Bloch oscillations, Zener tunneling and Wannier-Stark ladders in the time-domain

Jon Rotvig\textsuperscript{a}, Antti-Pekka Jalilho\textsuperscript{b}, and Henrik Smith\textsuperscript{a}
\textsuperscript{a}Ørsted Laboratory, H.C.Ørsted Institute, Universitetsparken 5, University of Copenhagen, DK-2100 Copenhagen \text{Ø}, Denmark
\textsuperscript{b}MIC, Technical University of Denmark, DK-2800 Lyngby, Denmark
(March 23, 2022)

We present a time-domain analysis of carrier dynamics in a semiconductor superlattice with two minibands. Integration of the density-matrix equations of motion reveals a number of new features: (i) for certain values of the applied static electric field strong interband transitions occur; (ii) in static fields the complex time-dependence of the density-matrix displays a sequence of stable plateaus in the low field regime, and (iii) for applied fields with a periodic time-dependence the dynamic response can be understood in terms of the quasiequilibrium spectra.

Bloch oscillations (BO) are one of the most striking predictions of the semiclassical theory of electronic transport: in any system of independent electrons in a periodic potential the electron velocity becomes a periodic function of time with characteristic frequency $\omega_B = eEd/\hbar$, where $d$ is the lattice period and $E$ is the applied field \[2\]. In ordinary bulk materials these oscillations cannot be seen, because collisions dephase the coherent motion of electrons on a time-scale which is much shorter than $T_B = 2\pi/\omega_B$. However, as pointed out by Esaki and Tsu \[3\], the conditions for observing BO’s are much less stringent for high-quality semiconductor superlattices. Recent years have witnessed an intense experimental activity in this area, culminating in the observation of terahertz radiation from coherently oscillating electrons \[4\].

There has been equal activity on the theoretical side. Holthaus \[5\] analyzed the semiclassical motion of electrons in a single mini-band subjected to a strong \textit{alternating} electric field. Studies of this kind have gained importance due to the emerging free-electron lasers, which open the possibility of experimental probing of the theoretical predictions. For certain values of the system parameters a dynamical localization takes place \[6\]: the average velocity vanishes. This phenomenon can alternatively be called band collapse \[7\]. Ignatov et al. \[8\] pointed out an interesting analog between Bloch electrons and the Josephson effect. Very recently, Meier et al. \[9\] considered coherent motion of photoexcited carriers in the presence of Coulomb interaction, and found out that BO’s should persist even in the limit where the exciton binding energy is comparable to the miniband width.

The papers quoted above have mainly concentrated on studying systems with one miniband \[8\]; the central theme in the present work is to study the dynamics of electrons in a \textit{two-band} superlattice. The second miniband adds an essential feature to the model: it is possible to study how Zener tunneling affects the dynamics of the carriers. Our method consists of setting up, and solving, the density-matrix equations of motion for the two-band system. In this paper we focus on the coherent part of the motion. This coherent motion displays in its own right a number of interesting features, which we shall describe after having sketched the general formalism.

First we need to define the microscopic model underlying the density matrix calculation. The model Hamiltonian is

$$H = \sum_n \left[ (\Delta_n^a + n eEd)a_n^\dagger a_n + (\Delta_n^b + n eEd)b_n^\dagger b_n \right. $$

$$\left. - \frac{\Delta_n^a}{4}(a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1}) - \frac{\Delta_n^b}{4}(b_{n+1}^\dagger b_n + b_n^\dagger b_{n+1}) + eE R(a_n^\dagger b_n + b_n^\dagger a_n) \right].$$

The integers $n$ label the lattice sites and the operators $a$ and $b$ refer to electrons in the two minibands; the first two terms give the (field-dependent) site-energies, the next two describe site-to-site hopping, and the last one is the term responsible for the interband transfer. The overlap matrix-element $R$ is model-dependent and may depend on time through its momentum argument; we take it as a constant corresponding to a Kronig-Penney model. At zero applied field \[1\] leads to two mini-bands, $e^{a,b}(k) = \Delta_n^{a,b} \mp (\Delta_n^{a,b}/2) \cos(kd)$, while at finite static fields the spectrum consists of two interpenetrating Stark-ladders \[10\]: $e_{n}^{a,b} = \Delta_n^{a,b} + eEdn^{a,b} - meEd$. The numbers $n^{a,b}(E)$ must be determined numerically, and results of such a calculation are shown in Fig. \[1\]. It is important to notice that for certain field values the two levels come very close to each other; as we shall show below this leads to profound effects on Zener-tunneling.

