Zener transitions between dissipative Bloch bands. II: Current Response at Finite Temperature

Xian-Geng Zhao
CCAST (World Laboratory) P.O. Box 8730, Beijing 100080, China
Institute of Applied Physics and Computational Mathematics,
P.O. Box 8009, Beijing 100088, China

Daniel W. Hone
Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106

We extend, to include the effects of finite temperature, our earlier study of the interband dynamics of electrons with Markoffian dephasing under the influence of uniform static electric fields. We use a simple two-band tight-binding model and study the electric current response as a function of field strength and the model parameters. In addition to the Esaki-Tsu peak, near where the Bloch frequency equals the damping rate, we find current peaks near the Zener resonances, at equally spaced values of the inverse electric field. These become more prominent and numerous with increasing bandwidth (in units of the temperature, with other parameters fixed). As expected, they broaden with increasing damping (dephasing).

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I. INTRODUCTION

In a previous paper (henceforth referred to as I) we began a study of the effects on interband transitions of the scattering of electrons from static imperfections in a semiconductor superlattice. A uniform static electric field was applied. It has long been recognized that scattering destroys the coherence necessary to sustain the Bloch oscillations predicted in such a field, and in practice this delayed the observation of these oscillations until the development of semiconductor superlattices. But the scattering destroys other types of interesting coherent motion, as well. Dunlap and Kenkre, in particular, looked at the effects on dynamic localization of electrons in time periodic electric fields. We were interested in I in a multiband effect, the Rabi oscillations of electron population between bands of a crystal in a uniform static electric field of appropriate magnitude — near an avoided crossing of the two interpenetrating Wannier-Stark Ladders (WSL) arising essentially from different bands. These are the so-called Zener resonances. Within a simple two-band tight-binding model we demonstrated the destruction of localization (of occupied electron states) to a single miniband by the dephasing associated with the scattering. The decay rate for the approach to steady state band populations exhibits sharp peaks at values of the static electric field which give Zener resonances in the absence of scattering. The specific approximations in I, however, effectively limited the results to the case of infinite temperature. In particular, the steady state was assumed to be equal population of the two bands. In this paper we remove that restriction, to discuss these effects at finite temperature. The necessary modification was described in Ref. (4), namely relaxation of band populations toward values set by the Boltzmann factors describing thermal equilibrium. This will allow us, in particular, to look at the electric current, a quantity of obvious experimental interest which vanishes in the infinite temperature limit.

II. MODEL

We consider the same model that we treated in I, a standard simple tight-binding model of a two-band system in a static electric field $E$. The Hamiltonian can be written as

$$H = \sum_n \left[ (\Delta_a + n\omega_B) a_n^\dagger a_n + (\Delta_b + n\omega_B) b_n^\dagger b_n ight.$$

$$- (W_a/4) (a_{n+1} a_n + h.c.) + (W_b/4) (b_{n+1} b_n + h.c.)$$

$$+ eE R (a_n b_n + b_n^\dagger a_n). \right] \tag{1}$$
Here the subscripts label the lattice sites and the lower and upper minibands are designated by symbols $a$ and $b$, respectively. We have introduced the notation $\omega_k \equiv eEd$, where $d$ is the lattice constant, for the Bloch frequency, which will appear often below. The first two terms describe the site energies of the Wannier states in the presence of the electric field, and $W_{a,b}$ are the widths of the isolated ($E = 0$) minibands induced by nearest neighbor hopping: $\epsilon_{a,b}(k) = \Delta_{a,b} \mp (W_{a,b}/2) \cos k$, where the dimensionless wave vector $k$ is in units of the inverse lattice constant $d$.

The last term is the on-site electric dipole coupling between minibands: $eR$ is the corresponding dipole moment. This Hamiltonian does neglect Coulomb interactions and electric dipole elements between Wannier states on different sites, but it contains the essential physics for the problem. Note that the hopping parameters $W_{a,b}$ are written here with opposite signs, so that with both parameters positive the band structure at $E = 0$ is of the standard nearly free electron character, with direct band gaps at the zone boundary. But the calculation to follow is valid for arbitrary signs of the parameters.

