Landau–Zener tunnelling in 2D periodic structures in the presence of a gauge field: I. Tunnelling rates

Andrey R Kolovsky

Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia
Siberian Federal University, Institute of Engineering Physics and Radio Electronics, 660041 Krasnoyarsk, Russia
E-mail: andrey.r.kolovsky@gmail.com

Received 6 March 2013, in final form 26 April 2013
Published 13 June 2013
Online at stacks.iop.org/JPhysB/46/145301

Abstract
We study the interband Landau–Zener tunnelling of a quantum particle in the Hall configuration, i.e., in the presence of gauge field (for example, magnetic field for a charged particle) and in-plane potential field (electric field for a charged particle) normal to the lattice plane. The interband tunnelling is induced by the potential field and for the vanishing gauge field is described by the common Landau–Zener theory. We generalize this theory for a nonzero gauge field. The depletion rates of low-energy bands are calculated by using a semi-analytical method of the truncated Floquet matrix.

1. Introduction
In recent years, we have seen a recovery of interest in the Landau–Zener (LZ) tunnelling in periodic structures. Although this phenomenon was originally discussed with respect to Bloch oscillations (BOs) of crystal electrons in a strong electric field [1–4], nowadays the most successful experimental systems are semiconductor superlattices [5–7], one-dimensional (1D) arrays of optical waveguides [8–11] and cold atoms in quasi-1D optical lattices [12–27]. These systems allow access to many different aspects of LZ tunnelling including the resonant tunnelling [6, 13, 16, 20, 23, 26], LZ tunnelling in binary (double-periodic) lattices [11, 21, 22, 25], time-resolved LZ tunnelling [15, 24], modification of LZ tunnelling by nonlinearity caused by atom–atom interactions [18–20, 22, 23, 26], etc.

The above-cited papers refer to 1D systems. Another direction of research is BO and LZ tunnelling in two-dimensional (2D) periodic structures [28–34]. In comparison with 1D lattices, LZ tunnelling in 2D lattices depends not only on the field magnitude but also on the lattice geometry (square, hexagonal, etc), direction of the field vector with respect to the lattice primary axes and particular properties (for example, separability) of the periodic potential. In this work, we address LZ tunnelling in 2D lattices in the presence of magnetic field (electron systems) or artificial gauge field (cold atoms and twisted waveguide arrays) normal to the lattice plane, which mimic the magnetic field for charge neutral particles [33, 35–38]. Using the solid-state terminology, we shall refer to these systems as a quantum particle in the Hall configuration. In what follows, we define the notion of LZ tunnelling for the quantum particle in the Hall configuration and obtain an estimate on its rate. This estimate is highly demanded to formulate the validity condition of the tight-binding approximation, that is widely used in the physical literature to analyse the cyclotron–Bloch dynamics of the quantum particle in the Hall configuration [39–45].

2. The system
Let us consider a square lattice, where the electric field is aligned with the y axis. Then, using the Landau gauge for a magnetic field, the Hamiltonian of the quantum particle in the Hall configuration reads
\[
\hat{H} = \frac{1}{2M} \left[ \hat{p}_x^2 + \left( \hat{p}_y - \frac{e}{c} B y \right)^2 \right] + V(x, y) + e F y,
\]
where \(M\) is the particle mass, \(e\) is the charge, and \(B\) and \(F\) are the magnitudes of the magnetic and electric fields,
respectively. For vanishing electric and magnetic fields, the spectrum of the Hamiltonian (1) consists of the ground Bloch band separated from the rest of the spectrum by a finite energy gap and we assume that the initial state of the particle belongs to this ground band. A finite $F$ induces BOS in the band and simultaneously causes LZ tunnelling across the energy gap. In what follows, we shall consider the separable periodic potential:

$$V(x, y) = v_x \cos \left(2\pi \frac{x}{a}\right) + v_y \cos \left(2\pi \frac{y}{a}\right),$$

where $a$ is the lattice period). In this case, the rate of tunnelling can be readily calculated because the 2D Hamiltonian factorizes into two 1D Hamiltonians if $B = 0$:

$$\tilde{H}_x = \frac{\hat{p}_x^2}{2M} + v_x \cos \left(2\pi \frac{x}{a}\right),$$

$$\tilde{H}_y = \frac{\hat{p}_y^2}{2M} + v_y \cos \left(2\pi \frac{y}{a}\right) + eFy.$$  