Let us next consider the equation of motion for the density matrix for $a$- and $b$-electrons. With accelerated Bloch states as the basis \[1\], the diagonal elements of the density matrix give the electron density at a $k$-point following the semiclassical trajectory in reciprocal space, $k(t) = K - (e/\hbar) \int_0^t E(t') dt'$. We assume equilibrium at $t = 0$, when the density matrix is diagonal. Defining $\rho_\pm(K,t) = \rho_\pm^k(t) \pm \rho_\mp^k(t)$, we find the following equations of motion \[12\]:

$$\dot{\rho}_\pm(K,t) = 0 ,$$

(2)
\[ \dot{\rho}_-(K, t) = -\text{Re} \left\{ h(K, t) \int_0^t dt' h^*(K, t') \rho_-(K, t') \right\}, \tag{3} \]

where

\[ h(K, t) = 2\frac{e}{\hbar} E(t) R \exp \left[ -\frac{i}{\hbar} \int_0^t \Delta \epsilon(k(t')) dt' \right] \equiv ue^{i\phi}. \tag{4} \]

In the above equations we have defined \( \Delta \epsilon(k) = \epsilon^b(k) - \epsilon^a(k) \), and assumed that the intraband couplings are identical \[13\].

Eqs.\((\ref{eq:3})\) require several comments. If the interband coupling is turned off, they reduce to the normal collisionless Boltzmann equation (for two minibands), and thus contain, as special cases, the following standard results: (i) for static field one finds standard Bloch oscillations; and (ii) a harmonic \(E\)-field leads to the analog with Josephson effect of Ref. \[7\], and in particular, reproduces the band collapse discussed by Holthus \[8\]. Note that only \( \rho_- \) is affected by interband transitions, while \( \rho_+ \), which fixes the particle density, is a constant of motion.

By differentiating the equation of motion for \( \rho_- \) with respect to time, one finds \[12\]

\[ \dot{\rho}_- - \frac{\dot{u}}{u} \rho_- + u^2 \rho_- + u\phi \int_0^t dt' \dot{\rho}_- / u = 0. \tag{5} \]

Eq.\((\ref{eq:5})\) forms the basis of our analysis, and the rest of this paper will describe the numerical results obtained from it under a number of specific physical conditions.

a. Steady fields. In this case the dc-field is turned on abruptly at \( t = 0 \). From Eq.\((\ref{eq:4})\) \( u \) is time-independent, and Eq.\((\ref{eq:5})\) can be reduced to an ordinary third order differential equation:

\[ \ddot{\rho}_- - \dot{\phi} \dot{\rho}_- + \phi (u^2 + \dot{\phi}^2) \dot{\rho}_- - u^2 \ddot{\rho}_- = 0. \tag{6} \]

The accompanying initial conditions are \( \rho_- (0) = \rho^0_- \), \( \dot{\rho}_-(0) = 0 \), and \( \ddot{\rho}_-(0) = -u^2 \rho_-(0) \). Thus, the initial values are determined by the miniband parameters, the \( k \)-point in the Brillouin zone and the temperature (which enters through \( \rho_- (0) \)). From Eq.\((\ref{eq:5})\) it follows that \( \rho_-(K, 0) \) can be chosen equal to 1 without loss of generality.

Fig. \[2\] displays a typical time-dependence of \( \rho_- \), obtained from Eq.\((\ref{eq:5})\) by numerical integration. One observes a very sensitive behavior with respect to variations of the applied field: for certain field values an 'inversion' takes place: \( \rho_- \) reaches \(-1\), which is the negative of its initial value, while for other nearby field values \( \rho_- \) stays close to its initial value. This behavior can be understood by examining Fig. \[1\] the two energy levels are very close to each other for certain electric field strengths, and in the corresponding neighborhoods a strongly enhanced band-to-band transfer takes place. This situation is quite different from what one expects from simple Zener tunneling theory \[3\]: there the tunneling rate is a monotonic function of the applied field. The situation is summarized in Fig. \[3\] where we plot these Zener resonances as a function of the applied field. One can assign an index to the resonances: the resonance at the highest field (which corresponds approximately to aligning the levels at adjacent quantum wells), is called the first resonance, the next highest the second resonance (the case of Fig. \[2\]), and so forth. Adopting this numbering scheme we observe that in the low field limit \( E^{(n)} \approx \Delta^{ba}/ned \) (here \( \Delta^{ba} = \Delta^0_b - \Delta^0_a \)).

