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Effects of periodic modulation on the Landau–Zener transition

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Abstract

We study the quantum tunnelling of a two-level crossing system which extends the standard Landau–Zener model with applying a periodic modulation on its energy sweep. By directly integrating the time evolution operator we obtain the analytic expressions of tunnelling probability in the cases of high and low modulation frequency limit as well as in weak inter-level coupling limit. Our formula clarify the conditions for resonance occurrence, with the help of it we can readily manipulate the system in a desired way, say, to enhance or suppress the tunnelling probability effectively through adjusting the modulation properly.

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Avoided crossing of energy levels is a universal character for quantum nonintegrable systems where the break of system's symmetry leads to the splitting of degenerate energy levels forming a tiny energy gap. Around the avoided crossing point, the Landau–Zener (LZ) model provides an effective description for the tunnelling dynamics of the system with assuming that the energy bias of two levels undergoes a linear change with time [1]. LZ model is a rather general and fundamental model in quantum mechanics and has versatile applications in quantum chemistry [2], collision theory [3], and more recently, in the spin tunnelling of nanomagnets [4], Bose–Einstein condensates [5] and quantum computing [6].

There exist some extensions of the LZ model, including nonlinear LZ model [7], LZ problem with nonlinear energy sweep (square function of time) [8], LZ model with a fast noise mimic system's interaction with environment [9], to name only a few. On another aspect, there has been growing interest in the population dynamics of two-level systems under a periodic or quasi-periodic perturbation because of advances in the laser physics and fabrication techniques of mesoscopic systems. The probability of quantum tunnelling of an electron in a double-

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well potential is shown to be successively controlled by applying a periodic modulation of the relative energy of the wells [10]. As is mentioned above, the LZ model is a rather general and fundamental model in quantum mechanics, investigating its response to the external periodic modulation is a topics of great interest. Recently, Kayanuma and Mizaumoto [11] have discussed this issue. They emphasize on the population dynamics and find a series of step-like changes on the temporal evolution of level populations with using a transfer-matrix formalism.

In this Letter, we study this problem in a different way, i.e. directly integrating the time evolution operator. We concentrate on the total tunnelling probability, i.e. the population at final time, which is most concerned in practical situation. By directly integrating the evolution operator of Hamiltonian describing the LZ model with a periodic modulation, we are able to obtain the analytical expressions of total tunnelling probability. We find that, in both low and high frequency limits of periodic modulation the probability takes the same exponential form as the LZ formula but the energy gap is renormalized by modulation parameters; In the weak inter-level coupling limit, it takes a sinusoidal-like function predicting some resonance structures. Compared with the transfer-matrix method [11], our method is rather straight and our result is more concise and shows a better agreement with the numerical simulations.

We consider a time-dependent external electric field $\vec{E}(t)$, applied to the system modulating the energy bias between two states, denoted by $|1\rangle$ and $|2\rangle$. The operator for the electric-dipole moment $\vec{\mu}$ may be written as follows provided that the charge distribution of $|1\rangle$ and $|2\rangle$ is well separated,

$$\vec{\mu} = \frac{e\vec{a}}{2}\big(|1\rangle\langle 1| - |2\rangle\langle 2|\big), \tag{1}$$

where e is the electric charge of the electron and $\vec{a}$ is the vector connecting the two equilibrium points of the wells. The perturbation energy is then written as $-\vec{\mu}\cdot\vec{E}(t)$. We consider a case where $\vec{E}(t)$ is composed of two components, $\vec{E}(t) = \vec{E}_0 t + \vec{E}_1 \cos\omega t$. The model Hamiltonian then takes the form,

$$H(t) = \gamma\big(|1\rangle\langle 1| - |2\rangle\langle 2|\big) + \Delta\big(|1\rangle\langle 2| + |2\rangle\langle 1|\big), \tag{2}$$

where $\gamma = \frac{1}{2}(vt - A\cos\omega t)$, $v \equiv -e\vec{a}\cdot\vec{E}_0$, $A \equiv e\vec{a}\cdot\vec{E}_1$. Here the parameter γ denotes the energy bias between the two states.

