PHYSICAL REVIEW B VOLUME 33, NUMBER 12 15 JUNE 1986

k·p theory of semiconductor superlattice electronic structure. I. Formal results

D. L. Smith
Los Alamos National Laboratory, University of California, Los Alamos, New Mexico 87545

C. Mailhiot
Xerox Corporation, Webster Research Center, 800 Phillips Road (0114-41D), Webster, New York 14580

(Received 27 January 1986)

This is the first of a two-paper series in which we present a complete **k**·**p** theory of semiconductor superlattices. Here we present the formal theoretical results. In the second paper, numerical implementation of these results is described and examples of superlattice electronic structure calculations are presented. A single basis set for the constituent materials is provided by a zone-center pseudopotential calculation with a reference Hamiltonian. The Γ_{15} valence and Γ_1 conduction states are coupled with a spinor and treated explicitly. Near-in energy states are treated in Löwdin perturbation theory with the **k**·**p** operator and the difference between the material pseudopotential and the reference pseudopotential as the perturbation. The calculation is carried out to first order for wave functions and second order for energies. Spin-orbit and stress interactions are included between the explicitly included states. Bloch and evanescent states are computed for each material. Interface matching of the constituent material bulk eigenfunctions is accomplished using results derived for the normal component of the current density operator. Superlattice symmetry is used to derive an eigenvalue equation for the superlattice wave vector and eigenfunctions. The formalism has the advantage of involving only small-dimensionality matrices (typically, 12×12). It is well suited to optical and transport property calculations.

I. INTRODUCTION

Semiconductor superlattices consist of alternating thin layers of different semiconductors. The electronic structure of a superlattice depends on the layer thicknesses, as well as on the constituent materials.[1] Because the layer thicknesses can be precisely controlled, superlattices offer the possibility of being able to design the electronic band structure of semiconducting materials. The flexibility in superlattice electronic properties that are introduced by this design possibility makes them useful in several technological applications, including semiconductor diode lasers,[2] electro-optical modulators,[3] nonlinear optical devices,[4] and infrared detectors.[5]

Those electronic states whose mean free path is comparable to or longer than the superlattice period are significantly influenced by the spatial modulation of the superlattice. States whose mean free path is much less than a superlattice period are essentially kinetically confined within a particular material. Such states are, thus, not much modified by superlattice modulation. As a result, electronic states relatively close in energy to the conduction- and valence-band edges, which have relatively long lifetimes and mean free paths, are of greatest interest in superlattice materials. In bulk semiconductors, **k**·**p** theory is particularly effective at describing states near the conduction- and valence-band edges. For this reason, it is natural to develop a **k**·**p** theory description of these states in semiconductor superlattices.

Previous work on the electronic structure of semiconductor using **k**·**p** models includes the results of White and Sham,[6] Bastard,[7,8] and Altarelli.[9] White and Sham, and Bastard, used different approaches to arrive at essentially the same result. They considered a two-band model which describes the conduction and light-hole bands. The model is essentially one dimensional in the sense that only states whose wave vector is normal to the plane of the superlattice interfaces are described. Altarelli uses a three-band model which is capable of describing states whose wave vector lies in a plane which includes the vector normal to the plane of the superlattice interfaces. (States with any direction of **k** can thus be described, but it is necessary to use different basis sets for different directions of **k**.) It is also necessary to diagonalize rather large-dimensionality (e.g., 72×72) in this method. In the above approaches, the zone-center Bloch functions are taken to be identical in the two materials, only the very large spin-orbit splitting case is considered, and stress effects are usually ignored.

This is the first of a two-paper series in which we present a complete **k**·**p** theory of semiconductor superlattices. In this paper, we present the formal theoretical results. In the second paper,[10] numerical implementation of the formal results is described and examples of superlattice electronic-structure calculations are presented.

