Theory of coherent time-dependent transport in one-dimensional multiband semiconductor superlattices

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We present an analytical study of one-dimensional semiconductor superlattices in external electric fields, which may be time dependent. A number of general results for the (quasi)energies and eigenstates are derived. An equation of motion for the density matrix is obtained for a two-band model and the properties of the solutions are analyzed. An expression for the current is obtained. Finally, Zener tunneling in a two-band tight-binding model is considered. The present work gives the background and an extension of the theoretical framework underlying our recent Letter [J. Rotvig *et al.*, Phys. Rev. Lett. **74**, 1831 (1995)], where a set of numerical simulations was presented. $[$0163-1829(96)04148-3]$

I. INTRODUCTION

Studies of Bloch electrons under the influence of external electric fields attract at present intensive theoretical attention (some recent papers can be found in Refs. $1-14$); this is a natural consequence of recent experimental advances, which include the observation of Bloch oscillations¹⁵ and studies of photon-assisted transport.^{16–18} Thus the classic predictions of B loch¹⁹ and Zener²⁰ finally have been verified, and the arena is open for new investigations and ideas. The physics of superlattices in external fields is extremely rich due to the large number of parameters that can be controlled quite freely. Many of the physical properties are sensitive functions of these parameters and hence slight adjustments in their values allow one to move between different physical regimes, both experimentally and theoretically. Examples of such parameters are the miniband structure of the superlattice (which can be controlled by varying the composition and/or thickness of the layers comprising the superlattice to meet the requirements of the particular investigation) or the intensities and frequencies of the external fields. This flexibility allows one to study many different physical phenomena. The papers quoted above have addressed such varying physical phenomena as (i) dynamical localization or band collapse (originally discussed in Ref. 21) either in dc or ac electric fields, (ii) interplay of field-induced localization and Anderson localization due to disorder, (iii) chaotic motion of charge carriers, or (iv) full-scale numerical integration of semiconductor Bloch equations, which allow one to study interaction effects, such as exciton dynamics.

Much of the interest has been caused by the need of understanding the interplay of Bloch oscillations (i.e., coherent time-periodic motion of charge carriers in one band), Zener tunneling between Bloch bands, and interaction effects. We studied recently²² a two-band tight-binding model and found via a direct numerical solution of the density-matrix equation

of motion a rather complicated temporal behavior for the diagonal (in miniband index) component. This structure, however, could be interpreted in terms of intuitive physical arguments. Our numerical study was facilitated by a substantial amount of analytic background work, and the purpose of this paper is to provide a full account of the formal developments. In subsequent sections we shall derive a number of formal results, which we believe to be generalizations of previously known results, and we give mathematical proofs of several statements made in our previous work 22 . We also give a detailed discussion of the density-matrix equation of motion, upon which our previously reported numerical work was based, which can be used as a starting point for future studies, for example, consideration of relaxation or loss of phase coherence due to scattering.

The paper is organized as follows. In Sec. II we derive the energy spectrum for a superlattice with a finite number of finite bands, in static and time-dependent fields, and apply the general results to the tight-binding two-band superlattice of Ref. 22. Section III is devoted to the equation-of-motion analysis of the density matrix and a derivation of an expression for the current, from which semiclassical intraband and quantum-mechanical tunneling contributions can be identified. We also give some analytic results for Zener tunneling, which we used in the interpretation of our numerical results of Ref. 22. Sec. IV gives our conclusions.

II. ENERGY SPECTRA

In this section we consider the energy spectrum of an electron in a superlattice in the presence of a static or timeperiodic electric field, which causes coupling between the bands. The general Bloch problem can be divided into two cases: the zero-field spectrum consists of (i) an infinite number of finite bands and (ii) a finite number of finite bands and an upper infinite band. In general, the spectrum is replaced

A. Electronic motion in a superlattice

lations of Ref. 22 and establish a connection to the general

results derived in the beginning of this section.

We consider a semiconductor superlattice with a growth direction parallel to the *x* axis. The lattice period is denoted by *d* and is repeated $N_p = L/d$ times, where *L* is the length of the superlattice. In the effective-mass approximation²⁴ the wave function satisfies the usual Schrödinger equation with the scalar-potential Hamiltonian H_{ϕ} given by

$$
H_{\phi}(x,t) = \frac{p_x^2}{2m} + V_c(x) + eE(t)x,
$$
 (1)

where *m* is the effective mass, $V_c(x)$ is the periodic potential with period *d*, and $\mathbf{E}(t) = (E(t),0,0)$ is the electric field. For *E*(*t*)=0, the eigenstate problem $H_{\phi}(x)\psi(x) = \epsilon \psi(x)$ is solved by the usual Bloch states $(BS's)$

$$
\phi_{nK}(x) = \frac{1}{\sqrt{L}} e^{iKx} u_{nK}(x),\tag{2}
$$

with eigenvalues $\epsilon_n(K)$ associated with the miniband indexed by n . In a finite electrical field we follow²⁶ and introduce accelerated Bloch states (ABS's) when calculating the energy spectrum. We assume that the field is applied at $t=0$ and define the vector potential $A(t) = (A(t),0,0)$ by $A(t) = -\int_0^t E(t')dt'$. Then the semiclassical time evolvement of the crystal momentum $\mathbf{k}(t) = (k(t),0,0)$ is given by

$$
k(t) = K - (e/\hbar) \int_0^t E(t')dt' = K + eA(t)/\hbar.
$$
 (3)

At this point it is useful to introduce the Hamiltonian H_A in which the electrical field is represented by the vector potential instead of the scalar potential

$$
H_A(x,t) = \frac{[p_x + eA(t)]^2}{2m} + V_c(x).
$$
 (4)

The ABS's, defined as

$$
\psi_{nK}(x,t) = \frac{1}{\sqrt{L}} e^{iKx} u_{nk(t)}(x),\tag{5}
$$

are instantaneous eigenstates to the time-dependent Hamiltonian $H_A(x,t)$,

$$
H_A(x,t)\psi_{nK}(x,t) = \epsilon_n[k(t)]\psi_{nK}(x,t). \tag{6}
$$

The set of ABS's forms an orthonormal basis. The so-called Houston function²⁵ $\phi_{nk(t)}(x)$ can be expressed in the ABS basis as

$$
\phi_{nk(t)}(x) = e^{ieA(t)x/\hbar} \psi_{nK}(x,t) = e^{ieA(t)x/\hbar} \frac{1}{\sqrt{L}} e^{iKx} u_{nk(t)}(x)
$$

$$
= \frac{1}{\sqrt{L}} e^{ik(t)x} u_{nk(t)}(x). \tag{7}
$$

The Houston function is thus an ordinary BS corresponding to the wave vector $\mathbf{k}(t)$.

We shall write solutions to the Schrödinger equation

$$
H_{\phi}(x,t)\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}
$$
 (8)

in the form $\psi(x,t) = e^{-i\epsilon t/\hbar}u(x,t)$, where $u(x,t)$ is spatially periodic with period *L*. We thus have

$$
H_{\phi}(x,t)u(x,t) = \epsilon u(x,t) + i\hbar \frac{\partial u(x,t)}{\partial t}.
$$
 (9)

For a static electric field the function *u* can be chosen to be independent of time and ϵ is the energy. If the field is periodic in time with a period T_{ac} , Floquet's theorem states that *will have the same periodicity. The Floquet solutions de*fine the quasienergy ϵ , which is a generalization of the energy.