Further insight into the physical meaning of the various oscillations of Fig. \[2\] can be obtained by considering the Fourier transform of \( \rho_- \). Let us first try to establish a qualitative picture of what to expect. The initial state of the system is described by some wave-function, say \( |\Psi(0)\rangle \), which is not an eigenstate after the field has been turned on. However, it can be expanded in terms of the eigenstates: \( |\Psi(0)\rangle = \sum_n c_n \psi_n^a + d_n \psi_n^b \). Since \( \rho(t) = |\Psi(t)\rangle \langle \Psi(t) | \), and each eigenstate evolves according to \( \psi_n^{ab}(t) = \exp(-ie_n^{ab}t)\psi_n^{ab} \), large Fourier components in \( \rho_- \) are expected to occur at \( \hbar \omega = meEd \) and \( \hbar \omega = \pm eEd (r^a - r^b) + meEd \ [14] \). This expectation is fully born out by the numerical evaluation of \( \rho_- (\omega) \).

Fig. \[4\] shows the results of the two independent calculations: the continuous lines are obtained based on Fig. \[2\], while the asterisks come from the Fourier transform of \( \rho_- (t) \). Naturally, the more laborious calculation based on \( \rho_- (t) \) contains also more information: the magnitudes of the Fourier components are needed in the evaluation of other physical quantities, such as the current, which will be addressed elsewhere \[12\].

It is also of interest to examine the effect of varying the superlattice parameters. Fig. \[5\] shows the time-dependence of \( \rho_- (K = 0) \) when the field is tuned to the eighth Zener resonance, and we have increased the bandwidths and interband coupling. A distinctive set of stable plateaus has developed. The transitions between the plateaus occur at instants \( t = \frac{1}{2}T_B, \frac{3}{2}T_B, \frac{5}{2}T_B \ldots \) after the field was turned on. Thus, the life-time of a plateau is (approximately) equal to the Bloch period, and transitions occur every time the \( k \)-point reaches the Brillouin zone edge \[15\]. This behavior is generic to the low field regime, \( E \leq \Delta^{ba}/ed \), and we can qualitatively understand features in the time-dependence of \( \rho_- (t) \) by considering the semiclassical motion of a \( k \)-point between the extrema of the Brillouin zone; transitions to the other miniband occur mainly at zone-edges, where the energy separation between the minibands is at minimum.

We can also understand the number of oscillations on a given plateau by examining Eq.\((\ref{eq:5})\) under some simplifying assumptions. In particular, if we assume that \( \Delta \epsilon \) has a weak time-dependence, it is easy to solve \( \phi \) analytically. The solution suggests defining a 'local' time-dependent frequency for a general, but sufficiently slowly varying \( \Delta \epsilon \) to be \( \omega_t^2 (t) = \omega_0^2 + \omega_0^2 (k(t)) \). Here \( \omega_0 = 2(R/d) \omega_B \) and \( \hbar \omega_B (k) = \Delta \epsilon (k) \). Thus, in the
low field limit we can identify the number of oscillations $N_{osc} \equiv (\omega_{c}(t))/\omega_{B} = \Delta ba/\hbar \omega_{B}$, where the time-average was calculated over the Bloch period $T_{B}$. Consequently, at the $n$th Zener resonance, we find $N_{osc} = n$. In Fig. 2 one can distinguish two periods of oscillation in any of the plateaus (even though the plateaus are not very clearly resolved for this particular set of parameters), while Fig. 3 clearly shows eight periods of oscillation within a plateau.

In the high field regime, $E > \Delta ba/ed$, the situation differs drastically from semiclassical expectations: the plateaus vanish, and we find from Eq. (6), both numerically and analytically, that $\rho_{-}(t)$ oscillates between -1 and +1 with a single frequency $\omega_{c}$.

6. Alternating fields. In the case of a temporally periodic driving field one can make a close parallel to Floquet’s theorem applied to the Schrödinger equation. Hamiltonian with periodic driving field one can make a close parallel to $\omega$ and +1 with a single frequency $\omega_{c}$.

In summary, we have presented a time-dependent formulation of transport in superlattices. We have found that the dynamics of the two-band model can show, in addition to conventional Bloch oscillations, significant additional structure: Zener resonances, stable plateaus, and band collapses.