The energy spectra of the system, as a function of the parameter γ, can be readily obtained by diagonalizing the above Hamiltonian. They show two straight lines of $\pm\gamma$ for asymptotic large energy bias, and an avoided crossing at the origin with the energy gap of Δ. Initially provided the energy bias is negative infinity, the two states is decoupled and both $|1\rangle$ and $|2\rangle$ are eigenstates. We suppose our particle populates on the lower level, i.e. $|1\rangle$ state. As we increase the energy bias from negative infinity to positive infinity, the particle has probability to tunnel to upper level due to quantum resonance occurred near avoided crossing point. Clearly the tunnelling process as well as the total transition probability at final time strongly depends on the way how we change the energy bias. The most simple way is the linear change with time, which gives the standard LZ model. In our case, we put a periodic modulation on the linear energy sweep, want to see how the periodic perturbation affects the quantum tunnelling. Here we mainly consider the total tunnelling probability, for it is most interest in physics.

For the state vector given by (we put $\hbar = 1$ throughout this Letter)

$$\big|\psi(t)\big\rangle = C_1(t)\exp\big\{-ivt^2/4 + i(A/2\omega)\sin\omega t\big\}|1\rangle + C_2(t)\exp\big\{ivt^2/4 - i(A/2\omega)\sin\omega t\big\}|2\rangle, \tag{3}$$

the Schrödinger equation is written as

$$i\frac{d}{dt}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \big[X(t)\sigma_x + Y(t)\sigma_y\big]\begin{pmatrix} C_1 \\ C_2 \end{pmatrix}, \tag{4}$$

where σ_x and σ_y are the Pauli matrices, and $X(t)$ and $Y(t)$ are defined as

$$X(t) = \Delta\cos\left(\frac{v}{2}t^2 - \frac{A}{\omega}\sin\omega t\right), \qquad Y(t) = -\Delta\sin\left(\frac{v}{2}t^2 - \frac{A}{\omega}\sin\omega t\right). \tag{5}$$

The solution of the above equations can be expressed formally with the help of time evolution operator,

$$\begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix} = U(t)\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{6a}$$

where $U(t)$ is the time evolution operator, taking following form,

$$U(t) = \sum_{n=0}^{\infty}(-i)^n \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{n-1}} dt_n\, H_F(t_1)H_F(t_2)\cdots H_F(t_n), \tag{6b}$$

in which

$$H_F(t) = X(t)\sigma_x + Y(t)\sigma_y = \Delta\begin{pmatrix} 0 & e^{i(vt^2/2 - A/\omega \sin\omega t)} \\ e^{-i(vt^2/2 - A/\omega \sin\omega t)} & 0 \end{pmatrix}. \tag{7}$$

Since $H_F(t)$ is a 2×2 off-diagonal matrix, only even multiple times of $H_F(t)$ in the expansion of Eq. (6) give nonzero contribution to $C_1(\infty)$. With using the formula of the ordinary Bessel function J_n,

$$\exp(\pm iz \sin\omega t) = \sum_{n=-\infty}^{\infty} J_n(Z)\exp(\pm in\omega t), \tag{8}$$

we can rewrite the expression of $C_1(\infty)$ as,

$$C_1(\infty) = \sum_{n=0}^{\infty}\left(-\Delta^2/v\right)^n \sum_{m_1=-\infty}^{\infty}\sum_{m_2=-\infty}^{\infty}\cdots\sum_{m_{2n}=-\infty}^{\infty} J_{m_1}(A/\omega)J_{m_2}(A/\omega)\cdots J_{m_{2n}}(A/\omega)e^{i\frac{1}{2}\sum_{j=1}^{2n}(-1)^j m_j^2\omega^2/v}$$
$$\times \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{2n-1}} dt_{2n}\, e^{-i\frac{1}{2}\sum_{j=1}^{2n}(-1)^j (t_j - m_j\omega/\sqrt{v})^2}. \tag{9}$$

