LZ) tunneling caused by the varying sweeping rate of the external field, and solve the problem about the LZ tunneling rate among many levels. The LZ tunneling rate is essentially changed by the unsteady variation of the time-dependent sweeping field and is different from the steadily varying sweeping field, which makes the particles in lower states transit periodically to upper states within a finite time.

Keywords: Landau–Zener tunneling, varying sweeping rate, transition probability, n-level state
PACC: 3270F, 3280B

1. Introduction

As a basic quantum mechanical process, Landau–Zener (LZ) tunneling proposed by Landau and Zener describes the particles in level-crossings where the particles transit each other within a specific probability.[1,2] Based on LZ theory, extensive researches were conducted on their applications, such as atoms in accelerating optical lattices,[3] slow atomic and molecular collisions,[4] field-driven superlattices[5] and molecular predissociation.[6] Especially, Brundobler *et al.* pointed out a direction for solving the many-level problems although some of them are still open.[7−10] The generalization of this problem, such as the multiple variation of single particle level energies, could affect the many-particle state,[11] which reveals the mechanism of cavity quantum electrodynamics (cavity QED) experiments.[12−16] Therefore the research on a photon mode in a cavity provides a helpful way to understand the Feshbach resonance,[17] the variation of the molecular energy caused by Feshbach resonance in cold atomic gases.[11,18] After generalizing the many-body LZ problem, it was found that adiabatic driving did not keep the system in its many-particle ground state; rather, a finite fraction of particles still remain in high-lying states.[11] For the LZ tunneling between nonlinear two energy levels, it depends on the occupation of the levels within a periodic potential.[19] Therefore, the LZ tunneling between Bloch bands of a Bose–Einstein condensation in an accelerated optical lattice can be easily understood.[20]

As is well known, in the linear case, for the sweeping field $\gamma(t) = \alpha t$, we can derive the LZ transition in the nearly adiabatic regime $\alpha \to 0$ by the way of solving the eigenvalues and eigenstates of Hamiltonian. Now there arises a point, that is, how the system will evolve if the variation of the sweeping rate depends on time, particularly, when the periodical variation makes the system stay in an adiabatic state periodically at some specific time moments. Although, the forms of the LZ tunneling probability in these two cases are similar, their essential difference makes the physical property of the latter far-reaching which will be shown in the following after studying this situation with a special method. Thus, the first aim of the present paper is to derive the transition probability that is different from that obtained from the classical LZ model with considering the forms of sweeping field. Besides, the second aim is to provide a theoretical understanding of the effect of the LZ tunneling caused by the varying sweeping rate of external field, which leads to the time-dependent transition, and it corresponds to one of the hot topics in nanophysics, i.e. the time-dependent external magnetic field induces the transition in the system containing interacting spins.[21,22]

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2. The Hamiltonian

In order to discuss conveniently, we divide the Hamiltonian into three parts. The first one is the external field $H_{\rm e}$; the second one is the spin–spin interaction $H_{\rm s}$; and the last one is the level–level interaction with considering only the neighbourhood levels. The first one can be written as

$$\begin{aligned} H_{\rm e} &= \frac{1}{8\pi v}\sum_{\boldsymbol{k}}\sum_{\alpha=1,2} c^2\frac{2\pi\hbar}{\omega}\varepsilon_{\boldsymbol{k}}^{2(\alpha)}\int\left[\left|(\hat{a}_{\boldsymbol{k},\alpha}(t)\ \ \hat{a}^+_{\boldsymbol{k},\alpha}(t))\nabla\times\begin{pmatrix}\boldsymbol{u}(\boldsymbol{k},\boldsymbol{r})\\ \boldsymbol{u}^*(\boldsymbol{k},\boldsymbol{r})\end{pmatrix}\right|^2\right. \\ &\quad \left.+\frac{1}{c^2}\left|(\boldsymbol{u}(\boldsymbol{k},\boldsymbol{r})\ \ \boldsymbol{u}^*(\boldsymbol{k},\boldsymbol{r}))\frac{\partial}{\partial t}\begin{pmatrix}\hat{a}_{\boldsymbol{k},\alpha}(t)\\ \hat{a}^+_{\boldsymbol{k},\alpha}(t)\end{pmatrix}\right|^2\right]{\rm d}V \\ &= \frac{1}{8\pi v}\sum_{\boldsymbol{k}}\sum_{\alpha=1,2} c^2\frac{2\pi\hbar}{\omega}\varepsilon_{\boldsymbol{k}}^{2(\alpha)}\int\left[\left|2[{\rm Re}(a_{\boldsymbol{k},\alpha}(t))\ \ {\rm Im}(\hat{a}_{\boldsymbol{k},\alpha}(t))]\nabla\times\begin{bmatrix}{\rm Re}(\boldsymbol{u})\\ -{\rm Im}(\boldsymbol{u})\end{bmatrix}\right|^2\right. \\ &\quad \left.+\frac{1}{c^2}\left|2[{\rm Re}(\boldsymbol{u})\ \ {\rm Im}(\boldsymbol{u})]\frac{\partial}{\partial t}\begin{pmatrix}{\rm Re}(\hat{a}_{\boldsymbol{k},\alpha}(t))\\ -{\rm Im}(\hat{a}^+_{\boldsymbol{k},\alpha}(t))\end{pmatrix}\right|^2\right]{\rm d}V, \end{aligned} \tag{1}$$