[1] F. Bloch, Z. Physik 52, 555 (1928).
[2] C. Zener, Proc. Roy. Soc. A145, 523 (1934).
[3] L. Esaki and R. Tsu, IBM Journal of Res. Develop. 14, 61 (1970).
[4] C. Waschke, H. G. Roskos, R. Schwedler, K. Leo, H. Kurz, and K. Köhler, Phys. Rev. Lett. 70, 3318 (1993). This paper also contains references to other relevant experimental work.
[5] M. Holthaus, Phys. Rev. Lett. 69, 351 (1992); Z.Phys. B - Cond. Matter 89, 251 (1992).
[6] A. A. Ignatov and Y. A. Romanov, phys. stat. sol. (b) 73, 327 (1976); D. H. Dunlap, and V. M. Kenkre, Phys. Rev. B 34, 3625 (1986).
[7] A. A. Ignatov, K. F. Renk, and E. P. Dodin, Phys. Rev. Lett. 70, 1996 (1993).
[8] T. Meier, G. von Plessen, P. Thomas, and S. W. Koch, Phys. Rev. Lett. 73, 902 (1994).
[9] See, however, the very recent paper by M. Holthaus and D. W. Hone, Phys. Rev. B 49, 16605 (1994), which analyzes a finite multiband superlattice in an ac field.
[10] H. Fukuyama, R. A. Bari, and H. C. Fogedby, Phys. Rev. B 8, 5579 (1973).
[11] J. B. Krieger and G. J. Iafrate, Phys. Rev. B 33, 5394 (1986); ibid. 35, 9644 (1987); ibid. 38, 6324 (1988).
[12] J. Rotvig, A. P. Jauho, and H. Smith (unpublished).
[13] Explicitly, we assume that $R_{11} = R_{22}$, where $R_{nn}(k) = \frac{1}{2} \sum_{\alpha} \int_{-d/2}^{d/2} dx \hat{u}_{n,k}(x) \hat{v}_{n,k}(x)$. This assumption is valid e.g. for the Kronig-Penney model.
[14] Here we used the known energy spectrum of the biased superlattice [13].
[15] Since $K = 0$ in Fig. 1, which corresponds to the center of the Brillouin zone, the first transition occurs at $t = T_{B}/2$.
[16] In our numerical calculation we used the method suggested by X. - G. Zhao, R. Jahnke, and Q. Niu (unpublished).

FIG. 1. Energy spectrum for a two-band superlattice as a function of applied dc-field; continuous line corresponds to Eq. (8), while asterisks represent a model with no interband coupling ($R = 0$). The superlattice parameters are $d = 10$nm, $\Delta^{1}_{b} = 0.8 \times 10^{-2}$eV, $\Delta^{1}_{a} = 0.92 \times 10^{-2}$eV, $\Delta^{0}_{b} = \Delta^{0}_{a} = 2.0 \times 10^{-2}$eV, and $R = -\frac{16}{3\pi d}$. 

\[ T_{B} \]

\[ T_{B} \]

\[ T_{B} \]

\[ T_{B} \]
FIG. 2. Time-dependence of $\rho_-(K=0)$ for three different field values, top: $\varepsilon E = 0.9 \times 10^6$; middle: $1.1 \times 10^6$; and bottom: $1.02 \times 10^6$ eV/m, respectively. For clarity, we have shifted the top and middle curve upwards by 0.4 and 0.2, respectively. The superlattice parameters are as in Fig. 1 and the unit on the time axis is $10^3 \hbar/eV \simeq 4.14$ ps.

FIG. 3. The negative of $\rho_{\min}^-$ as a function of applied field. If $-\rho_{\min}^\text{min} \simeq 1$, a strong band-to-band transfer is taking place ('Zener resonance'). The dashed lines mark where the Wannier-Stark-ladder separation has local minima.

FIG. 4. Fourier spectrum of $\rho_-(K=0,t)$. A dot corresponds to each significant peak in the Fourier spectrum and the continuous lines are energy differences between the interpenetrating Stark ladders.

FIG. 5. Time-dependence of $\rho_-(K=0)$ for superlattice parameters $\Delta^{a}_1 = \Delta^{b}_1 = 1.8 \times 10^{-2}$ eV, $\Delta^{ba} = 2.0 \times 10^{-2}$ eV, and $R = -0.9d$. Units for the time-axis are as in Fig 2, and the field is $E = 0.232 \times 10^6$ V/m, corresponding to the eighth Zener resonance.

FIG. 6. Quasienergy spectrum for the superlattice of Fig. 1. We display the field-dependence of 17 $k$-points, which are evenly distributed in the positive half of the Brillouin zone, $k \in [0, \pi/d]$ (due to evenness of the quasienergy spectrum negative $k$'s would be redundant). The vertical lines indicate where the band collapse would occur for non-interacting minibands. The modulation frequency is $\omega_\text{ac} = 1.5 \times 10^{-2}$ eV/$\hbar$, and the quasienergies are given in units of $\omega_\text{ac}$.