In this work, an empirical pseudopotential calculation[11] is first performed at the zone center of a reference Hamiltonian, formed by averaging the pseudopotential form factors of the constituent materials, to provide a spatial basis set. The Γ_{15} valence states and Γ_1 conduction state are coupled with a spinor and treated explicitly. The near-in energy (typically 23, as actually implemented) spatial states are treated in Löwdin perturbation theory[32] with the **k**·**p** operator and the difference between the material pseudopotential and the reference Hamiltonian pseudopotential as the perturbation. The calculation is carried out to first order for wave functions and second order for energies. The spin-orbit and stress (for strained-layer superlattices) interactions are included between the explicitly treated states. Bloch and evanescent states for each bulk material are computed. Matching of the bulk Bloch and evanescent states at the superlattice interfaces is accomplished using results derived about the normal component of the current-density operator. The superlattice translational symmetry is used to derive an eigenvalue equation for superlattice wave vectors and eigenfunctions. The resulting eigenvalue equation has the advantage of involving only rather small-dimensionality matrices (typically 12×12).

The formal structure presented here can describe superlattice states with wave vector in any direction using the same basis set. It is well suited for optical properties and transport calculations. Assumptions concerning the similarity of the zone-center Bloch states in the two materials (in our case, the assumption is that first-order perturbation theory in the difference between material and averaged pseudopotentials is adequate) can be explicitly checked. It is not necessary to assume large spin-orbit splittings. The effects of stress resulting from lattice mismatch is explicitly included. The results presented here reduce to those of White and Sham,[3] and Bastard,[7,8] if only wave vectors normal to the interface plane are considered and an additional series of approximations is made.

We explicitly consider superlattices made from two zinc-blende crystal-structure semiconductors with a [100] growth direction. The basic theoretical approach we use is equally applicable to other cases. Detailed results, of course, depend on the physical geometry. We chose to consider the zinc-blende [100]-growth-direction case because most superlattices currently grown have this geometry.

The paper is organized in the following way: In Sec. II our description of the individual materials is presented, in Sec. III we describe our treatment of a single interface, in Sec. IV the superlattice periodicity is used to derive an eigenvalue equation for the superlattice wave vectors and state functions, and in Sec. V we summarize our conclusions. Calculational details and reduction to previous results are presented in the Appendixes.

II. DESCRIPTION OF THE CONSTITUENT MATERIALS

In this section we present our description of the individual materials making up the superlattice. For these calculations, it is desirable to have a single zone-center basis set to describe the states in both of the constituent materials.[13] For this reason, we define a reference Hamiltonian by

$$H_R=\frac{p^2}{2m}+\tfrac{1}{2}[V^a(r)+V^b(r)]\ , \tag{1}$$

where a and b label the constituent materials and $V^l(r)$ is the pseudopotential of material l described in terms of pseudopotential form factors.[11] The lattice constant in the reference Hamiltonian is the average of the constituent-material lattice constants. Alloy materials are treated in a virtual-crystal approximation.

The reference Hamiltonian is solved at the zone center, in terms of a plane-wave basis, to give a set of energies and cell-periodic, zone-center, eigenfunctions, ε_β and $U_\beta(r)$. We have

$$U_\beta(r)=\frac{1}{\sqrt{\Omega}}\sum_{\mathbf{G}} R_{\beta\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}}\ , \tag{2}$$

where β labels the various eigensolutions, Ω is the unit cell volume, $\mathbf{G}$ is a reciprocal-lattice vector, and R is an expansion coefficient. We choose phases such that $U_\beta(r)$ are real. For degenerate representations, the partner functions are chosen to transform according to the convention of Ref. 14. In terms of H_R, the Hamiltonians describing the constituent materials can be written as

$$H_l=H_R+\Delta V^l+H^l_{\text{s.o.}}+H^l_{\text{st}}\ , \tag{3a}$$

where

$$\Delta V^l=V^l-\tfrac{1}{2}(V^a+V^b)\ , \tag{3b}$$

$H^l_{\text{s.o.}}$ represents the spin-orbit interaction, and H^l_{st} represents the stress interaction (owing to lattice mismatch) in material l.