Now let us expand $\psi(x,t)$ in the ABS's according to

$$
\psi(x,t) = \sum_{n,K} C_{nK}(t) e^{ieA(t)x/\hbar} \psi_{nK}(x,t). \tag{10}
$$

We then insert (10) into (8) and use

$$
i\hbar \frac{\partial \psi_{nK}(x,t)}{\partial t} = i\hbar \frac{e^{iKx}}{\sqrt{L}} \nabla_k u_{n(k)}(x) \dot{k}, \qquad (11)
$$

where we defined $\vec{k} \equiv \partial k / \partial t$. Since $\nabla_k u_{nk}$ is a periodic function with period *d*, it may be expanded in terms of the functions $u_{n'k}$ according to

$$
i\nabla_k u_{nk(t)} = \sum_{n'} u_{n'k(t)} R_{n'n}[k(t)], \qquad (12)
$$

where the expansion coefficients $R_{n^{\prime}n}$ are the matrix elements

$$
R_{n'n}(k) = \frac{i}{d} \int_{-d/2}^{d/2} dx u_{n'k}^{*}(x) \nabla_k u_{nk}(x).
$$
 (13)

Combining Eqs. (11) and (12) with $\dot{k} = -eE/\hbar$ results in the following coupled equations for the expansion coefficients $C_{nK}(t)$:

$$
i\hbar \frac{\partial C_{nK}(t)}{\partial t} = \epsilon_n [k(t)] C_{nK}(t) - F(t) \sum_{n'} R_{nn'} [k(t)] C_{n'K}(t),
$$
\n(14)

where $F(t) = -eE(t)$. Equations similar to Eq. (14) were derived by Krieger and Iafrate.²⁶ Our formulation differs from theirs in that they use a gauge transformation in order to eliminate the spatially nonperiodic term $eE(t)x$. We avoid the gauge transformation and thereby keep the notion of energy. Instead we introduce a common factor $exp[i\epsilon A(t)x/\hbar]$ in the ABS expansion of the wave function. As seen from Eq. (10) , this is the same as using an ordinary BS expansion of the wave function:

$$
\psi(x,t) = \sum_{n,K} C_{nK}(t) \phi_{nk(t)}(x)
$$

$$
= e^{-i\epsilon t/\hbar} \sum_{n,K} c_{nK}(t) \phi_{nK}(x), \qquad (15)
$$

where $c_{nK}(t) = C_{n,K-eA(t)/\hbar}(t)e^{i\epsilon t/\hbar}$. The function *u* is found from Eq. (15) ,

$$
u(x,t) = \sum_{n,K} c_{nK}(t) \phi_{nK}(x).
$$
 (16)

The set of coupled equations (14) for the coefficients $C_{nK}(t)$ together with a boundary condition will now be used to derive properties for the (quasi)energy spectra.

1. Static fields

In the following we consider a model periodic potential corresponding to a finite number *N* of energy bands and demonstrate the WS form of the spectrum in static fields. For a static field, $F(t) = F(0)$, the c_{nK} 's in Eq. (16) are independent of time. From this condition and the periodicity of the c_{nK} 's in *K* it follows that

$$
C_{nK}(t+T_B) = C_{nK}(t)e^{-i\epsilon T_B/\hbar},\qquad(17)
$$

where $T_B = 2\pi/\omega_B$ and $\omega_B = F d/\hbar$. For each *K* in the Brillouin zone (BZ) there are N linearly independent solutions $C_{K_i}(t)$, $j = 1, ..., N$, to the system Eq. (14). From Eq. (17) we see that the energy for a specific solution $C_{Ki}(t)$ is only determined mod $\hbar \omega_B$. The system of equations (14) has periodic coefficients with period T_B . By applying the *N*-dimensional Floquet theorem we know that the solutions can be found of the form $\mathbf{C}_{Kj}(t) = e^{i\omega_{Kj}t}\mathbf{P}_{Kj}^{0}(t)$, where ω_{Kj} is only determined modulo ω_B and $\mathbf{P}_{Kj}^0(t+\widetilde{T}_B)=\mathbf{P}_{Kj}^0(t)$. From Eq. (17) the energies of the Floquet solution $C_{Ki}(t)$ are $\epsilon_{Kj}^p = -\hbar \omega_{Kj} + p\hbar \omega_B$, *p*=integer. Solving Eq. (14) with *K* replaced by $K' = K + (2\pi/d)t_0/T_B$ we obtain solutions $\mathbf{C}_{K}^{'}$ $(t) = e^{i\omega_{K}j(t+t_0)} \mathbf{P}_{K}^0(t+t_0)$. Comparing with the Floquet solutions $\mathbf{C}_{K'j}(t) = e^{i\omega_{K'j}t} \mathbf{P}_{K'j}^{0}(t)$ we conclude that ω_{Kj} can be chosen to be independent of *K*. The energy spectrum is then

$$
\epsilon_j^p = -\hbar \omega_j + p\hbar \omega_B; \quad j = 1, ..., N; \quad p \text{ an integer.}
$$
\n(18)

We see that the spectrum can be visualized as *N* WS energy ladders.

Another way to obtain the WS spectrum is to eliminate the K dependence in Eq. (14) : the semiclassical motion of $k(t)$ is monotonic and can therefore be inverted to yield $t(k) = \hbar (k - K)/F$. By use of the definition $D_n(k) = c_{nk}e^{-i\epsilon k/F}$ we obtain $C_{nK}(t) = D_n[k(t)]e^{i\epsilon K/F}$. Equation (14) is then reduced to a system of equations that is independent of the initial momentum *K*,

$$
iF\frac{\partial D_n(k)}{\partial k} = \epsilon_n(k)D_n(k) - F \sum_{n'} R_{nn'}(k)D_{n'}(k). \quad (19)
$$

A direct calculation shows that

$$
D_n(k+2\pi/d) = D_n(k)e^{-i\epsilon T_B/\hbar}.
$$
 (20)

As before the energy is only determined mod $\hbar \omega_B$. If for a definite solution $\mathbf{D}_i(k)$ to Eq. (19) we make the replacement $\epsilon \rightarrow \epsilon + p\hbar \omega_B$, where *p* is an integer, then $\mathbf{c}_{Kj} \rightarrow \mathbf{c}_{Kj}e^{iKpd}$. Therefore the displaced energy corresponds to a spatial translation of the solution by $-pd$, *i.e.*, the eigenstates in terms of the $\mathbf{D}_i(k)$'s are only determined within a direct lattice displacement. The system of equations (19) has periodic coefficients with period $2\pi/d$. Appealing again to the *N*-dimensional Floquet theorem, we conclude that the solutions are of the form $\mathbf{D}_j(k) = e^{ikr_j}\mathbf{P}_j^1(k)$, $j = 1, ..., N$. The Floquet functions $P_j^1(k)$ are periodic with period $2\pi/d$. By calculating $\mathbf{D}_i(k+2\pi/d)$ and using Eq. (20) we therefore obtain the energy spectrum

$$
\epsilon_{jp} = -F r_j + p \hbar \omega_B, \quad j = 1, ..., N, \quad p \text{ an integer.} \tag{21}
$$

We see again that the spectrum can be visualized as *N* WS energy ladders. The relative positions of these are expressed in terms of the Floquet coefficients r_j . The system (19) and (20) will later be used to evaluate the point spectrum for a two-band superlattice.