It is easily shown[4] that the exact spectrum of $H$ is two interpenetrating Wannier-Stark Ladders. But what do the corresponding states represent in terms of the occupation of the original bands as a function of time, and what is the influence of scattering? For vanishing dipole matrix element between bands, $R = 0$, there is no interband mixing. Each of the two bands gives rise to a single WSL. Clearly, when the electric field amplitude is such that the ladders become degenerate, even small values of $R$ lead to strong interband mixing. The crossing of the ladders is “avoided” by any finite $R$, and the behavior near those avoided crossings (the Zener resonances) is of particular importance and interest. In general there are peaks in the current response at those values of the electric field, but the peaks are broadened by increasing temperature, as well as by decreasing bandwidth relative to band separation.

We start by defining the density matrix in the representation of the two bands,

$$ \rho(t) = \sum_{ij,mn} \rho_{ij,mn}^O \xi_{m,n}^i \xi_{m,n}^j, $$

where $i, j = 1$ or $2$ are band indices: $\xi_{m}^1 (\xi_{m}^2)$ and $\xi_{m}^2 (\xi_{m}^1)$ designate $a_{m}^\dagger (a_{m})$ and $b_{m}^\dagger (b_{m})$, respectively. Since we are interested in the dynamics of occupation of various band states, it is convenient to work in a wave vector basis, by Fourier transforming the density matrix. In general, since $\rho_{mn}$ is not translationally invariant (a function only of $m - n$), we have a full set $\rho_{kq}^{ij} = \sum_{mn} \rho_{mn}^{ij}(t) \exp[-i(k + q)n + iqn]$ of Fourier components. But we will be interested in the wave vector diagonal band occupation numbers $\rho_{kk}^{ij}(t) \equiv \rho^{ij}(k, t)$. Then at finite temperature $T$ we insist that the wave vector and band diagonal occupation number relax to the thermal equilibrium value,

$$ \rho_{kk}^{ij} \to \rho_T^{ij}(k) \equiv e^{-\beta \epsilon_k^{ij}} \sum e^{-\beta q^{ij}}, $$

where $\beta = 1/k_B T$, the sum in the partition function is over $j = 1, 2$ and over all wave vectors $q$, and the band energies are those given above,

$$ \epsilon_{1,2}(k) = \Delta_{a,b} \mp (W_{a,b}/2) \cos k. $$

Within a constant relaxation rate approximation[4], the density matrix $\rho(k, t)$ satisfies the following stochastic Liouville equation (SLE) (we set $\hbar = 1$ throughout this paper),

$$ i \frac{d\rho}{dt} = [H, \rho(t)] - i\Gamma [\rho(t) - \rho_T]. $$

Here each of $H$, $\rho$, and $\rho_T$ is labelled by (the same) wave vector $k$. The operator $\Gamma$ describes the relaxation of the off-diagonal elements of $\rho$ through dephasing:

$$ \Gamma[\rho - \rho_T] = \sum_{ij} \alpha_{ij} \left[ \rho^{ij}(k, t) - \delta_{ij} \rho_T(k) \right] \xi_{m,n}^i \xi_{m,n}^j. $$

The utility of this simplest form of the SLE has been discussed by Kenkre and collaborators (see Ref. 4 and references therein). The parameters $\alpha_{ij}$ measure the loss of phase coherence between sites, or the scattering lifetime of band states labeled by quasimomentum.

As in I it is convenient to introduce the linear combinations of density matrix elements:

$$ \rho_+(k, t) = \rho^{11}(k, t) + \rho^{22}(k, t), $$

$$ \rho_-(k, t) = \rho^{11}(k, t) - \rho^{22}(k, t), $$

$$ \rho_{+-}(k, t) = \rho^{12}(k, t) + \rho^{21}(k, t), $$

$$ \rho_{-+}(k, t) = i[\rho^{21}(k, t) - \rho^{12}(k, t)]. $$
For simplicity, we also take $\alpha_{11} = \alpha_{22} = \alpha_{12} = \alpha_{21} = \alpha$ to reduce the number of parameters in the theory. Then the SLE (3) has the explicit components

\begin{equation}
\frac{\partial}{\partial t} \rho_+(k, t) - \omega_B \frac{\partial}{\partial k} \rho_+(k, t) = -\alpha \left[ \rho_+(k, t) - \rho_T^+(k) \right],
\end{equation}

\begin{equation}
\frac{\partial}{\partial t} \rho_-(k, t) - \omega_B \frac{\partial}{\partial k} \rho_-(k, t) = -2eER \rho_-(k, t) - \alpha \left[ \rho_-(k, t) - \rho_T^-(k) \right],
\end{equation}