We use the zone-center states $U_\beta(r)$ as a basis set to describe cell-periodic functions in each material. We divide the set of states $U_\beta(r)$ into two groups. One group consists of the threefold Γ_{15} valence-band states and the Γ_1 conduction-band state combined with a spinor. These eight states are treated explicitly. We will use the notation $U_d(r)$, where d runs over the eight states, to label them. The other spatial states, also combined with a spinor, form the second group of states. These states will be included to first order for the wave function in Löwdin perturbation theory.[12] The perturbation consists of $\Delta V^l+m^{-1}\mathbf{k}\cdot\mathbf{p}$. (These two operators are considered to be of the same order.) Thus we construct, in each material, the cell-periodic functions,

$$U^l_{dj}(r)=U_d(r)+\sum_\beta W^l_{d\beta j}U_\beta(r)\ , \tag{4a}$$

where

$$W^l_{d\beta j}=\frac{\langle U_\beta\,|\,\Delta V^l+m^{-1}\mathbf{k}_j\cdot\mathbf{p}\,|\,U_d\rangle}{\varepsilon_d-\varepsilon_\beta}\ , \tag{4b}$$

the sum over β does not include the explicitly treated states labeled by d, and $\mathbf{k}_j$ is a point in $\mathbf{k}$ space. The Bloch and evanescent states in each material are written as

$$\psi^l_j(r)=\frac{e^{i\mathbf{k}^l_j\cdot\mathbf{r}}}{\sqrt{N}}\sum_d C^l_{dj}U^l_{dj(r)}\ , \tag{5}$$

where N is the number of bulk primitive cells (two atoms in the zinc-blende structure) in the superlattice. The cell-periodic states U are normalized to a unit cell and the C's are taken so that $[(\psi_{j*})^*\psi_j]$ integrates to unity over the superlattice volume. We construct the 8×8 matrices defined by

$$H^l_{dd'}(\mathbf{k}^l_j)\equiv\langle U_d\,|\,e^{-i\mathbf{k}^l_j\cdot\mathbf{r}}H_l\,e^{i\mathbf{k}^l_j\cdot\mathbf{r}}\,|\,U^l_{d'j}\rangle\ . \tag{6}$$

The expansion coefficients C_{dj}^{l} are found by solving the eigenvalue equation

$$[H_{dd'}^{l}(\mathbf{k}_j^l)-\varepsilon\delta_{dd'}]C_{d'j}^{l}=0\ , \tag{7}$$

where ε is the state energy.

In the construction of $H_{dd'}^{l}(\mathbf{k}_j^l)$, we neglect the commutator of $H_{\text{s.o.}}^{l}$ and H_{st}^{l} with $\exp(i\mathbf{k}_j^l\cdot\mathbf{r})$ and first-order matrix elements with $H_{\text{s.o.}}^{l}$ and H_{st}^{l}.[15] Matrix elements of $\Delta V^l+m^{-1}\mathbf{k}\cdot\mathbf{p}$ are kept through second order. In essence, we treat ΔV^l and $m^{-1}\mathbf{k}\cdot\mathbf{p}$ as first-order perturbations, $H_{\text{s.o.}}^{l}$ and H_{st}^{l} as second-order perturbations, and compute $H_{dd'}^{l}(\mathbf{k}_j^l)$ through second order. As usual, energy denominators for off-diagonal second-order matrix elements are symmetrized.

For the problem considered here, we wish to calculate the wave vectors normal to the interfaces $k_{\perp j}^{l}$, in each material at fixed values of $\mathbf{k}_{\parallel}$, the projection of the wave vector on the interface plane, and energy ε. (For notational convenience we will use the symbol k_j, without a vector sign, to refer to the normal component of the wave vector and the symbol $\mathbf{k}_j$, with a vector sign, to refer to a three-dimensional wave vector.) For this purpose, it is convenient to display the k dependence of $H_{dd'}^{l}(\mathbf{k}_j^l)$ explicitly. We rewrite Eq. (7) as

$$[H_{dd'}^{2}(k_j^l)^2+H_{dd'}^{1l}(k_j^l)+H_{dd'}^{0l}]C_{d'j}^{l}=0\ , \tag{8}$$

where the matrix H^2 is the same for the two materials. The matrices are given by

$$H_{dd'}^{2}=\frac{\hbar^2}{2m}\delta_{dd'}+\left[\frac{\hbar}{m}\right]^2\sum_{\beta}\left[\frac{\langle U_d\,|p_\perp|\,U_\beta\rangle\langle U_\beta\,|p_\perp|\,U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}\right], \tag{9a}$$