Thus, we can use the known results for 1D lattices where the population of the ground Bloch band decreases exponentially in time with the rate $\Gamma$ given by the inverse lifetime (resonance width) of the ground Wannier–Stark states [16]. Ignoring the phenomenon of resonant tunnelling the $F$ dependence of the rate $\Gamma$ is given by the celebrated LZ equation,

$$\Gamma(F) \sim F \exp \left(-\frac{b}{F}\right),$$

where $b$ is proportional to the square of the energy gap $\Delta_y$ of the Hamiltonian (3). For the purpose of future comparison, the dashed line in figure 1 shows the population of the ground Bloch band $N(t)$ as the functions of time for $v_x = 0.5E_R$, $v_y = 0.25E_R$ and $eFa = 0.05E_R$, where $E_R = \hbar^2/Ma^2$ sets the relevant energy scale. The initial wavefunction corresponds to the ground state of the Hamiltonian (1) for vanishing electric and magnetic fields, i.e., to the Bloch wave with zero quasi-momentum. The steps in $N(t)$ occur when the quasi-momentum $\kappa_y$, which evolves according to the linear law $\kappa_y = eFl/\hbar$, crosses the boundary of the Brillouin zone.

### 3. Magnetic bands

Before proceeding to LZ tunnelling for $B \neq 0$, we shall discuss the notion of ground magnetic bands. By those bands, we mean the magnetic bands that have originated from the ground Bloch band. One easily finds them by using the tight-binding approximation to the original Hamiltonian (see, for example, [46]):

$$\tilde{H}_{ib} = E_0 \sum_{l,m} |l, m\rangle \langle l, m| - \frac{J_y}{2} \sum_{l,m} (|l, m\rangle \langle l, m| + \text{h.c.})$$

$$- \frac{J_x}{2} \sum_{l,m} (|l, m\rangle \langle l, m| e^{2\alpha x l} + \text{h.c.}),$$  

where $|l, m\rangle$ denote the Wannier functions associated with the ground Bloch band, $E_0$ is the on-site energy, $J_{xy}$ are the hopping matrix elements and $\alpha$ is the Peierls phase given by the ratio of the magnetic flux $\Phi = Ba^2$ to the flux quantum $\Phi_0 = \hbar/e$. If $\alpha = 0$, the spectrum of (5) is given by

$$E(\kappa_x, \kappa_y) = E_0 - J_x \cos(\kappa_x) - J_y \cos(\kappa_y)$$

and the eigenfunctions are Bloch waves, $|\psi\rangle \sim \sum_{l,m} \exp[ia(\kappa_x l + \kappa_y m)l, m]$. If $\alpha \neq 0$, solutions of the stationary Schrödinger equation with the Hamiltonian (5) have the form $|\psi\rangle \sim \sum_{l,m} \exp[ia(\kappa_x m)b l l, m]$, where the coefficients $b_l$ satisfy the Aubry–André equation:

$$- \frac{J_x}{2} (b_{l+1} + b_{l-1}) - J_y \cos(2\pi \alpha l + a\kappa_x) b_l = Eb_l,$$

where $J_x = J_y$ coincides with the Harper equation [47]. If $\alpha$ is a rational number, then we can apply the Bloch theorem and, hence, eigenfunctions of (6) are labelled by the quasi-momentum $\kappa_y$ defined in the reduced Brillouin zone. Thus, for rational $\alpha = r/q$, the ground Bloch band splits into $q$ magnetic bands. As an example, the lower panel in figure 2 shows the ground magnetic bands for $\alpha = 1/8$ and $(J_x, J_y) = (0.0431, 0.0741)E_R$, which corresponds to $(v_x, v_y) = (0.5, 0.25)E_R$ in the continuous Hamiltonian (1). Note that in figure 2 we use the extended Brillouin zone picture. We also mention that in the considered case $J_x > J_y$, the magnetic bands are almost flat in the $\kappa_y$ direction.