It should be noted that the ω_i 's and r_i 's are connected. This can be demonstrated as follows. Floquet solutions for $\mathbf{D}(k)$ can also be found by using the Floquet solutions for $C_K(t)$. For an arbitrary choice of *K* we set $\mathbf{D}_j(k) = e^{-i\epsilon K/F} \mathbf{C}_{Kj}(k) = e^{i\hbar \omega_j k/F} e^{-i(\epsilon + \hbar \omega_j)K/F} \mathbf{P}_{Kj}^0(k)$. The energy spectrum is thus given by Eq. (18) . Uniqueness of the spectrum implies that the energies $\{\hbar \omega_j | j = 1, \ldots, N\}$ are equal to the WS ladder positions $\{Fr_j | j = 1, \ldots, N\}$ except for individual multiples of $\hbar \omega_B$.

2. Time-periodic fields

In this section we consider time-periodic solutions $u(x,t)$ to Eq. (9). We can derive general results concerning the quasienergy spectrum using the properties of the C_K coefficients. As we shall see, the interplay between the spatial periodicity and the temporal periodicity can have significant consequences for the quasienergy spectrum.

Specifically, let us consider a time-dependent electric field with period T_{ac} . Since the coefficients $c_{nK}(t)$ in Eq. (16) are periodic in *t* and $A(t+T_{ac})=A(t)+A(T_{ac})$, we find that

$$
C_{nK}(t+T_{ac}) = C_{n,K+\Delta K}(t)e^{-i\epsilon T_{ac}/\hbar},\qquad(22)
$$

where $\Delta K = eA(T_{ac})/\hbar$. The quasienergy ϵ for a given solution $C_{K_i}(t)$ to Eq. (14) is only given mod $\hbar \omega_{ac}$, where $\omega_{ac} = 2\pi/T_{ac}$.

Let us now consider two special cases for ΔK . First, if ΔK =0 mod 2 π/d , as for a harmonic field, the condition Eq. (22) is equivalent to Eq. (17) in the static case. All momenta in the BZ are then independent.

A special case arises if $\Delta K = (2\pi/d)(p/q)$, with *p* and *q* integers.⁹ Now a finite number of crystal momenta couple and the quasienergies are determined from

$$
C_{nK}(t+qT_{ac}) = C_{nK}(t)e^{-i\epsilon qT_{ac}/\hbar}.
$$
 (23)

The quasienergies are now only defined mod $\hbar \omega_{ac} / q$. The Brillouin zone collapses to $[-\pi/qd,\pi/qd]$ and the quasienergy spectrum consists of fractional quasienergy ladders.

We have so far assumed that the system stays in equilibrium until $t=0$, when it is instantaneously coupled to the electric field. This is obviously an idealization, and it is natural to ask whether a finite switch-on period will change the general results. We have repeated the above analysis, but allowed for a finite switch-on period $[0,T_0]$. The upshot is that all formal results for the quasienergy spectrum still apply; however, one must change the initial momentum label *K*. The new momentum values $K \rightarrow K - eA(T_0)/\hbar$ correspond to a translation in reciprocal space.²⁹

B. Tight-binding model

In the rest of this paper we consider a superlattice model with only two bands $n=a,b$. The Hamiltonian is

$$
H = \sum_{l} \left\{ \left[\Delta_0^a - F(t)X^a - F(t)Id \right] a_l^{\dagger} a_l \right\}
$$

+
$$
\left[\Delta_0^b - F(t)X^b - F(t)Id \right] b_l^{\dagger} b_l - \frac{\Delta_1^a}{4} (a_{l+1}^{\dagger} a_l + a_l^{\dagger} a_{l+1})
$$

+
$$
\frac{\Delta_1^b}{4} (b_{l+1}^{\dagger} b_l + b_l^{\dagger} b_{l+1}) - F(t)X^{ab} (a_l^{\dagger} b_l + b_l^{\dagger} a_l) \right\}.
$$
 (24)

The terms involving the constants X^a and X^b describe a siteindependent shift, due to the electric field, of the unperturbed energies Δ_0^a and Δ_0^b , while the band coupling is described by the term involving the constant *Xab*. The remaining terms in the Hamiltonian involve the site-dependent potential energy $-F(t)$ *ld* and the hopping between nearest-neighbor sites. Due to the terms involving X^a and X^b the model represents a generalization of the two-band model, which was solved in Ref. 30. The reason for introducing these parameters is that we can construct, as shown below, a mapping between the tight-binding model and a general two-band model (when the band couplings are described with the parameters R^a , R^b , and R^{ab}). The various energy parameters describing the twoband superlattice are summarized in Fig. 1.

We shall first consider static electric fields. Then the Schrödinger equation $H_{\phi}u = \epsilon u$ in the site representation is solved by making the ansatz $u = \sum_l (u_l^a a_l^{\dagger} + u_l^b b_l^{\dagger}) |0\rangle$ and projecting out the *l*th component, which results in the following coupled equations for the expansion coefficients:

$$
(\Delta_0^a - FX^a - Fld)u_l^a - \frac{\Delta_1^a}{4}(u_{l-1}^a + u_{l+1}^a) - FX^{ab}u_l^b = \epsilon u_l^a,
$$

$$
(\Delta_0^b - FX^b - Fld)u_l^b + \frac{\Delta_1^b}{4}(u_{l-1}^b + u_{l+1}^b) - FX^{ab}u_l^a = \epsilon u_l^b.
$$
 (25)

For vanishing field the spectrum consists of two bands

$$
\epsilon^{a,b}(K) = \Delta_0^{a,b} \mp (\Delta_1^{a,b}/2) \cos(Kd),\tag{26}
$$

corresponding to the plane-wave solutions $u_l^a = e^{iKld}$, $u_l^b = 0$ and $u_l^a = 0$, $u_l^b = e^{iKld}$, respectively. When

FIG. 1. Definitions of various energy parameters for the twoband superlattice. $\Delta_0^{a,b}$ are the band midpoints, $\Delta_1^{a,b}$ are their widths, and $\hbar \omega_d(K) = \epsilon_b(K) - \epsilon_a(K)$ is the band separation at K . Also, in the text, the following are used: (i) $\Delta \omega_d(I) = \max[\omega_d(K)] - \min[\omega_d(K)], K \in I;$ (ii) $\tilde{\omega}_d(K) = \omega_d(K)$ $+FX_-/\hbar$ [here $X_- = X^a - X^b$, where X^i are defined in Eq. (24)]; (iii) $\langle \omega_d \rangle$ _{*I*}, which is the average of $\omega_d(K)$, over a given part of the Brillouin zone *I*; (iv) $\omega_0 = \langle \omega_d(K) \rangle_{\mathcal{BZ}}$, i.e., the average band separation over the entire Brillouin zone; and, finally, (v) $\widetilde{\omega}_0 = \omega_0 + FX$ ₋/ \hbar .