Here $C_1(+\infty)$ is the tunnelling probability denoting the possibility of an particle tunneled to the upper level at the final time. Sometimes, what we concern is the probability of the particle remaining in the lower level, namely, transition probability, given by,

$$P = 1 - \left|C_1(\infty)\right|^2. \tag{10}$$

If the periodic perturbation is absent, one can obtain the Landau–Zener formula

$$P = 1 - \exp\left(-2\pi\Delta^2/v\right) \tag{11}$$

by directly integrating the Eq. (9) using the variable transformation [12], like $x_1 = t_1$, $x_p = t_1 + \sum_{j=1}^{p-1}(t_{2j+1} - t_{2j})$, $y_p = t_{2p} - t_{2p-1}$.

With the periodic modulation, generally it is not possible to derive an explicit analytic expression from the complicated integrations Eq. (9). However, in some limit cases we can successively integrate Eq. (9) explicitly and obtain an explicit analytic expressions for the quantum transition.

The first case we consider is the so-called high frequency limit, i.e. $A/\omega \ll 1$. In this case, the linear sweep of the energy bias undergoes a high frequency modulation. From our intuition the high-frequency field can be averaged over because its change is fast compared with the linear sweep term. With this fact in mind, we only keep the dominating term (zero-order term) in the expansion of the Bessel function, abandoning higher-order terms. Then, Eq. (9) can be immediately integrated out like what we do in the linear sweep case,

$$P = 1 - \exp\left(-2\pi\Delta'^2/v\right), \tag{12}$$

where the effective energy gap $\Delta' = J_0(A/\omega)\Delta$.

The second case we consider is that periodic field changes much slower than the linear sweeping, i.e., $\omega/\sqrt{v} \to 0$. In this case approximately we can ignore the related terms in the exponents of the integrations (9), and then make the integration of Eq. (9) directly, we obtain

$$C_1(\infty) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\pi\Delta^2/v\right)^n \left|\sum_{m=-\infty}^{\infty} J_m(A/\omega)e^{i\frac{1}{2}m^2\omega^2/v}\right|^{2n} = \exp\left(-\pi\Delta^2/v\right)\left|\sum_{m=-\infty}^{\infty} J_m(A/\omega)e^{i\frac{1}{2}m^2\omega^2/v}\right|^2, \tag{13}$$

and the final tunnelling probability P that the system resides in $|2\rangle$ at $t \to \infty$ is,

$$P = 1 - \left|C_1(\infty)\right|^2 = 1 - \exp\left(-2\pi\Delta'^2/v\right), \tag{14}$$

where

$$\Delta' = \Delta\left|\sum_{m=-\infty}^{\infty} J_m(A/\omega)e^{i\frac{1}{2}m^2\omega^2/v}\right|. \tag{15}$$

In the above two cases, we see that the final tunnelling probability can be expressed in the same form as the famous Landau–Zener formula, except that the energy gap is renormalized by the periodic modulation. The effective energy gap always shrinks compared to the original gap, providing more opportunity for an particle to tunnel to upper level. It leads to the monotonic decrease of the transition probability with increasing the scaled amplitude of periodic perturbation. To check the validity of our formula, we make numerical simulations by directly solving the Schrödinger Eq. (4), using the Runge–Kutta forth and fifth order integration method. The results are plotted Fig. 1, where we see our analytic results are in a very good agreement with numerical results for a wide range of parameters. As a comparison we also plot the results calculated from the transfer-matrix method [11] in the same figure, which shows a big deviation in the case of relatively small A/ω and relatively large coupling. The reason is that the assumption in the transfer-matrix method that successive crossing events are coherent but independent of each other breaks down in this case, moreover the role of the level crossing is not clear in their approach [13]. Note that in applying the transfer-matrix method to calculate the final tunnelling probability we have iterated a 2×2 matrix (i.e. transfer-matrix) even up to 100 times to get a converged result. It is obviously much time consuming compared to our concise formula (14).

