Time Periodic Behavior of Multiband Superlattices in Static Electric Fields

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Abstract

We use an analytic perturbation expansion for the two-band system of tight binding electrons to discuss Bloch oscillations and Zener tunneling within this model. We make comparison with recent numerical results and predict analytically the frequency of radiation expected from Zener tunneling, including its disappearance, as a function of the system parameters.

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One of the earliest predictions of the theory of electrons in periodic crystals is of Bloch oscillations — time periodic motion at frequency \( \omega_B = Fd/\hbar \) under application of a uniform constant field \( F \) in a crystal potential of lattice period \( d \), associated with Bragg reflection at Brillouin Zone boundaries. But in ordinary atomic crystals, subjected to accessible applied (electric) fields, scattering typically disrupts the coherence of electronic motion in times very short compared to the Bloch period \( T_B = 2\pi/\omega_B \), preventing observation of the phenomenon. However, the lattice constant \( d \) of semiconductor superlattices, typically two orders of magnitude larger, correspondingly reduces \( T_B \) by the same factor. Esaki and Tsu\(^1\) recognized 25 years ago, at the dawn of this new technology, that this greatly improved the prospects of experimental observation of Bloch oscillations and related phenomena. Moreover, the characteristic frequencies lie in the interesting far infrared region. Not surprisingly, then, there has been a great deal of subsequent activity, both experimental\(^2\) and theoretical\(^3\), in the study of high quality semiconductor superlattices under the influence of static and time periodic electric fields. Transport and both linear and nonlinear optical response have been of special interest. In particular, Bloch oscillations have been shown\(^4\) to survive the addition of Coulomb interactions to the simple theory, and far infrared radiation from such oscillations has now\(^5\) been observed.

The one-dimensional periodicity of a quantum well superlattice gives as the eigenstates for independent (noninteracting) electrons a set of “minibands” associated with motion in the growth direction, perpendicular to the wells. For obvious reasons of simplicity, much of the theoretical study has been limited to consideration of a single isolated miniband. But, as emphasized particularly in a recent Letter\(^6\) by Rotvig, Jauho and Smith (RJS), there are essential interesting phenomena — notably Zener tunneling — introduced by additional bands in the presence of a static electric field. These authors reported a numerical study of the density matrix of a two-band model, exhibiting a number of interesting types of periodic behavior of the electrons. It is the purpose of the present paper, (i) to make use of analytic results in the form of an exact perturbation expansion to explore the corresponding behavior throughout the space of the parameters characterizing the two-band superlattice, and (ii) to
make use of our analytically predicted behavior to compare with selected numerical results in order to test the convergence of the perturbation series so as to define its range of validity for application to other problems and properties. The structure of the series suggests (correctly, we will show) that the convergence is much more rapid than imposed by the obvious limits that can be set analytically.

The two-band model is, of course, the simplest extension beyond the single band picture, and it does introduce those features characteristic of interband communication. But is it a reasonable approximation to any physical situation to focus on a single pair of minibands while neglecting the higher bands which inevitably also exist? As we have pointed out before, there is at least one realistic situation where this should capture the dominant physical behavior. A superlattice can be grown dimerized, with the unit cell consisting, e.g., of a pair of quantum wells, separated from the adjacent pair by a larger (wider) barrier than that which separates the two wells of the basis pair. Then the lowest level of an individual well is split within the “molecular” pair. These two levels form a pair of bands in the superlattice which are well separated energetically from those arising from higher levels in the well, and it is then reasonable to neglect all except that lowest pair of bands.

We will use the standard two-band tight-binding Hamiltonian in a uniform static electric field $E$:

$$\mathcal{H} = \sum_n \left[ (\Delta_a + neEd) a_n^\dagger a_n + (\Delta_b + neEd) b_n^\dagger b_n 
- (W_a/4)(a_{n+1}^\dagger a_n + h.c.) + (W_b/4)(b_{n+1}^\dagger b_n + h.c.) 
+ eER(a_n^\dagger b_n + b_n^\dagger a_n) \right].$$

(1)

Here the subscripts label the lattice sites and the lower and upper minibands are designated by symbols $a$ and $b$, respectively. 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: $\epsilon^{a,b}(k) = \Delta_{a,b} \mp (W_{a,b}/2) \cos(kd)$. The last term is the on-site electric dipole coupling between minibands; $eR$ is the corresponding dipole moment. This Hamiltonian, first used by Fukuyama, Bari and Fogedby in connection with
this type of system, 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.