\begin{equation}
\frac{\partial}{\partial t} \rho_{+-}(k, t) - \omega_B \frac{\partial}{\partial k} \rho_{+-}(k, t) = \left( \Delta - W \cos k \right) \rho_{+-}(k, t) - \alpha \rho_{+-}(k, t),
\end{equation}

\begin{equation}
\frac{\partial}{\partial t} \rho_{-+}(k, t) - \omega_B \frac{\partial}{\partial k} \rho_{-+}(k, t) = -\left( \Delta - W \cos k \right) \rho_{-+}(k, t) + 2eER \rho_{-+}(k, t) - \alpha \rho_{-+}(k, t).
\end{equation}

Here we have used the simplified notation $\Delta = \Delta_a - \Delta_b$ and $W \equiv (W_a + W_b)/2$. The equation (11) for $\rho_+$ is decoupled from the others, and is readily integrated to give

\begin{equation}
\rho_+(k, t) = e^{-\alpha t} \left\{ \rho_T^+(k + \omega_B t) + \alpha \int_0^t dt' e^{\alpha t'} \rho_T^+(k + \omega_B (t - t')) \right\}.
\end{equation}

The equations for $\rho_-(k, t)$, $\rho_{+-}(k, t)$, and $\rho_{-+}(k, t)$ can be reduced to the following ordinary differential equations in an accelerated basis, $k(t) = k - \omega_B t$ or, equivalently, in the transverse or vector gauge discussed in Ref. 10,

\begin{equation}
\frac{d}{dt} X(k, t) = -2eER Z(k, t) - \alpha [X(k, t) - \rho_T^-(k - \omega_B t)],
\end{equation}

\begin{equation}
\frac{d}{dt} Y(k, t) = [\Delta - W \cos(k - \omega_B t)] Z(k, t) - \alpha Y(k, t),
\end{equation}

\begin{equation}
\frac{d}{dt} Z(k, t) = -[\Delta - W \cos(k - \omega_B t)] Y(k, t) + 2eER X(k, t) - \alpha Z(k, t).
\end{equation}

Here $X(k, t) = \rho_-(k - \omega_B t, t)$, $Y(k, t) = \rho_{+-}(k - \omega_B t, t)$, and $Z(k, t) = \rho_{-+}(k - \omega_B t, t)$. The structure is exactly the same as Eqs. (17 - 19) in I, except for the $k$-dependent relaxation of $X$ here. As we did there, we can integrate these equations analytically as a perturbation series in the parameter $\mu \equiv 2eER$, which characterizes the electric dipole coupling between bands. To lowest nontrivial (second) order in $\mu$ we find

\begin{equation}
\rho_-(k, t) = e^{-\alpha t} \left\{ \rho_T^-(k + \omega_B t) + \alpha \int_0^t dt' e^{\alpha t'} \rho_T^-(k + \omega_B (t - t')) \right\} \cos \int_{t'}^{t} dt'' \left[ \Delta - W \cos(k + \omega_B (t - t'')) \right].
\end{equation}

### III. CURRENT

We turn now to the calculation of the interesting physical quantity, the current $j(t)$ along the superlattice direction. In the band $i = a, b$ the instantaneous current is given by the sum over wave vectors of the relevant electron velocity $v_i(k) = (W_i d/2) \sin k$ times the number density in that band at that wave vector, $n_0 \rho_i(k, t)$, where $n_0$ is the number of carriers per unit area in each cell of the superlattice. In terms of the convenient quantities $\rho_{\pm}(k, t)$ we then have

\begin{equation}
\dot{j}(t) = \int_0^{2\pi} \frac{dk}{8\pi} [(W_a - W_b) \rho_{+}(k, t) + 2W \rho_{-}(k, t)] n_0 d \sin k.
\end{equation}

Of particular interest is the steady state long time average of this,
\[ \langle j \rangle = \lim_{T_0 \to \infty} \frac{1}{T_0} \int_0^{T_0} dt \langle j(t) \rangle. \] (21)