the field is finite, we depart from the procedure used in Ref. 30 by applying the discrete Fourier transformation

$$
u_l^{\nu} = \sum_K u_K^{\nu} e^{iKld},
$$

$$
u_K^{\nu} = \frac{1}{N_p} \sum_l u_l^{\nu} e^{-iKld}
$$
 (27)

directly on Eq. (25). With the notation $u_K^{\nu} = P_K^{\nu} e^{i\epsilon K/F}$ the result is

$$
iF\frac{\partial}{\partial K}\begin{pmatrix}P_K^a\\P_K^b\end{pmatrix}=\begin{pmatrix}\epsilon^a(K)-FX^a & -FX^{ab}\\-FX^{ab} & \epsilon^b(K)-FX^b\end{pmatrix}\begin{pmatrix}P_K^a\\P_K^b\end{pmatrix}
$$
(28)

and

$$
P_{K+2\pi/d}^{\nu} = P_K^{\nu} e^{-i\epsilon T_B/\hbar}.
$$
 (29)

The form of Eq. (29) is analogous to Eq. (20) . Furthermore, Eq. (28) in the tight-binding model has the form of Eq. (19) if the bands are identical. In addition, the band couplings in the general model must be time independent and satisfy $X^a = R^a$, $X^b = R^b$, and $X^{ab} = R^{ab} = R^{ba}$. The last equation requires that X^{ab} is real. If these conditions are fulfilled, the tight-binding model describes exactly the energy spectrum Eq. (21). The condition $X^a - R^a = X^b - R^b = 0$ can be relaxed in the case where only the difference spectrum between the two WS ladders is required to be exact. Then it is sufficient that $X^a - R^a = X^b - R^b = \Delta R$.³¹

We now return to the solution of Eq. (28) . The diagonal matrix elements in this equation can be eliminated by transmatrix elements in this equation can be eliminated by transforming $P_K^{\nu} = \overline{P}_K^{\nu} \exp[-(i/F)\int_0^K (\epsilon^{\nu} - FX^{\nu})dK']$. One then $\frac{1}{2}$ finds³⁰ \widetilde{P}_K^a

$$
\frac{\partial^2 \widetilde{P}_K^a}{\partial K^2} + i \frac{\hbar \,\widetilde{\omega}_d}{F} \frac{\partial \widetilde{P}_K^a}{\partial K} + (X^{ab})^2 \widetilde{P}_K^a = 0 \,, \tag{30}
$$

where we defined $\tilde{\omega}_d(K) = \omega_d(K) + FX$ / \hbar . Here the band separation is given by $\hbar \omega_d(K) = \epsilon^b(K) - \epsilon^a(K)$, and we also introduced $X = X^a - X^b$. The boundary condition is

$$
\widetilde{P}_{K+2\pi/d}^a = \widetilde{P}_{K}^a e^{-i(\epsilon - \Delta_0^a + FX^a)T_B/\hbar}.\tag{31}
$$

Let us next consider a part *I* of the Brillouin zone, where $\omega_d(K)$ is a weak function of *K* (i.e., the bands are almost flat). Specifically, we demand that $\Delta \omega_d(I) = \max[\omega_d(K)]$ $-\min[\omega_d(K)], \quad K \in I$, is small compared to $|\langle \omega_d \rangle_I + FX_-/\hbar|$ (the average is calculated over *I*). In this case Eq. (30) is easily solved and one finds

$$
\widetilde{P}_K^a = e^{-i\hbar(\widetilde{\omega}_d \pm \omega_l)K/2F}.\tag{32}
$$

Here the frequency ω_l is given by $\omega_l^2 = \omega_c^2 + \tilde{\omega}_d^2$ with $\omega_c = 2(|X^{ab}|/d)\omega_B$. Let us define the mean band separation $\omega_0 = \langle \omega_d \rangle_B$ and $\tilde{\omega}_0 = \omega_0 + F X$ / \hbar . The integration interval can be extended to the whole Brillouin zone when $\Delta \omega_d(\mathcal{B}) \ll |\tilde{\omega}_0|$. The solutions Eq. (32) then correspond to the spectrum

$$
\epsilon^{\pm} = \frac{\Delta_0^a + \Delta_0^b}{2} - F\frac{X_+}{2} \pm \frac{\hbar \Omega_l}{2} + p\hbar \omega_B, \quad p \text{ an integer}
$$

$$
\Omega_l^2 = \omega_c^2 + \tilde{\omega}_0^2,
$$
 (33)

where $X_+ = X^a + X^b$. Thus the two interpenetrating WS ladders are positioned symmetrically around the band midpoint, translated by $-FX_+/2$, and the ladder separation is $\hbar \Omega_1$. The exact form of the spectrum (33) can also be obtained in a much more direct way by looking for localized solutions to Eq. (25) . We restrict the solution to be confined within the *p*th unit cell. Solving

$$
\begin{vmatrix} \Delta_0^a - F(X^a + pd) - \epsilon & -FX^{ab} \\ -FX^{ab} & \Delta_0^b - F(X^b + pd) - \epsilon \end{vmatrix} = 0 , (34)
$$

we find the spectrum (33) . The difference spectrum obtained under the flat-band (or localization) condition will reappear in Sec. III when we discuss the electronic response in a static field in the case of nearly flat bands.

Next let us turn to time-periodic fields, when the righthand side of Eq. (25) acquires the additional terms $i(\hbar \partial/\partial t) u_l^{a(b)}$. Following Refs. 7–9 we substitute

$$
u_l^{\nu} = Q_l^{\nu} \exp\{i[\epsilon t + eA(t)ld]/\hbar\}
$$
 (35)

and Fourier transform, whence

$$
i\hbar \frac{\partial}{\partial t} \left(\frac{Q_K^a}{Q_K^b} \right) = \begin{pmatrix} \epsilon^a [k(t)] - F(t)X^a & -F(t)X^{ab} \\ -F(t)X^{ab} & \epsilon^b [k(t)] - F(t)X^b \end{pmatrix}
$$

$$
\times \begin{pmatrix} Q_K^a \\ Q_K^b \end{pmatrix}.
$$
(36)

From the Fourier transform of (35) we get the boundary condition

$$
Q_K^{\nu}(t+T_{ac}) = Q_{K+\Delta K}^{\nu} e^{-i\epsilon T_{ac}/\hbar}, \qquad (37)
$$

with $\Delta K = eA(T_{ac})/\hbar$, as above. A comparison of Eq. (36) with Eq. (14) , and Eq. (37) with Eq. (22) , shows that in order to obtain a correspondence we must set the Fourier variable *K* equal to the initial crystal momentum in the general model. The (difference) quasienergy spectrum in the tightbinding model and the (difference) spectrum obtained in the general model are then seen to be identical under the same conditions as in the static case.

III. RESPONSE

We have thus far examined the general properties of the energy spectrum and the wave functions of a superlattice in an external field. The next step is to compute the physical quantities, such as densities or drift velocities. To this end we must construct an appropriate kinetic equation. The simplest approach would be to consider the Boltzmann equation. However, since we are interested in the properties of systems with two or more occupied minibands, where a coherent band-to-band transfer plays an essential role, it is necessary to use a method that allows one to consider quantummechanical tunneling. In the following sections we shall use the density-matrix description.