where $\boldsymbol{\varepsilon}_{\boldsymbol{k}}^{(\alpha)}$ is a polarization vector, and the direction of $(\boldsymbol{\varepsilon}_{\boldsymbol{k}}^{(1)},\boldsymbol{\varepsilon}_{\boldsymbol{k}}^{(2)},\boldsymbol{k}/|\boldsymbol{k}|)$ is determined by the right-hand rule. The base vector $\boldsymbol{u}(\boldsymbol{k},\boldsymbol{r})$ satisfies the normalizing condition

$$\frac{1}{V}\int \boldsymbol{u}_{\boldsymbol{k},\alpha}\cdot\boldsymbol{u}_{\boldsymbol{k}',\alpha'}{\rm d}V=\delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\alpha,\alpha'}. \tag{2}$$

The conjugate forms of $\hat{a}^+_{\boldsymbol{k},\alpha}$ and $\boldsymbol{u}^*(\boldsymbol{k},\boldsymbol{r})$ make the multiple integration result H a real number. In the meantime, the operators $\hat{a}^+_{\boldsymbol{k},\alpha}$ and $\hat{a}_{\boldsymbol{k},\alpha}$ are given by

$$\begin{aligned} \hat{a}^+_{\boldsymbol{k},\alpha} &= (2\hbar\omega)^{1/2}(\omega\hat{Q}_{\boldsymbol{k},\alpha}-{\rm i}\hat{P}_{\boldsymbol{k},\alpha}),\\ \hat{a}_{\boldsymbol{k},\alpha} &= (2\hbar\omega)^{1/2}(\omega\hat{Q}_{\boldsymbol{k},\alpha}+{\rm i}\hat{P}_{\boldsymbol{k},\alpha}), \end{aligned} \tag{3}$$

and

$$\begin{aligned} \hat{Q}_{\boldsymbol{k},\alpha} &= \frac{1}{c\sqrt{4\pi}}(C_{\boldsymbol{k},\alpha}+C^*_{\boldsymbol{k},\alpha}),\\ \hat{P}_{\boldsymbol{k},\alpha} &= \frac{-{\rm i}\omega}{c\sqrt{4\pi}}(C_{\boldsymbol{k},\alpha}-C^*_{\boldsymbol{k},\alpha}), \end{aligned}$$

where $C_{\boldsymbol{k},\alpha}$ and $C^*_{\boldsymbol{k},\alpha}$ are the coefficients of the Fourier expansion for the vector potential at the initial time. So the $\hat{a}_{\boldsymbol{k},\alpha}(t)$ with its relation can be written as $[\hat{a}_{\boldsymbol{k},\alpha}(t),\hat{a}^+_{\boldsymbol{k},\alpha}(t)]=\delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\alpha,\alpha'}$, and the relationship between $\hat{P}_{\boldsymbol{k},\alpha}$ and $\hat{Q}_{\boldsymbol{k},\alpha}$ can be indicated by regular equation as follows:

$$\frac{\partial H_{\rm e}}{\partial Q_{\boldsymbol{k},\alpha}}=-\dot{P}_{\boldsymbol{k},\alpha},\quad \frac{\partial H_{\rm e}}{\partial P_{\boldsymbol{k},\alpha}}=\dot{Q}_{\boldsymbol{k},\alpha}. \tag{4}$$