Now we consider the case that the inter-level coupling is very weak, i.e. $\Delta/\sqrt{v} \to 0$. In this case we neglect the time-order operator and suppose that the Hamiltonian (7) at successive times is commutative, we can approximately get the state vector at $t \to \infty$,

$$\begin{pmatrix} C_1(\infty) \\ C_2(\infty) \end{pmatrix} = e^{-i\Delta\sqrt{\frac{2\pi}{v}}(\bar{X}\sigma_x + \bar{Y}\sigma_y)} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{16}$$

where

$$\bar{X} = \sum_{m=-\infty}^{\infty} J_{2m}(A/\omega)\cos\left(\frac{2m^2\omega^2}{v} - \frac{\pi}{4}\right), \qquad \bar{Y} = \sum_{m=-\infty}^{\infty} J_{2m}(A/\omega)\sin\left(\frac{2m^2\omega^2}{v} - \frac{\pi}{4}\right). \tag{17}$$

The final transition probability P that the particle resides in $|2\rangle$ at $t \to \infty$, is then given by

$$P = \sin^2\sqrt{\frac{2\pi\Delta^2}{v}\left(\bar{X}^2 + \bar{Y}^2\right)} = \sin^2\left(\sqrt{\frac{2\pi\Delta^2}{v}}\left|\sum_{m=-\infty}^{\infty} J_{2m}\left(\frac{A}{\omega}\right)e^{i\frac{2m^2\omega^2}{v}}\right|\right). \tag{18}$$

This analytic expression shows that, the total transition probability is modulated by the periodic perturbation through two scaled parameters, namely, A/ω and ω^2/v. It is a periodic function about the dimensionless parameter ω^2/v, i.e. $P(\omega^2/v + \pi) = P(\omega^2/v)$. Moreover, in the following three resonance cases, the expressions of transition probability take extreme simple forms:

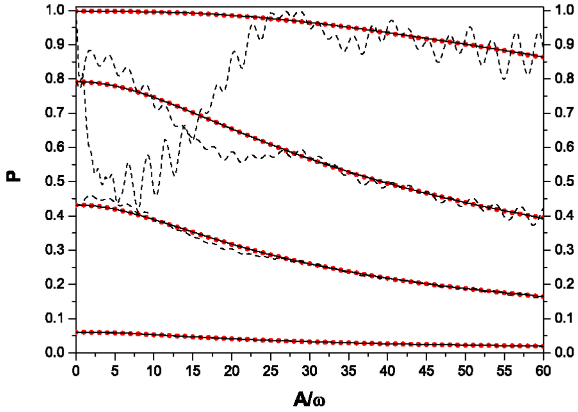

Fig. 1. The final tunnelling probabilities versus the dimensionless amplitude A/ω for different $\Delta/\sqrt{v}$ with the modulation frequency $\omega/\sqrt{v} = 0.2$. The solid line is the predication of the Eq. (14), dashed line is the result from transfer-matrix method [11] showing a big deviation for relatively small A/ω and relatively large coupling, and the circle dots are the numerical results. From the top to bottom, the four line correspond to $\Delta/\sqrt{v} = 1$, 0.5, 0.3, and 0.1, respectively.

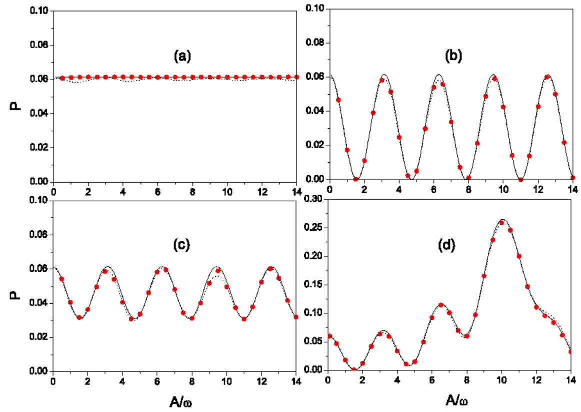

Fig. 2. The final tunnelling probabilities versus the dimensionless amplitude A/ω for different frequencies (a) $\omega^2/v = \pi$, (b) $\omega^2/v = \pi/2$, (c) $\omega^2/v = \pi/4$ and (d) $\omega^2/v = 1.695$. Here $\Delta/\sqrt{v} = 0.1$. The solid line shows the results of Eq. (18), and the square dots do the numerical results of Eq. (4). The dashed line is from transfer-matrix [11] showing small discrepancy.