A. Density-matrix equations of motion

In order to describe the coherent transport we shall start from the equations of motions for the density matrix in the limit where collisions may be neglected. Such equations of motions were derived by Krieger and Iafrate.^{27,28} Thus we take as our starting point Eq. (51) of Ref. 27, adapted to the case of two minibands. The density matrix is defined as

$$
\rho_{nKn'K'}(t) = \langle \psi_{nK}(x,t) | \rho(x,t) | \psi_{n'K'}(x,t) \rangle, \qquad (38)
$$

and for coherent motion its diagonal elements ($\rho_K^a \equiv \rho_{aKaK}$ etc.) satisfy

$$
\frac{\partial \rho_K^a(t)}{\partial t} = \frac{1}{2} \text{Re} \Bigg\{ h(K,t) \int_0^t h^*(K,t') [\rho_K^b(t') - \rho_K^a(t')] dt' \Bigg\},\tag{39}
$$

$$
\frac{\partial \rho_K^b(t)}{\partial t} = \frac{1}{2} \text{Re} \Bigg\{ h^*(K,t) \int_0^t h(K,t') [\rho_K^a(t') - \rho_K^b(t')] dt' \Bigg\},\tag{40}
$$

where

$$
h(K,t) = -\frac{2F(t)R^{ab}[k(t)]}{\hbar}
$$

$$
\times \exp\left(-i\int_0^t \{\omega_d[k(t')] + F(t')R - [k(t')]/\hbar\}dt'\right)
$$
(41)

and $R_{-}(k) = R^{a}(k) - R^{b}(k)$. Defining $\rho_{\pm}(K,t) = \rho_{K}^{a}(t)$ $\pm \rho_K^b(t)$ we get, from Eqs. (39) and (40),

$$
\dot{\rho}_+(K,t) = 0,\tag{42}
$$

$$
\dot{\rho}_{-}(K,t) = -\operatorname{Re}\left\{ h(K,t) \int_{0}^{t} h^{*}(K,t') \rho_{-}(K,t') dt' \right\},\tag{43}
$$

where we defined $\rho \equiv \partial \rho / \partial t$. Equation (42) is simply a statement of particle number conservation, while the integrodifferential equation (43) determines the kinetic properties of our system.

As it stands, Eq. (43) is unsuited for analytical applications because of the non-Markovian "collision term" (presently, the ''collisions'' consist of band-to-band transfers, dressed with the effects of the external fields). However, it can be solved numerically by the technique described in Ref. 32. We now prove that Eq. (43) can be reduced to a thirdorder differential equation and then handled by standard numerical techniques, if we assume that $h \neq 0$ except in equilibrium. In addition, it will be shown that the form of this equation is invariant after a finite switch-on period $[0,T_0]$. At the end of this time interval the response belonging to an initial momentum *K* depends only on the position $k(T_0)$ of the semiclassical motion of *K* and on the boundary conditions of ρ ₋ at $t=T_0$.

Since the different K components do not mix in (43) , we can keep the initial momentum *K* fixed. In order to ease the notation we write Eq. (41) as $h=ue^{i\phi}$. Then the relation $u\dot{h} = (\dot{u} + i\dot{u}\dot{\phi})h$ holds. Using this and differentiating Eq. (43) we get

$$
u\ddot{\rho}_{-} = u\dot{\rho}_{-} - u\dot{\phi}\text{Re}\left\{ih\int_{0}^{t} h^* \rho_{-} dt'\right\} - u^3 \rho_{-}.
$$
 (44)

An auxiliary function *w* is next defined by $w = -\text{Im}\{hf_0^th*\rho_-dt'\}$. It satisfies the equation

$$
uw = uw + u\,\phi\rho_- \,. \tag{45}
$$

We proceed by expressing *w* in terms of another auxiliary function $w = u\tilde{w}$. Using $u\tilde{w} = \dot{\phi}\rho$ _{*=*}, we obtain

$$
w(t) = u(t) \int_0^t \frac{\phi(t')\rho_-(t')}{u(t')}dt'.
$$
 (46)

This allows one to rewrite Eq. (44) as

$$
\ddot{\rho}_{-} - \frac{\dot{u}}{u} \dot{\rho}_{-} + u^2 \rho_{-} + u \phi \int_0^t \frac{\dot{\phi} \rho_{-}}{u} dt' = 0.
$$
 (47)

Finally, dividing Eq. (47) by $u\dot{\phi}$, differentiating, and multiplying by $u^3\dot{\phi}^2$, we arrive at the third-order differential equation

 $p = 3i$

$$
p_3 \ddot{\rho}_- + p_2 \ddot{\rho}_- + p_1 \dot{\rho}_- + p_0 \rho_- = 0 , \qquad (48)
$$

where

$$
p_3 = u \quad \phi,
$$

\n
$$
p_2 = -u(2u\dot{u}\phi + u\ddot{\phi}),
$$

\n
$$
p_1 = (-u\ddot{u} + 2\dot{u}^2 + u^4 + u^2\dot{\phi}^2)\dot{\phi} + u\dot{u}\ddot{\phi},
$$

$$
p_0 = u^3(\dot{u}\dot{\phi} - u\ddot{\phi}).
$$
 (49)

From Eqs. (43) and (47) above we get the boundary conditions ρ ^{*i*} $(K,0) = 0$ and ρ ^{*i*} $(K,0) = -u^2 \rho$ ^{*i*} $(K,0)$. These equations are readily numerically integrated, and a few special cases were described in our recent paper.²²

Current

The results derived above can be used to obtain an expres-The results derived above can be used to obtain an expression for the drift velocity $\bar{v}(t)$. The result can be expressed as a sum of a semiclassical, intraband term and a term with quantum-mechanical origin, which incorporates Zener tunneling.

Omitting the details, we state our result:

$$
\overline{v}(t) = \sum_{\nu, K} \rho_K^{\nu}(t) v_K^{\nu}(t) + 2 \sum_K \left[\text{Re} \rho_K^{ba}(t) \text{Re} v_K^{ab}(t) - \text{Im} \rho_K^{ba}(t) \text{Im} v_K^{ab}(t) \right],
$$
\n(50)

where

$$
v_K^{\nu}(t) = \frac{1}{\hbar} \frac{\partial \epsilon^{\nu}[k(t)]}{\partial k},
$$
\n(51)

$$
v_K^{ab}(t) = -i\omega_d[k(t)]R^{ab}[k(t)].
$$
 (52)

The nondiagonal density-matrix elements ρ_K^{ba} can be expressed in terms of the diagonal elements

$$
u(t)\rho_K^{ba}(t) = -\frac{i}{2}h(K,t)\int_0^t h^*(K,t')\rho_-(K,t')dt'.
$$
\n(53)

Using the auxiliary function *w* defined in the previous section, we obtain

$$
\operatorname{Re}\{u(t)\rho_K^{ba}(t)\} = -\frac{u}{2}\int_0^t \frac{\dot{\phi}\dot{\rho}_-}{u} dt',\tag{54}
$$