For deep lattices, the above tight-binding approach provides a reasonable approximation to the ground magnetic bands¹. However, to address LZ tunnelling, we need to find not only ground bands but also the spectrum above the energy gap. In the rest of this section, we discuss a different method of calculating the ground magnetic bands which accomplishes this task. To simplify equations, we use from now on dimensionless variables where the length is measured in units of $a/2\pi$, the energy in units of $E_R = \hbar^2/Ma^2$ and the

¹ For the considered separable potential, ‘the deep lattices’ mean $v_x, v_y > 0.5E_R$. 

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**Figure 1.** Survival probability as the function of time for $eFa/2\pi = 0.05E_R$ ($E_R = \hbar^2/Ma^2$) and $B = 0$, dashed line, and $a^2B = \Phi_0/8$ ($\Phi_0 = \hbar/e$), solid line. The lattice parameters are $v_x = 0.5E_R$ ($J_x = 0.0431E_R$) and $v_y = 0.25E_R$ ($J_y = 0.0741E_R$). The time is measured in units of the Bloch period $T_B = h/eFa$. Inset shows the data in the semi-logarithmic scale.
time in units of $\hbar/E_R$. In these units, the Hamiltonian (1) takes the form
\[ \hat{H} = \frac{1}{2} \left( \hat{p}_x^2 + (\hat{p}_y - Bx)^2 \right) + v_x \cos x + v_y \cos y + Fy, \]
\[ B = \frac{\alpha}{2\pi}, \]
where the magnetic field is characterized by the Peierls phase $\alpha$ and the dimensionless electric field is given by the ratio of the Stark energy over the one lattice period to the recoil energy.

Let us assume that $v_x$ is large enough to justify the tight-binding approximation in the $x$ direction. Then we can use the ansatz
\[ \psi_{l}(x, y) = \sum_{l=-\infty}^{\infty} \psi_{l}(y) \phi_{l}(x), \]
where $\phi_{l}(x)$ are the 1D Wannier functions associated with the ground Bloch band of the Hamiltonian (2). Substituting (8) into the stationary Schrödinger equation with the Hamiltonian (7), where we temporarily set $F = 0$, we have
\[ E_0 \psi_{l}(y) - \frac{J_x}{2} \left[ \psi_{l+1}(y) + \psi_{l-1}(y) \right] + \hat{H}_{y}^{(l)} \psi_{l}(y) = E \psi_{l}(y), \]
where
\[ \hat{H}_{y}^{(l)} = \frac{1}{2} \left( \hat{p}_y - \alpha l \right)^2 + v_y \cos y. \]

The eigenfunctions of the Hamiltonians (10) are Bloch waves with the shifted dispersion relation. Namely, if $E(\kappa_y)$ is the Bloch spectrum of the Hamiltonian $\hat{H}_{y}^{(0)}$, then for $l \neq 0$ we have
\[ E^{(l)}(\kappa_y) = E^{(0)}(\kappa_y + \alpha l), \]
see figure 3(a). Next, using the Fourier expansion for the Bloch wave,
\[ \psi_{l}(y) = \exp(i\kappa_y) \sum_{n=-\infty}^{\infty} c_{l}^{(n)}(\kappa_y) \exp(iny), \]
the system of partial differential equations (9) reduces to the system of algebraic equations for the coefficients $c_n^{(j)}$:

$$\begin{align*}
- \frac{J_y}{2} [c_n^{(j+1)} + c_n^{(j-1)}] + \frac{1}{2} (n + \kappa_y + \alpha l) c_n^{(j)} \\
\frac{\nu_y}{2} [c_n^{(j)} + c_{n+1}^{(j)}] &= E c_n^{(j)}. 
\end{align*}$$

(13)

In the general case of arbitrary $\alpha$, the index $l$ in (9)–(13) runs from minus to plus infinity. However, if $\alpha = r/q$ is a rational number, we can restrict $l$ to one magnetic period, $1 \leq l \leq q$. In this case, equation (13) should be supplemented by the periodic boundary condition

$$c_n^{(q+1)} = e^{2\pi \kappa_x l} c_n^{(1)},$$

(14)

where the dimensionless quasi-momentum $\kappa_x$ in the Bloch phase factor is defined in the reduced Brillouin zone $|\kappa_x| \leq 1/2q$. The system of algebraic equations (13) together with the boundary condition (14) provide an alternative method for calculating the ground magnetic bands.