Above all, the Hamiltonian describing a particle in the nth level under the action of external field can be written as a matrix form as follows:

$$\boldsymbol{H}_{\rm e}(n)=\boldsymbol{I}_n H_{\rm e}, \tag{5}$$

where $\boldsymbol{I}_n$ is a unitary matrix. Here, it must be pointed out that we suppose the external field acting on the system is a homogeneous field. Thus the Hamiltonian $\boldsymbol{H}_{\rm e}(n)$ only couples with the nth level where the particle stays. Meanwhile, the Hamiltonian $H_{\rm s}$ describing the spin–spin interaction and the Hamiltonian $H_{\rm i}$ depicting the level–level interaction can be expressed, respectively, as

$$\begin{aligned} H_{\rm s} &= \lim_{\varepsilon\to 0}\int_{t-\varepsilon}^{t+\varepsilon}\omega(t)\sigma_{nz}{\rm d}\varepsilon\\ &= \begin{Bmatrix}\omega(t)\,|\uparrow\rangle\\ \omega(t)\,|\downarrow\rangle\end{Bmatrix}\\ &\equiv E_n(t)_{\pm}, \end{aligned} \tag{6}$$

$$\begin{aligned} H_{\rm i} &= \lim_{h\to 0}\int_{t-h}^{t+h}[\Delta\varepsilon(n-1,n)-\Delta\varepsilon(n,n+1)]{\rm d}t\\ &\equiv \overline{\Delta\varepsilon_n(t)}, \end{aligned} \tag{7}$$

where σ_{nz} is the Pauli matrix, and $\Delta\varepsilon(n,n+1)$ is the difference in energy between the nth and the $(n+1)$th levels, meanwhile the difference in energy between the nth and the $(n+2)$th levels is neglected. Note that the reduction form of $E_n(t)_{\pm}$ represents that the spin–spin interaction is time-dependent and thus Hamiltonian $H_{\rm e}$ is also time-dependent. Yet, the part $\overline{\Delta\varepsilon_n(t)}$ in expression (7) that shows the average interaction of particles in the nth level with its nearest neighbour level is also time-dependent, but we can regarded it

as a time-independent form because it varies slightly with time, so it may be equivalently written as $\varepsilon_{\rm i}$.

For the general case of an arbitrary linear Hamiltonian, we assume that $H(t) = E + C(t)$. If $C(t)$ is a diagonal, there is no general solution, but for some survival probabilities, some exact results have been conjectured[7] and derived.[8,9,23,24] Especially in Ref. [7], Brundobler and Elser considered that the formula for the certain diagonal elements of the S matrix contained an approximation, but the numerical results were still very accurate when the approximation was assumed to break down even at strong coupling. To obtain a general solution, we expand the diagonal matrix into the complex one which was called three-diagonal one.

Based on the above discussion, it is natural to organize a Hamiltonian formula that covers all information of energy, into a special matrix as shown below:

$$\boldsymbol{H} = \begin{pmatrix} H_1 & \varepsilon_1 & 0 & 0 & \cdots & 0 \\ -\varepsilon_1 & H_2 & \varepsilon_2 & 0 & \cdots & 0 \\ 0 & -\varepsilon_2 & H_3 & \varepsilon_3 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & -\varepsilon_{n-2} & H_{n-1} & \varepsilon_{n-1} \\ 0 & 0 & \cdots & 0 & -\varepsilon_{n-1} & H_n \end{pmatrix}, \quad (8)$$

where $H_{nn} = H_{en} + H_{sn} = H_{en} + E_n(t)_{\pm}$ represents the sum of Hamiltonian in the nth level, and $\varepsilon_n = H_{\rm i} = \overline{\Delta\varepsilon_n(t)}$ indicates the interaction with its neighbour. Unfortunately, it cannot be added to the H_n because it is seen as a constant discussed above, unlike Hamiltonian $H_{\rm e}$ and $H_{\rm s}$.