Im{
$$
u(t)\rho_K^{ba}(t)
$$
} = $-\frac{1}{2}\rho_{-}(K,t)$. (55)

If R^{ab} is real, Eq. (50) can be further reduced and one finds

$$
\overline{v}(t) = \sum_{\nu, K} \rho_K^{\nu}(t) v_K^{\nu}(t) - \frac{1}{2F(t)} \sum_K \dot{\rho}_-(K, t) \hbar \omega_d[k(t)].
$$
\n(56)

In Eq. (50) or (56) the first sum is the semiclassical contribution to the drift velocity, while the second sum accounts for Zener tunneling. Since $\rho_K^a(t) + \rho_K^b(t) = \text{const}$ (determined by the initial conditions), we can express Eq. (56) in terms of $\rho_{-}(K,t)$ alone. Thus a numerical solution of the third-order differential equation derived in the previous section, Eq. (48) , is sufficient to determine the full time depention, Eq. (48), is sufficient to determine the full time dependence of $\bar{v}(t)$. This, however, must be done for each initially occupied *K* value and we leave applications for future work.

B. Zener tunneling

The numerical calculations of Zener resonances based on (48) were discussed in our recent paper.²² Since tunneling between bands plays an important role in the interpretation of our results we now consider the condition for Zener tunneling in the present two-band model. The electrical field is assumed to be static $F(t)=F(0)$.

1. Analytical considerations

(a) *Weak coupling limit*. We shall show how a two-band version of Eq. (14) can give Zener resonances, following the perturbative method used by Mullen *et al.*, ³³ which is valid for weak band coupling. The two-band system is

$$
i\hbar \frac{\partial}{\partial t} \begin{pmatrix} C_K^a \\ C_K^b \end{pmatrix} = \begin{pmatrix} \epsilon^a - FR^a & -FR^{ab} \\ -FR^{ba} & \epsilon^b - FR^b \end{pmatrix} \begin{pmatrix} C_K^a \\ C_K^b \end{pmatrix}.
$$
 (57)

The system is linear and time periodic with period T_B . The solution $(C_K^a (NT_B), C_K^b (NT_B))^t$ can then be obtained from the initial state $(C_K^a(0), C_K^b(0))^t$ by applying the time propagator U_0 *N* times on the initial state. The propagator \mathbf{U}_0 is found as follows. By defining $C_K^{\nu}(t)$ \mathbf{U}_0 is found as follows. By defining $C_K(t)$
= $\tilde{C}_K^{\nu}(t) \exp[-(i/\hbar)] \int_0^t (\epsilon^{\nu} - FR^{\nu}) dt'$ the diagonal in Eq. (57) is eliminated,

$$
\frac{\partial}{\partial t} \begin{pmatrix} \widetilde{C}_{K}^{a} \\ \widetilde{C}_{K}^{b} \end{pmatrix} = \begin{pmatrix} 0 & G^{ab} \\ -(G^{ab})^* & 0 \end{pmatrix} \begin{pmatrix} \widetilde{C}_{K}^{a} \\ \widetilde{C}_{K}^{b} \end{pmatrix},
$$
(58)

where $G^{ab}=i(FR^{ab}/\hbar)$ exp($-i\int_0^{T_B}\tilde{\omega}_d dt'$). We work in the limit of small band couplings $|G^{ab}(t)T_B| \ll 1$. To first order in $\Gamma^{ab} = \int_0^{T_B} G^{ab} dt'$ the initial state $(1,0)^t$ develops in a Bloch period T_B to $(1,-(\Gamma^{ab})^*)^t$ and the orthogonal state $(0,1)$ to $(\Gamma^{ab},1)^t$. The time propagator is then

$$
\mathbf{U}_0 = \exp\left(-\frac{i}{2\hbar} \int_0^{T_B} \left[\,\epsilon^a + \epsilon^b - F(R^a + R^b)\,\right] dt'\,\right) \\
\times \left(\begin{array}{cc} M & \Gamma^{ab} M \\ -(\Gamma^{ab} M)^* & M^* \end{array}\right),\tag{59}
$$

where $M = \exp[(i/2)\int_0^{T_B} \tilde{\omega}_d dt']$. According to Ref. 33, the resonance condition is that there should be a phase difference $2\pi p$, where p is an integer, between the diagonal elements. In our case, the resonance condition is therefore $\int_0^{T_B} \widetilde{\omega}_d dt' = 2 \pi p$ or

$$
\frac{1}{Fd} = \frac{1}{\hbar \omega_0} \left(p - \frac{\langle R_- \rangle}{d} \right), \quad p \text{ an integer.}
$$
 (60)

(b). *Static flat-band limit*. Let us now discuss the case where the band coupling is not assumed to be small. For a static field Eq. (48) reduces to²²

$$
\ddot{\phi}\ddot{\rho}_{-} - \ddot{\phi}\ddot{\rho}_{-} + \dot{\phi}(u^2 + \dot{\phi}^2)\dot{\rho}_{-} - u^2\ddot{\phi}\rho_{-} = 0.
$$
 (61)

We restrict ourselves to the case when $|\omega_1| \ll |\tilde{\omega}_0|$, where $\omega_1 = \omega_d - \omega_0$. Furthermore, it is assumed that the band couplings *R* are independent of time and we denote $X^a = R^a$, $\overline{X}^b = \overline{R}^b$, and $\overline{X}^{ab} = \overline{R}^{ab} = R^{ba}$. We have

$$
u = 2(|X^{ab}|/d)\omega_B \equiv \omega_c,
$$

$$
\dot{\phi} = -(\tilde{\omega}_0 + \omega_1).
$$
 (62)

Equation (61) is then

$$
-(\tilde{\omega}_0 + \omega_1)\ddot{\tilde{\rho}}_- + \dot{\omega}_1\ddot{\tilde{\rho}}_- - (\tilde{\omega}_0 + \omega_1)(\omega_c^2 + (\tilde{\omega}_0 + \omega_1)^2)\dot{\rho}_- + \omega_c^2\dot{\omega}_1\rho_- = 0.
$$
 (63)

We write Eq. (63) in the form

$$
(L_0 + L_1 + L_r)(\rho_0 + \rho_1 + \rho_r) = 0 , \qquad (64)
$$

where L_{μ} and ρ_{μ} , $\mu=0,1,r$, are of the zeroth, first, and higher order in ω_1 . We get

$$
L_0 \rho_- = -\tilde{\omega}_0 \ddot{\rho}_- - \tilde{\omega}_0 \Omega_l^2 \dot{\rho}_-,
$$

\n
$$
L_1 \rho_- = -\omega_1 \ddot{\rho}_- + \dot{\omega}_1 \ddot{\rho}_- - \omega_1 (\Omega_l^2 + 2\tilde{\omega}_0^2) \dot{\rho}_- + \dot{\omega}_1 \omega_c^2 \rho_-,
$$

\n
$$
L_r \rho_- = -\omega_1^2 (3\tilde{\omega}_0 + \omega_1) \dot{\rho}_-. \tag{65}
$$