The right panel in figure 3 shows the solution of equations (13) and (14) for $\alpha = 1/8$, $\nu_y = 0.25$ and $J_y = 0.0431$, which corresponds to $\nu_y = 0.5$. Magnetic bands are plotted as functions of the quasi-momentum $\kappa_y$ for a single value of the quasi-momentum $\kappa_x = 0$. This figure should be compared with figure 2(b) showing the magnetic bands in the tight-binding approximation. We note that in figure 3, we intentionally restricted the upper limit of the energy axis to a relatively low value because for higher energies the second Bloch band of the Hamiltonian $H_2$ contributes the spectrum. However, for our aim of studying LZ tunnelling, it is sufficient to have a fragment of the actual energy spectrum just above the energy gap.

4. LZ tunnelling

The structure of the eigenvalue equation (9) provides an insight into the physics of LZ tunnelling in the presence of a magnetic field. To address this phenomenon, the 1D Hamiltonians (10) should be complemented with the term $F y$ and we should solve the non-stationary Schrödinger equation instead of the stationary one. Thus, the original 2D problem reduces to $q$ coupled 1D Landau–Zenner problems. Below we analyse the effect of this coupling on the tunnelling dynamics by using two different approaches.

In our first approach, we numerically solve the time-dependent Schrödinger equation and project the solution on the subspace of ground magnetic bands. In more detail, we solve the following differential equations for the coefficients $c_n^{(j)}$:

$$\begin{align*}
\dot{c}_n^{(j)} &= -\frac{J_y}{2} (c_n^{(j+1)} + c_n^{(j-1)}) + \frac{1}{2} (n + \kappa + \alpha l) c_n^{(j)} \\
&+ \frac{\nu_y}{2} (c_{n+1}^{(j)} + c_{n-1}^{(j)}),
\end{align*}$$

(15)

where the quasi-momentum $\kappa'$ linearly depends on time as $\kappa' = \kappa_y + F t$. (This equation follows from (12) where one substitutes $\kappa'$ instead of $\kappa_y$.) The initial wavefunction corresponds to one of the multi-degenerate ground states of the system for $F = 0$. Thus, initially only the lowest magnetic band is populated. Depending on the electric field magnitude $F$, we observed three different regimes of the tunnelling dynamics. For very small $F$, the population of the lowest magnetic band stays close to unity during the whole simulation time. If $F$ exceeds some critical value $F_c$, then all $q$ ground magnetic bands become involved in the dynamics, yet their populations sum up to unity with high accuracy. Finally, for even larger $F$, we observe a decrease in the total population of the ground magnetic bands; see figure 1. Comparing $N(t)$ for $\alpha = 1/8$ (solid line) and $\alpha = 0$ (dashed line), it is seen that the finite magnetic field decreases the rate of LZ tunnelling and smoothes oscillations of $N(t)$, although the overall decay remains exponential (see inset in figure 1).

In the above simulations, the initial wavefunction belongs to the lowest magnetic band. In fact, the rate of tunnelling across the main energy gap strongly depends on which magnetic band is initially populated. To find decay rates $\Gamma_j$ of the individual magnetic bands, we employ the truncated Floquet matrix method of [28], adopted to the currently considered problem. Namely, using the ansatz (12) and the Schrödinger equation (15), we calculate the (formally infinite) matrix of the evolution operator over one Bloch period $T_B = 1/F$ and truncate it to a finite size. Note that when calculating the Floquet matrix, we explicitly use the periodic boundary condition (14). Thus, the matrix is truncated only with respect to the index $n, |n| \leq n_{\text{max}}$. (The method rapidly converges if $n_{\text{max}}$ is increased: in our calculations we use $n_{\text{max}} = 7$.) The eigenvalues $\lambda_j$ of the truncated Floquet matrix are known to be the complex poles of the scattering matrix. Then the individual decay rates $\Gamma_j$ of ground magnetic bands are found from the equation $|\lambda_j|^2 = \exp(-\Gamma_j T_B)$, where $\lambda_j$ are the first $q$ eigenvalues which are closest to the unit circle.