The application of a static electric field localizes all electronic energy eigenstates, with a localization length which decreases with increasing electric field strength \( E \). The energy spectrum associated with the Hamiltonian (1) above becomes two interleaved Stark ladders:

\[
\epsilon_1^m = \Omega_{1,2} + m\omega_B, \quad (2)
\]

where \( \omega_B = eEd \) is the Bloch frequency defined above (we have taken units with Planck’s constant equal to unity), \( m \) is an arbitrary integer, and the Stark ladder offsets \( \Omega_{1,2} \) depend on the field amplitude \( E \). The result so far can be established in several ways. A particularly satisfying proof based on the symmetries evident in a suitably chosen gauge is given in the Appendix. But one of us has established, in addition, an analytic solution which includes an explicit expression for the offset between the two ladders \( \Omega \equiv \Omega_2 - \Omega_1 \). As noted by RJS, the Zener tunneling behavior undergoes dramatic changes when \( \Omega \) approaches zero.

We first analyze that interplay between ordinary Bloch oscillations and Zener tunneling with the use of those analytic results, to understand how the behavior is affected by the parameters of the superlattice. One of the most attractive features of the semiconductor systems is, after all, that those parameters are to a considerable extent under the control of the fabricator.

Formally, the analytic results are in the form of a perturbation series in the ratio \( R/d \) of the interband dipole coupling to the Bloch frequency. It is therefore natural to compare the exact energy eigenvalues to those of the decoupled bands (for the Hamiltonian (1) with \( R = 0 \)). These are of the same form as (2):

\[
\epsilon_0^{a,b} (n) = \Delta_{a,b} + n\omega_B, \quad (3)
\]
but the offsets $\Delta_{a,b}$ are now the bare energy parameters of the Hamiltonian, independent of the applied field $E$. These energies are plotted in Fig. 1, as in RJS, in the form $(\epsilon^0 - \Delta_a)/\omega_B$, which equals $n$ (for $p = a$) or $(\Delta_a - \Delta_b)/\omega_B + n$ (for $p = b$), as a function of $(\Delta_a - \Delta_b)/\omega_B$, giving a set of horizontal lines at the integers and a set of parallel lines of unit slope for bands $a$ and $b$, respectively. Away from the crossing points of this unperturbed spectrum, $\Delta_b - \Delta_a = n\omega_B$, where the two Stark ladders are degenerate, the exact full energies are expected (and found) to show only small corrections due to finite interband coupling $R$ for reasonable values of $R/d < 1$. Similarly, the eigenstates are largely those of individual bands $a$ and $b$. Then significant Zener tunneling is to be found only near the crossing points, and we will concentrate on those special values of the field,

$$\omega_B \equiv eEd = (\Delta_b - \Delta_a)/\ell, \quad (4)$$

where $\ell$ is an integer. At these fields the eigenstates will be mixtures of comparable weights of states in the two bands. If the system is prepared initially in one of the bands, Zener tunneling will exhibit oscillations of the weight between the two bands with a dominant frequency of the Stark ladder offset $\Omega$. We will show, moreover, that there are special circumstances where this offset vanishes and the tunneling disappears.

The results of Ref. 9 can be expressed for the resonance condition of Eq.(4) in the form

$$\Omega = \frac{\omega_B}{\pi} \cos^{-1} \sum_{m=0}^{\infty} (R/d)^{2m}U^{(2m)}[\ell, (W_b + W_a)/\omega_B], \quad (5)$$

where we have explicitly indicated the dependence of the terms $U^{(2m)}$ of the perturbation series on the parameters of the system. The contribution $U^{(2m)}$ (other than the first: $U^{(0)} = 1$) is a sum of $2^{2m}$ terms, each of which is an ordered integral of the form

$$\int_0^{2\pi} dk_1 \int_0^{k_1} dk_2 \cdots \int_0^{k_{2m-1}} dk_{2m} F_1(k_1) F_2(k_2) \cdots F_{2m}(k_{2m}), \quad (6)$$

where each function $F_n(k)$ is of one of the two forms:

$$C(k) = \cos(\alpha \sin k - 2\ell k)$$

$$S(k) = \sin(\alpha \sin k - 2\ell k). \quad (7)$$
Here \( \alpha = (W_b + W_a)/(2\omega_B) \), and the integer \( \ell \) is again the resonance parameter of Eq. (4). The formal derivation of the perturbation series shows that \( |U^{(2m)}| < (2\pi)^{2m}/(2m)! \), so the series is convergent for all values of the ratio \( R/d \). On the other hand, the number of terms and their algebraic complexity increase very rapidly with index \( (2m) \), so the result is of practical use only when it converges so rapidly that one or two terms suffice. In that regard the simple limit just invoked, which puts an upper bound on the term of order \( n \) of \( (2\pi R/d)^n/n! \), is not very helpful for typical values of \( 2\pi R/d \), which are of order unity. But the highly oscillatory character of the integrands suggests that the series converges, in fact, much more rapidly than this. Our results below verify that this is indeed the case. We will keep only the first nontrivial correction in \( R/d \), namely the \( m = 1 \) term, for which the integrals can readily be expressed in closed form:

\[
U^{(2)} = 2\left[\pi J_\ell(\alpha)\right]^2,
\]

where \( J_\ell(\alpha) \) is the Bessel function of order \( \ell \). Already we see the substantial reductions from the oscillatory integrands from the crude limit above, though we have been unable to establish rigorous lower analytic limits than this. Near \( x = 1 \), \( \cos^{-1} x \) has a square root singularity; for \( (R/d)^2U^{(2)} \ll 1 \) we have as the offset between closest steps on the two ladders,

\[
\Omega \approx \frac{\omega_B R}{\pi d} \sqrt{2U^{(2)}} \\
= 2\frac{(\Delta_b - \Delta_a) R}{\ell d} J_\ell(\alpha)
\]

We note, in particular, that this drops off rapidly with increasing \( \ell \) (with decreasing field \( E \) for fixed \( (\Delta_b - \Delta_a) \), as defined in (4)), or as we move to the right in the level crossings shown in Fig. 1. This can be observed in the numerical results of Fig. 1 of RJS. The parameters used there are: \( \Delta_b - \Delta_a = 20 \text{ meV} \), \( R/d = -16/9\pi^2 = -0.18 \), and \( \alpha = 0.43\ell \), giving for the first three gaps (\( \ell = 1, 2, 3 \)) the values \( \Omega = 1.51, 0.306, 0.030 \text{ meV} \). For more direct comparison with the figure we reduce this by the Bloch frequency in each case: \( \Omega/\omega_B = 0.076, 0.031, 0.015 \), which appears to be in good agreement with those numerical
results.

How accurate, in general, is the theory cut off at this lowest nontrivial order? To answer that, as well as to understand more easily the nature of the Zener tunneling, it is useful to rederive the result (9) without the full machinery of the exact solution, but rather using standard degenerate perturbation theory. For the independent band problem \((R = 0)\) the Wannier-Stark eigenstates for band \(a\) are given explicitly as

\[
\phi^a_n = \sum_m J_{n-m} \left( \frac{W_a}{2\omega_B} \right) a_m^\dagger |0\rangle,
\]

with energy \(\epsilon^a_0\) given by (3). The wave function for band \(b\) is, of course, of precisely the same form. The resonance condition (4) then gives as degenerate the states \(\phi^a_n\) and \(\phi^b_{n+\ell}\) for each integer \(n\). The degeneracy is lifted by the interband dipole matrix elements, which are given explicitly between degenerate unperturbed states as

\[
\langle \phi^a_n | H_{\text{int}} | \phi^b_{n+\ell} \rangle = \frac{R}{d} \omega_B \sum_m J_{n-m} \left( \frac{W_a}{2\omega_B} \right) J_{n+\ell-m} \left( \frac{W_b}{2\omega_B} \right) = \frac{R}{d} \omega_B J_\ell(\alpha) .
\]

Then the degenerate states are split by twice this amount in lowest order, in agreement with (9), and the corresponding eigenstates are the symmetric and antisymmetric combinations,

\[
\psi_n^{s,a} = (\phi^a_n \pm \phi^b_{n+\ell})/\sqrt{2} .
\]

Now the nature of the Zener tunneling is transparent. Let us prepare the system in the (lower) band \(a\) before turning on the field at time \(t = 0\). Then the subsequent time development is given by

\[
\psi(t) = \sum_n A_n \left( \psi^a_n + \psi_n^a e^{-i\Omega t} \right) e^{-i(n\omega_B+\Omega)t} ,
\]

where the symbols, other than the arbitrary constant coefficients \(A_n\) which determine the initial state, have all been defined above. Clearly, the state becomes completely made of contributions from band \(b\) after time \(t = \pi/\Omega\) and returns to band \(a\) in twice that time — i.e., with a full cycle of frequency \(\Omega\), as seen in the numerical results of RJS. In particular,
at the zeroes of the Bessel function, $J_\ell(\alpha) = 0$, the splitting of the ladders $\Omega$ also vanishes, and Zener tunneling also disappears. Although this is tunneling between bands rather than between the spatially separated sides of a standard double well, the physical manifestations are not dissimilar. Corresponding degenerate states from the two bands are shifted by $\ell$ lattice sites, and there will therefore be an ac current, or oscillating dipole associated with the Zener tunneling, and corresponding radiation at the frequency $\Omega$. Therefore, the prediction of the theory to this order is that such radiation will be observed at a frequency $\Omega \propto J_\ell(\alpha)$, except for the special points where the Bessel function vanishes, at which the radiation will disappear, as well. These special points for various resonance ratios $\ell$ (electric field given by (4)) are given by

$$\alpha = \frac{\ell(W_a + W_b)}{2(\Delta_b - \Delta_a)} = x_\ell,$$

(14)

where $x_\ell$ is a zero of $J_\ell(x)$.