The boundary conditions are $\rho_0(K,0) = \rho_-(K,0)$, $\rho_1(K,0) = \rho_r(K,0) = 0,$ $\rho_\mu(K,0) = 0,$ and $\rho_\mu(K,0)$ $\dot{L}_0 = -\omega_c^2 \rho_\mu(K,0)$. The zeroth-order equation $L_0 \rho_0 = 0$ is readily integrated:

$$
\ddot{\rho}_0 + \Omega_I^2 \rho_0 = \tilde{\omega}_0^2 \rho_0(0). \tag{66}
$$

Using the zeroth-order equation and Eq. (66) in the firstorder equation $L_0\rho_1 + L_1\rho_0 = 0$ and integrating, we find

$$
\ddot{\rho}_1 + \Omega_l^2 \rho_1 = -\tilde{\omega}_0 \bigg[\omega_1 [\rho_0 - \rho_0(0)] + \int_0^t \omega_1 \dot{\rho}_0 dt' \bigg].
$$
 (67)

It is now clear that ρ_0 contains only the frequency Ω_l . If $\omega_1(K)$ is an analytic function then the spectrum of ω_1 is $p\omega_B$, where *p* is an integer. From Eq. (67) we see that the Fourier spectrum of ρ_1 consists of the frequencies Ω_l + $p\omega_B$, where *p* is an integer.

Let us turn to the particular case with cosine bands Eq. (26) . As shown in Sec. II B, the cosine bands can be generated by a simple tight-binding model. For finite field values the energy spectrum is given by Eq. (33) . Performing the integrals we obtain

$$
\rho_0(K,t) = \frac{\rho_0(K,0)}{\Omega_l^2} (\overline{\omega}_0^2 + \omega_c^2 \cos \Omega_l t),
$$

$$
\rho_1(K,t) = \frac{\tilde{\omega}_0(\Delta_1^a + \Delta_1^b)\omega_c^2 \rho_0(K,0)}{2\hbar \Omega_l^2(\Omega_l^2 - \omega_B^2)\omega_B}
$$

$$
\times \left\{\omega_B \cos K d + \omega_B \cos(\omega_B t + K d) + (\Omega_l - \omega_B) \cos K d \cos \Omega_l t - \Omega_l \cos(\Omega_l t + K d) + \frac{\Omega_l - \omega_B}{2} \cos[(\Omega_l + \omega_B)t + K d] - \frac{\Omega_l + \omega_B}{2} \cos[(\Omega_l - \omega_B)t - K d]\right\}, \tag{68}
$$

where Ω_l was defined in (33). Thus, to first order in ω_1 the response contains the first intra-WS transition ω_B and the inter-WS transitions Ω_l , $\Omega_l \pm \omega_B$.

The structure of the perturbative solution (68) seems to suggest that the response frequency spectrum always corresponds to intra- and intertransitions between (quasi)energy ladders. This expectation is proven analytically in the Appendix for static fields. The numerical examples in Ref. 22 also support this conclusion for time-periodic fields.

2. Numerical example

In our recent paper²² we presented examples of a numerical solution of the equation of motion for the density matrix ρ _{(K⁻⁰,*t*). It was found that at certain, relatively sharp} defined values of the applied field the time dependence of $\rho_-(0,t)$ exhibited a full inversion, i.e., its values ranged from $+1$ (the initial value corresponding to a carrier in band *a*) to -1 (carrier in band *b*). The sharp resonances, corresponding to complete band-to-band transfer, were termed ''Zener resonances.'' These features were shown to be intimately related to the Wannier-Stark ladder structure of the system: The resonances occurred when the level differences of the double ladder (corresponding to the two-band system) was at minimum. In the present section we describe the results of extensive simulations that generalize our earlier results in the following two respects: (i) We allow the interband coupling, described by a parameter $\xi = X^{ab}/d$, to vary from zero to large values and (ii) we examine the equation of motion for 41 different *K* points, covering the entire Brillouin zone.

We next comment on the choice of the parameters defining our model. Our numerical investigations show that the plateaus are most clearly resolved when the following conditions are met: (i) The bandwidths $\Delta_1^{a,b}$ should be as large as possible and (ii) the band separation at the zone boundary should be small. Under these conditions the inversion of $\rho_{-}(K,t)$ occurs on a time scale that is of the order of a few Bloch periods, which is essential for distinguishing the plateaus.

One should next address the question whether these conditions can be realized within existing semiconductor materials, such as GaAs-Al_xGa_{1-x}As heterostructures. We have used equal bandwidths of 14 meV for the two minibands, and a band separation of 20 meV. A possible experimental realization of such a system with two minibands can be obtained in a superlattice that contains a *pair* of quantum wells in its unit cell.^{2,13} It is not difficult to see that in this case the

FIG. 2. The first five Zener resonances as a function of the band coupling parameter $\xi = X^{ab}/d$. The diamonds represent the field values at which the distance between WS ladders has a local minimum. The solid lines give the local minima for the flat-band model. The error bars indicate at which field strengths the electronic response shows a Zener resonance. The finite widths are a consequence of dispersion. See the text for further discussion. The superlattice parameters are $X_0 = 0$, $d = 10$ nm, $\Delta_1^a = 14$ meV, $\Delta_1^b = 14$ meV, and $\Delta^{ab} \equiv \Delta_0^b - \Delta_0^a = 20$ meV.

bandwidths and band separations are controlled by two parameters $exp(-\kappa l)$ and $exp(-\kappa b)$, where *l* is the barrier thickness separating the double well from the neighboring double well, *b* is the barrier between the pair of wells, and $k^2 = 2m(V_0 - E)/\hbar^2$ with $V_0 \approx 0.3$ eV and *E* is the energy of the bound state for an isolated quantum well. It is then possible to choose values for *l*, *b*, and the quantum-well width *a* so that the band parameters are comparable to the ones used in our numerical work. The conclusion is thus that the versatility of the GaAs- $Al_xGa_{1-x}As$ system allows one to fine tune the miniband structure so that the conditions for experimental verification are present.

The results of our numerical work, which consists of three separate calculations, are summarized in Fig. 2. The first calculation consists of an evaluation of the local minima of *the normalized WS ladder separation* as a function of field strength. These are represented by diamonds in Fig. 2. The normalized WS ladder separation is constructed in three steps: (i) Compute the differences of the energy levels in the two WS ladders, (ii) divide the differences by Fd , and (iii) select the part of the normalized difference spectrum that belongs to $[0,0.5]$. It is seen from Fig. 2 that by increasing the interband coupling the local minima are shifted monotonical towards higher-field values and that they vanish in succession. The local minima are numbered from the highfield end at zero band coupling. The first five local separation minima are depicted (when they exist) in Fig. 2.