(1) For $\omega^2/v = n\pi$ $(n = 0, 1, 2 \ldots)$, we have $P = \sin^2\sqrt{2\pi\Delta^2/v}$, which means that the final tunnelling probability keeps constant with changing the perturbation parameter A/ω, i.e., the external periodic perturbation does not affect the tunnelling probability no matter how strong it is. On the other hand, one can notice that when $\Delta^2/v \ll 1$ the expansion of our expression is approximately equivalent to that of the Landau–Zener formula in the first-order approximation [1]. The above prediction has been have confirmed by our numerical results as shown in Fig. 2(a).

(2) For $\omega^2/v = (n + 1/2)\pi$, we have $P = \sin^2(\sqrt{2\pi\Delta^2/v}\cos\frac{A}{\omega})$, which means that the final transition probability is oscillatory between 0 and $\sin^2\sqrt{2\pi\Delta^2/v}$ with increasing A/ω. When $A/\omega = (m + 1/2)\pi$, the final transition probability is zero, meaning that the particle is localized at its initial state $|1\rangle$ and the quantum transition is completely suppressed. When $A/\omega = m\pi$, the final transition probability is $\sin^2\sqrt{2\pi\Delta^2/v}$, which is the same as the case of $\omega^2/v = n\pi$. This result is also verified by our numerical simulation as shown in Fig. 2(b), in which we take the parameters to be $\omega^2/v = \pi/2$ and $\Delta/\sqrt{v} = 0.1$.

(3) For $\omega^2/v = (n \pm 1/4)\pi$, we have $P = \sin^2(\sqrt{\pi\Delta^2/v(1 + \cos^2\frac{A}{\omega}})$, which means that the final transition probability is oscillatory between $\sin^2\sqrt{\pi\Delta^2/v}$ and $\sin^2\sqrt{2\pi\Delta^2/v}$ with changing the dimensionless amplitude A/ω. When $A/\omega = (m + 1/2)\pi$, the final transition probability is $\sin^2\sqrt{\pi\Delta^2/v}$. When $A/\omega = m\pi$, the final transition probability is $\sin^2\sqrt{2\pi\Delta^2/v}$, sharing the same value as the case of $\omega^2/v = n\pi$. The result is also in agreement with our numerical simulation as shown in Fig. 2(c), in which we take the parameters to be $\omega^2/v = \pi/4$ and $\Delta/\sqrt{v} = 0.1$.

In the above three resonance cases, the transition probability either keeps consistent or tends to be suppressed by the periodic perturbation, compared to the standard LZ formula. The strongest suppression occur at $A/\omega = (m + 1/2)\pi$ in case (b), where the transition can be completely suppressed.

To see how the periodic modulation enhance the transition, we should choose the parameters away from the resonance regimes. In Fig. 2(d) we plot the dimensionless amplitude A/ω dependence of the final transition probability, with the parameters $\omega^2/v = 1.695$, $\Delta/\sqrt{v} = 0.1$. It shows a maximum enhancement on the transition probability occurred at $A/\omega = 3\pi$, where the total transition probability is five times larger than the prediction of the standard LZ formula. Our theoretical results are also confirmed by numerical simulations.

In conclusions, we study a modified LZ model analytically where the transition probability is shown to be modulated by the periodic perturbation through two scaled parameters, namely, A/ω and ω^2/v. We find that, in the low and high frequency limit of the modulation, the transition probability is always suppressed, compared to the standard LZ formula. Whereas, in the weak inter-level coupling case, we observe an interesting resonance phenomenon: We find that the transition probability is suppressed in the resonance regimes (i.e. $\omega^2/v = n\pi, (n + 1/2)\pi, (n + 1/4)\pi$) and enhanced only in the off-resonance regime, more effectively at some discrete values of A/ω, i.e. $(n\pi, (n + 1/2)\pi)$. Our results extend the famous LZ formula and applicable in future's practical physical systems.

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