The full theory predicts similar phenomena, but then the splitting of the Stark ladders $\Omega$ needs to be calculated to all orders. If the corrections are significant, then the predictions of (9) and (14) will be at least quantitatively incorrect.

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**APPENDIX A: PROOF OF INTERLEAVED STARK LADDER SPECTRUM**

The translational symmetry of the Hamiltonian (1) is broken by the scalar potential terms proportional to the intraband part of the position operator,
\[ x^0 \equiv d \sum_n n(a_n^\dagger a_n + b_n^\dagger b_n). \] (A1)

It is convenient to restore that translational symmetry by a suitable gauge transformation (different from the standard vector potential gauge, because only the intraband part of the position operator is involved):

\[ \psi' = e^{ieE^0 t} \psi, \] (A2)

which obeys the time-dependent Schrödinger equation \((i\partial_t - \mathcal{H}')\psi' = 0\), with

\[ \mathcal{H}' = \sum_k \mathcal{H}'_k \]

\[ \mathcal{H}'_k = \left[ \Delta_a - (W_a/2) \cos(kd - \omega_B t) \right] a^\dagger(k) a(k) \]
\[ + \left[ \Delta_b + (W_b/2) \cos(kd - \omega_B t) \right] b^\dagger(k) b(k) \]
\[ + eER \left[ a^\dagger(k) b(k) + b^\dagger(k) a(k) \right]. \] (A3)

Here \(a(k)\), the spatial Fourier transform of \(a_n\),

\[ a(k) = \frac{1}{N} \sum_n e^{inkd} a_n, \] (A4)

destroys a plane wave state of wave vector \(k\) in band \(a\), and the hermitian conjugate operator \(a^\dagger(k)\) creates that state. The operators \(b(k)\) and \(b^\dagger(k)\) are defined analogously for the other band. The dynamical equation thus separates into a set of independent two-level problems, one for each wave vector \(k\), described by \(\mathcal{H}'_k\). Moreover, \(\mathcal{H}'_k(t + T_B) = \mathcal{H}'_k(t)\), a discrete time translational symmetry which, by the Floquet theorem, implies solutions of the form

\[ \psi'_k(t) = u_k(t) \exp(-i\epsilon_k t), \] (A5)

with \(u_k(t) = u_k(t + T_B)\) periodic in time, and the “quasienergy” \(\epsilon_k\) defined only modulo \(\omega_B\). Further, the form (A3) of \(\mathcal{H}'_k\) makes it clear that \(\epsilon_k\) and \(u_k\) are, in fact, independent of \(k\): the parameter \(k\) merely shifts the origin of time, \(t' = t - kd/\omega_B\) in each term. Therefore, modulo \(\omega_B\) there are only two quasienergies, which we designate \(\Omega_{1,2}\). Finally, we can see that this is also the set of energies of the system. Transforming back to the original time independent (scalar) gauge, we have
\[ \psi_k(t) = e^{-iE_0 t} \left[ u^{(a)}(t) a^\dagger(k) + u^{(b)}(t) b^\dagger(k) \right] |0\rangle e^{-i\Omega_{1,2} t} \]
\[ = \frac{1}{N} \sum_n e^{i(kd-\omega_B t)} \left[ u^{(a)}(t) a^\dagger_n + u^{(b)}(t) b^\dagger_n \right] |0\rangle e^{-i\Omega_{1,2} t}, \] (A6)

as the basis set of solutions to the dynamical Schrödinger equation in that gauge \((u^{a,b}(t))\) are the parts of the Bloch periodic function \(u(t)\) belonging to each of the two bands, in an obvious notation). But these must be linear combinations \(\sum \phi_j \exp(-iE_j t)\) of energy eigenvalue solutions, and we see from (A6) that those energies are \(E_j = \Omega_{1,2} + n\omega_B\), for arbitrary integers \(n\) — two interleaved Stark ladders of rung spacing \(\omega_B\), offset from each other by \(\Omega = \Omega_2 - \Omega_1\).
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