3. Transition probability

It is revealed by expression (8) that the Hamiltonian of a system can be expressed by a three-diagonal matrix, which is quite concise and convenient to deal with. As is known, all microscopic systems can be described by the n-dimensional Schrödinger equation

$$\mathrm{i}\hbar\partial_t\psi_n(t) = H\psi_n(t), \quad (9)$$

with $\psi_n(t)$ is given by $\psi_n(t) = [\psi_1(t) \quad \psi_2(t) \quad \ldots \quad \psi_n(t)]^{\rm T}$.

Ostrovsky *et al.*[25] assumed that the transitions between the states could take place at the time when the energies were associated with two states crossing or had an avoided crossing according to the no-crossing rule of von Neumann and Wigner. So the method they applied is to fulfill the assumption by the way of expanding the adiabatic basis states of the system as shown below:

$$|\psi(t)\rangle = \sum_j c'_j \exp\left[-\mathrm{i}\int_{t_i}^{t} \varepsilon_j(t')\mathrm{d}t'\right]|\chi_j\rangle\,. \quad (10)$$

It is a useful way to research for the LZ tunneling. But we connect another direction by dealing with the form of Hamiltonian $H(t)$ whose state function is just formed as above.

Therefore, it is intuitively seen that the main problem is how to transfer the Hamiltonian to solve Eq. (9). The Hamiltonian shown in expression (8) can be transferred into

$$\boldsymbol{H} = \begin{pmatrix} h_1 & 0 & 0 & \cdots & 0 \\ -\varepsilon_1 & h_2 & 0 & \cdots & 0 \\ 0 & -\varepsilon_2 & h_3 & \cdots & 0 \\ \vdots & \vdots & \vdots\ddots & \ddots & \vdots \\ 0 & 0 & 0 & -\varepsilon_{n-1} & h_n \end{pmatrix} \equiv \Gamma^{(h_n)}_{(-\varepsilon_{n-1})}, \quad (11)$$

where the intermediate parameters h_n read as $h_1 = H_1$, $p_1 = \varepsilon_1^2/H_1$, $p_k = \varepsilon_k^2/h_k$, $h_{k+1} = H_k + p_k$ $(k = 2, 3\ldots, n)$. So we concisely rewrite the Hamiltonian $\boldsymbol{H}$ as $\boldsymbol{H} = \Gamma^{(h_n)}_{(-\varepsilon_{n-1})}$. Inserting it into expression (9) yields

$$\begin{aligned} &h_1\psi_1 = \mathrm{i}\hbar\dot{\psi}_1, \\ &-\varepsilon_{k-1}\psi_{k-1} + h_k\psi_k = \mathrm{i}\hbar\dot{\psi}_k, \\ &(k = 2, 3\ldots, n). \end{aligned} \quad (12)$$

Note that based on the expression of ψ in Eq. (12), we can insert it into the below formula for the case of $k = 2$, and the expression ψ becomes ψ_2. Therefore, we can obtain the final expression of $\psi_i(t)$ $(i = 1, 2, 3\ldots, n)$. Finally, it becomes easy to obtain the result for the LZ tunneling probability P.

Without loss of generality, the Hamiltonian $\boldsymbol{H}(t)$ in many cases can be transformed by Morris–Shore (MS) transformation,[26] and the form can be written as[27]

$$\boldsymbol{H}(\mathrm{T}) = \boldsymbol{S}\boldsymbol{H}(t)\boldsymbol{S}^{+} = \begin{bmatrix} 0 & \boldsymbol{V} \\ \boldsymbol{V}^{+} & \boldsymbol{D}(t) \end{bmatrix} \quad (13)$$

and

$$\boldsymbol{S} = \begin{bmatrix} \boldsymbol{A} & 0 \\ 0 & \boldsymbol{B} \end{bmatrix},$$

where $\boldsymbol{S}$ is a constant transformation matrix, which can be shown in the block matrix form, $\boldsymbol{A}$ and $\boldsymbol{B}$ are

the unitary square matrices with $N_{\rm a}$ and $N_{\rm b}$ dimensions, respectively, and $\boldsymbol{V} = \boldsymbol{A}\boldsymbol{V}\boldsymbol{B}^{+}$. Here, the $\boldsymbol{H}(t)$ matrix can be transformed into an upper-triangular matrix because $\boldsymbol{A}$ and $\boldsymbol{B}$ are determined by the condition that they can be diagnosed into $\boldsymbol{V}\boldsymbol{V}^{+}$ and $\boldsymbol{V}^{+}\boldsymbol{V}$ respectively.[26]