To second order in \( \mu \) we have the probability densities \( \rho_{\pm}(k, t) \), in Eqs. (18) and (19), and we find

\[
\frac{\langle j \rangle}{\rho_{\pm}} = \left( \frac{W_a}{2} \right) \left( \frac{\alpha \omega_B}{\alpha^2 + \omega_B^2} \right) [C_1 + (W_b/W_a)C_2] \\
- \left( \frac{W}{4} \right) \left( \frac{\alpha \mu}{\alpha^2 + \omega_B^2} \right)^2 [C_1 + C_2] \sum_{\ell = -\infty}^{\infty} [D_{\ell}^- + D_{\ell}^+] J_\ell^2(W/\omega_B),
\] (22)

with

\[
C_1 = \frac{e^{-\beta\Delta} I_1(\beta W_a/2)}{e^{-\beta\Delta} I_0(\beta W_a/2) + I_0(\beta W_b/2)},
\]

\[
C_2 = \frac{I_1(\beta W_b/2)}{e^{-\beta\Delta} I_0(\beta W_a/2) + I_0(\beta W_b/2)},
\]

\[
D_{\ell}^{\pm} = \frac{\alpha^2 - \omega_B^2 - 2\omega_B[(\ell + 1)\omega_B \pm \Delta]}{\alpha^2 + [(\ell + 1)\omega_B \pm \Delta]^2},
\]

where \( I_n \) is the modified Bessel function and \( J_n \) the ordinary Bessel function of order \( n \). The interband effects are all contained in the second term on the right hand side of (22), proportional to \( \mu^2 \). The Zener resonances, near \( \Delta = n\omega_B \), with \( n \) an integer, exhibit themselves as peaks in the factors \( D_{\ell}^{\pm} \).

We will look at the nonlinear conductance, the current as a function of increasing electric field, which is conveniently expressed in terms of \( n \) having been described by a single parameter characterizing the rate at which a nonequilibrium density is restored to thermal equilibrium, using a stochastic Liouville equation. We have been particularly interested in the interband

\[ \langle j \rangle = \lim_{T_0 \to \infty} \frac{1}{T_0} \int_0^{T_0} dt \langle j(t) \rangle. \] (21)

IV. CONCLUSIONS

Within a simple two-band tight binding model we have studied the electric current response of a semiconductor superlattice subject to a finite uniform electric field. Relaxation processes have been assumed Markoffian, and they have been described by a single parameter characterizing the rate at which a nonequilibrium density is restored to thermal equilibrium, using a stochastic Liouville equation. We have been particularly interested in the interband
transitions, which lead to current peaks near the values of external field where Zener resonances occur. We have exhibited the variation in height and width of these peaks, as well as in the overall current magnitude with temperature and with the various parameters of the theory, including bandwidth, band separation, interband dipole coupling, and relaxation rate.

The results we have obtained are perturbational in \( \mu \); we do require weak interband coupling. Moreover, we have limited the discussion to a single pair of bands, assuming the impact of all other bands to be negligible on the Zener tunneling between these two. This can be realized in practice by using a dimerized semiconductor superlattice with, for example, uniform wells but alternating thick and thin barriers between them. With weak alternation of barrier thickness one can adjust a pair of bands resulting from the doubling of the unit cell to be well isolated from all other bands, and the predictions of this paper can be studied in such a system by varying the external uniform electric field. Another way to observe the effects predicted here is to use ultracold atoms in accelerating optical potentials. Recently, Rabi oscillations were observed in such a system, where the interband coupling was generated by a small phase modulation. Very low temperatures can be realized in these systems, and it should be possible to observe the resonant structures in current that we have predicted in this paper.

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FIG. 1. Time averaged current in the absence of interband transitions (\( \mu = 0 \)). The ratio of relaxation rate to band center separation is \( \alpha/\Delta = 0.1 \). The bandwidths are \( W_a = W_b = W = 0.8\Delta \).

FIG. 2. Time averaged current, as in Fig. 1, but with \( \mu = W = 0.4\Delta \).

FIG. 3. Time averaged current, as in Fig. 2, but with \( W = 0.8\Delta \).

FIG. 4. Time averaged current, as in Fig. 2, but with \( \alpha = 0.05\Delta \).

FIG. 5. Time averaged current, as in Fig. 2, but with \( \alpha = 0.2\Delta \).
\[ \frac{2 \langle j \rangle}{W n_\theta d} \] vs. \[ \frac{\omega_B}{\Delta} \]
\[ \frac{2 \langle j \rangle}{\omega n_0 d} \] vs \[ \frac{\omega_B}{\Delta} \]