The second part of Fig. 2 is a comparison of part one with the local minima of the WS ladder separation in the case where the double ladder is given by Eq. (33) . The normalized difference spectrum $\epsilon_{\text{dif}} = \pm (\epsilon^+ - \epsilon^-)/Fd$ is

$$
\epsilon_{\text{dif}} = q \pm \sqrt{4\xi^2 + \left(\frac{\Delta^{ab} + FX}{Fd}\right)^2}, \quad q \text{ an integer.}
$$
\n(69)

In our numerical example we have set $X^a = X^b = 0$; thus $X_0 = 0$. The normalized WS ladder separation has local minima (equal to zero) whenever $q - \sqrt{4\xi^2 + (\Delta^{ab}/Fd)^2} = 0$ or

$$
\frac{1}{Fd} = \frac{1}{\Delta^{ab}}\sqrt{q^2 - 4\xi^2}.\tag{70}
$$

In the limit of zero band coupling we get $1/Fd = q/\Delta^{ab}$, in exact agreement with the correct result. In the high-field limit the local minima should be at $\xi = q/2$. As seen from Fig. 2, the flat-band (or localized) model tends to overshoot the exact findings, but it provides an important hint about where to find the local minima. In general, the flat-band model is not formally correct: the numerical calculations show that the two WS ladders never coincide (level repulsion) for nonzero band coupling. But even in our case, where the bands are far from being flat, it estimates well the local minima.

The last part of Fig. 2, denoted by error bars, is a calculation of Zener resonances, based on examining the time development of $\rho_{-}(K,t)$. As shown in our paper²² the number of oscillations in $\rho_{-}(K,t)$ within a plateau increases when the field is decreased. A plateau is better defined at the center than at the terminal points where the deviation from a constant value of $\rho_{-}(K,t)$ is largest. Thus for Zener resonances with high index it is not sufficient to calculate $\rho_{-}^{\min}(K)$. Instead we define the center of a plateau as the time where the oscillation amplitude of ρ (*K*,*t*) is at local minimum. A Zener resonance is then a field value at which any of the plateau center values have reached -1 . For a fixed interband coupling the first five Zener resonances have been estimated (when they exist) for 41 evenly distributed K points in the Brillouin zone. Some dispersion was detected, and this is indicated by the height of the error bars in Fig. 2. In the weak-coupling limit we find zero dispersion and the Zener resonances coincide with Eq. (60) . As seen from Fig. 2, there is an excellent overall correspondence between local minima of the normalized WS ladder separation on the one hand and the Zener resonances on the other hand.

IV. CONCLUSION

Our main results can be summarized as follows. (i) The wave function for an electron in a periodic potential, such as in a semiconductor superlattice, under the influence of a (time-dependent) uniform electric field is expanded in terms of accelerated Bloch states. The properties of the expansion coefficients allow us to give a unified treatment of several different results, obtained by a variety of techniques in the literature, for the superlattice. In static fields, the Wannier-Stark ladder spectrum can be deduced for a superlattice with a finite number of finite bands and in the time-dependent case with a periodic external field; a fractional quasienergy spectrum emerges for certain values of the external field. (ii) A mapping is constructed between a two-band tight-binding model and the general system considered in (i). This allows one to make several general statements concerning the properties of the two-band system, both in static and timedependent situations. (iii) A density-matrix equation of motion is developed and the resulting third-order differential equation is shown to be well suited for both analytic and numerical studies of Zener tunneling in the two-miniband system. We also give numerical results for Zener resonances, identified in our earlier work, 22 and interpret them analytically applying the tools developed in this work.

ACKNOWLEDGMENTS

We thank Dr. A. Sacchetti for his comments on the general Bloch problem.

APPENDIX: RESPONSE FREQUENCY SPECTRUM

We shall demonstrate that the response frequency spectrum in a dc field consists of elements corresponding to intraand inter-WS transitions. In Sec. II we found the linearly independent solutions

$$
\psi_j^p(x,t) = e^{-i\epsilon_j^p t/\hbar} \sum_{nK} c_{Kjn} \phi_{nK}(x)
$$
 (A1)

to the Schrödinger equation by using the *N*-dimensional Floquet theorem. Now expanding a general solution as

$$
\psi(x,t) = \sum_{j,p} \alpha_j^p \psi_j^p(x,t), \qquad (A2)
$$

we obtain, for the diagonal element $\rho_{nK}(t)$ of the density operator $\rho(x,t) = |\psi(x,t)\rangle \langle \psi(x,t)|$,

$$
\rho_{nK}(t) = \langle \psi_{nK}(x,t) | \rho(x,t) | \psi_{nK}(x,t) \rangle \n= \sum_{\substack{K',j',n',p'\\ K'',j'',n'',p''}} \alpha_{j'}^{p'} \alpha_{j''}^{p''*} c_{Kj'n'}^{p''*} c_{K''j''n''}^{p''} e^{-i(\epsilon_{j'}^{p'} - \epsilon_{j''}^{p''} t/\hbar)} \n\times \langle \psi_{nK}(x,t) | \phi_{n'K'}(x) \rangle \langle \phi_{n''K''}(x) | \psi_{nK}(x,t) \rangle.
$$
\n(A3)

The ABS's are time-periodic functions with period T_B . Thus $\rho_{nK}(t)$ contains only frequencies that are a subset of energy differences between the WS ladders.

In Sec. III the gauge was changed. We now show that the response frequency spectrum still consists of energy differences between the WS ladders for the scalar-potential Hamiltonian. In the new gauge the Schrödinger equation is of the form

$$
H_A(x,t)\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}.
$$
 (A4)

We expand the wave function directly in the ABS's $\psi(x,t) = \sum_{n,K} B_{nK}(t) \psi_{nK}(x,t)$ and find the system²⁶

$$
i\hbar \frac{\partial B_{nK}(t)}{\partial t} = \epsilon_n [k(t)] B_{nK}(t) - F(t) \sum_{n'} R_{nn'} [k(t)] B_{n'K}(t),
$$
\n(A5)

$$
\psi_{Kj}^{A}(x,t) = \sum_{n} C_{Kjn}(t) \psi_{nK}(x,t).
$$
 (A6)

Expanding the wave function $\psi(x,t) = \sum_{K,j} \alpha_{K,j} \psi_{K,j}^A(x,t)$, we get

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$$
\rho_{nK}(t) = \sum_{j',j''} \alpha_{Kj'} \alpha_{Kj''}^* e^{i(\omega_{j'} - \omega_{j''})t} P_{Kj'n}^0(t) P_{Kj''n}^0*(t).
$$
\n(A7)

The diagonal elements have a different appearance as compared to Eq. $(A3)$, but the conclusion concerning the response frequency spectrum is the same as before the gauge change.

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in Eq. (14) is compensated for by defining Eq. (14) is compensated for by in Eq. (14) is compensated for by defining
 $C_{nK}(t) = \tilde{C}_{nK}(t) \exp[(i/\hbar) \int_0^t F \Delta R dt']$. This brings Eq. (14) back to the original form. Equation (17) becomes back to the original form. Equation (17) becomes $\tilde{C}_{nK}(t+T_B) = \tilde{C}_{nK}(t)e^{-i(\epsilon+F(\Delta R))T_B/\hbar}$, where $\langle \rangle$ is the period average. We see that the WS ladders are translated by the same amount $-F(\Delta R)$. [For a time-periodic field and a timeindependent ΔR , Eq. (22) is replaced by
 $\widetilde{C}_{nK}(t+T_{ac}) = \widetilde{C}_{nK+\Delta K}(t)e^{-i(\epsilon+\langle F \rangle \Delta R)T_{ac}/\hbar}$, thus the quasienergy ladders are translated by $-\langle F \rangle \Delta R$.
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