The classical LZ model in the case of $\gamma(t) = \alpha t$ is the most basic process. According to the method discussed in this paper, we provide the external field $\gamma(t) = A\sin(\omega t)$ instead of $\gamma(t) = \alpha t$, and the transition probability in the adiabatic limit is as follows:

$$P(t) = \exp\left(-\frac{\pi\varepsilon^2}{2A\omega\cos(\omega t)}\right). \tag{14}$$

Figure 1 shows the distinction of transition between the classical LZ model and our case. In classical LZ model, shown in Fig. 1(a), the probability changes with the value of α. When $\alpha \to 0$, the transition probability between two levels has a break in the region. The probability steadily changes beyond the region. But in our case, just as shown in Fig. 1(b), the probability changes periodically with time. At some special time moments, particles have a high probability to transit to higher energy level. The system cuts down transition probability and reaches the adiabatic state with some particles located in high level. At the next special time moment, other particles will grasp another chance and reach a higher state. As time goes on, the system is excited to the higher energy state with the help of the external field. By the way, the transition probability is also correlated with the value of ω (shown in Fig. 1(b) with different lines). From Fig. 1(b), it can be found that the probability amplitude turns smaller while the value of ω becomes bigger. It means that the probability amplitude becomes larger in the case of the slowly varying sweeping rate of external field.

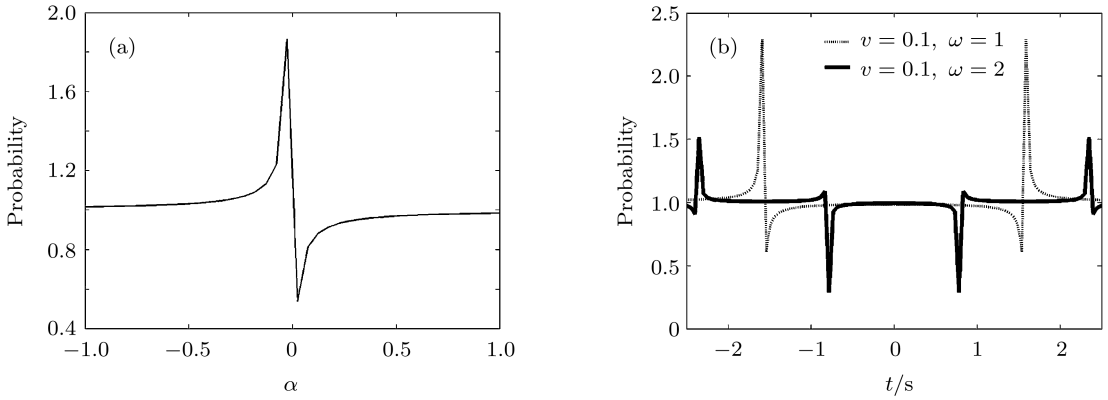


Fig. 1. Landau–Zener tunneling probabilities, where (a) is for the classical case, (b) is for the transition probability varying with time between two levels in our case, and a comparison between the cases $\omega = 1$ (dashed line) and $\omega = 2$ (solid line) at the same value of $v(v = 0.1)$ is also given.

Here, we have studied a many-body system in LZ tunneling, with n-level states although we consider only the neighbour levels interaction. The method of transferring three-diagonal matrix into lower triangular one can be applied to a five-diagonal matrix or even more-diagonal matrix, and the difference between three-diagonal and five-diagonal matrixes is that in the former only the neighbour interaction is considered but in the later the interaction with its two neighbour levels is taken into consideration. Surely, the later case is much more complicated than the former case, not only in the sense of calculation. Above all, this method could be applied theoretically to any case as long as its Hamiltonian can be transferred into lower triangular matrix.

4. Conclusion

We theoretically explore the effect of the varying sweeping rate of the external field on the LZ tunneling by an accurate method that has a wide application to physical processes. The main significance of the present paper lies in the fact that first, we find a new way to make the system transit to higher energy levels with the help of the external field; secondly, we provide a concise method to solve the Schrödinger equation

with a special Hamiltonian form, which makes it possible to describe many cases of physical models. For the future, we expect that the concise method could be applied to physical experiments and the LZ tunneling may be used to interpret the more interesting quantum dynamical phenomena.

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