The decay rates $\Gamma_j$ for $\alpha = r/q = 1/8$ are shown in figure 4(b) as functions of the inverse electric field magnitude. The right panel of this figure should be compared with the left panel, which shows the decay rate of the ground Bloch band

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1. These two regimes correspond to the transporting and ballistic regimes of the cyclotron-Bloch dynamics, respectively, that in the tight-binding approximation were studied in much detail in [43–45].
for $B = 0$. As mentioned in section 2, for $B = 0$ the functional dependence of the decay rate is approximately given by the LZ formula (4), where deviations are due to the phenomenon of the resonant tunnelling [16]. It can be seen in figure 4 that the resonant tunnelling also takes place if $B \neq 0$. Thus, we can decompose $\Gamma_j$ into two terms:

$$\Gamma_j(F) = \bar{\Gamma}_j(F) + \Gamma_j^s(F)$$  \hspace{1cm} (16)

where $\Gamma_j(F) \sim F \exp(-b_j/F)$ and $\Gamma_j^s(F)$ is the oscillating part. Analysing the values of the coefficients $b_j$ we conclude that LZ tunnelling is suppressed for lower magnetic bands, $j \ll q$, but enhanced for higher bands, $j \sim q$. Note that this effect is well pronounced only for weak electric fields, while in the strong field regime the decay rates $\Gamma_j$ approximately coincide with that for $B = 0$.

To conclude this section, we briefly discuss the case of irrational $\alpha$. Since in the wavefunction simulations we do not use any boundary conditions, we can directly compare the survival probability $N(t)$ for rational and irrational $\alpha$. However, this approach gives reliable results only for strong electric fields, where $N(t)$ essentially differs from unity, and we can ignore an error introduced by the integrator. On the other hand, using the Floquet matrix method, we can reliably treat weak electric fields but, since the method explicitly uses the boundary condition (14), an irrational $\alpha$ has to be approximated by a sequence of rational numbers, which makes calculations very time consuming. We did our best employing both methods but found no qualitative difference with the case of rational $\alpha$. This is consistent with results of [43, 44] where the rationality of $\alpha$ is shown to affect neither dynamics nor spectral properties of the system in the tight-binding approximation.

5. Conclusions

We analysed the interband Landau–Zener (LZ) tunnelling for a quantum particle in the Hall configuration. It was found that a strong electric field induces transitions to higher energy states also in the presence of a finite magnetic field $B$. Moreover, in the strong field regime the corrections to the LZ equation (4) due to finite $B$ was found to be relatively small. Thus, as the first approximation, one can use this equation to estimate the rate of LZ tunnelling. This result is crucial for understanding the cyclotron–Bloch dynamics of the quantum particle beyond the tight-binding approximation. In particular, it was shown in the recent works [44, 45] devoted to the system (1) in the tight-binding approximation that the particle is localized in the lattice for almost all directions of the electric field, where the localization length of the eigenstates tends to one lattice site when $F$ is increased. However, the present analysis shows that the tight-binding approximation is valid only up to certain $F$, while LZ tunnelling across the energy gap can be neglected. Thus the result about particle localization in the limit of large $F$ can be questioned. We address this problem in our subsequent work [48].

Acknowledgments

The authors acknowledge financial support of Russian Academy of Sciences through the SB RAS integration project no. 29 Dynamics of atomic Bose–Einstein condensates in optical lattices and the Russian Foundation for Basic Research (RFBR) project no. 12-02-00094 Tunneling of the macroscopic quantum states.

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