$$\begin{aligned}H_{dd'}^{1l}=&\frac{\hbar}{m}\langle U_d\,|p_\perp|\,U_{d'}\rangle+\frac{\hbar}{m}\sum_{\beta}\left[\frac{\langle U_d\,|p_\perp|\,U_\beta\rangle\langle U_\beta\,|\Delta V^l|\,U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}+\frac{\langle U_d\,|\Delta V^l|\,U_\beta\rangle\langle U_\beta\,|p_\perp|\,U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}\right]\\&+\left[\frac{\hbar}{m}\right]^2\mathbf{k}_{\parallel}\cdot\sum_{\beta}\left[\frac{\langle U_d\,|p_\perp|\,U_\beta\rangle\langle U_\beta\,|\mathbf{p}_{\parallel}|\,U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}+\frac{\langle U_d\,|\mathbf{p}_{\parallel}|\,U_\beta\rangle\langle U_\beta\,|p_\perp|\,U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}\right],\end{aligned} \tag{9b}$$

and

$$\begin{aligned}H_{dd'}^{0l}=&\left[\varepsilon_d+\frac{\hbar^2\mathbf{k}_{\parallel}^2}{2m}-\varepsilon\right]\delta_{dd'}+\langle U_d\,|\,\Delta V^l+H_{\text{s.o.}}^{l}+H_{\text{st}}^{l}\,|\,U_{d'}\rangle+\frac{\hbar\mathbf{k}_{\parallel}}{m}\cdot\langle U_d\,|\,\mathbf{p}_{\parallel}\,|\,U_{d'}\rangle\\&+\sum_{\beta}\left[\frac{\langle U_d\,|\,\Delta V^l\,|\,U_\beta\rangle\langle U_\beta\,|\,\Delta V^l\,|\,U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}\right]\\&+\frac{\hbar\mathbf{k}_{\parallel}}{m}\cdot\sum_{\beta}\left[\frac{\langle U_d\,|\,\mathbf{p}_{\parallel}\,|\,U_\beta\rangle\langle U_\beta\,|\,\Delta V^l\,|\,U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}+\frac{\langle U_d\,|\,\Delta V^l\,|\,U_\beta\rangle\langle U_\beta\,|\,\mathbf{p}_{\parallel}\,|\,U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}\right]\\&+\frac{\hbar\mathbf{k}_{\parallel}}{m}\cdot\sum_{\beta}\left[\frac{\langle U_d\,|\,\mathbf{p}_{\parallel}\,|\,U_\beta\rangle\langle U_\beta\,|\,\mathbf{p}_{\parallel}\,|\,U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}\right]\cdot\frac{\hbar\mathbf{k}_{\parallel}}{m}\ .\end{aligned} \tag{9c}$$

Each of the three H matrices is Hermitian. Explicit evaluation of these matrices is shown in Appendix A.

It is well known that Eq. (8) can be converted into a linear eigenvalue problem for k_j^l if the matrix H^2 is nonsingular.[16] In obvious notation, one has

$$\begin{bmatrix}0 & 1\\ -(H^2)^{-1}H^0 & -(H^2)^{-1}H^1\end{bmatrix}\begin{bmatrix}C\\ kC\end{bmatrix}=k\begin{bmatrix}C\\ kC\end{bmatrix}\ . \tag{10}$$

For the case we consider, the H matrices are 8×8 and thus the non-Hermitian matrix in Eq. (10) is 16×16. Thus there are 16 eigenvalues k for Eq. (10) and 16 corresponding eigenvectors. The eigenvalues may be complex describing evanescent states. We refer to Eq. (10) as describing a 16-band model.

The matrix H^2 is a nonsingular diagonal matrix [see Appendix A, Eq. (A1)]. Four of the matrix elements, which are equal to $M+\hbar^2/2m$, describe the second-order coupling, in the $\mathbf{k}\cdot\mathbf{p}$ interaction, of states which do not couple directly to other explicitly included states. These matrix elements are essential to give the heavy-hole bands downward curvature. Four other matrix elements, two equal to $A'+\hbar^2/2m$ and two equal to $L'+\hbar^2/2m$, describe the second-order coupling, in the $\mathbf{k}\cdot\mathbf{p}$ interaction, of states which do couple directly to other explicitly included states. These matrix elements are not necessary to give the heavy-hole band downward curvature. In essence, they slightly modify the curvature of the electron and light-hole bands at large k. (Typically, they are less than half the size of the $M+\hbar^2/2m$ matrix elements.[17]) Thus, to good approximation, one can neglect the matrix elements $A'+\hbar^2/2m$ and $L'+\hbar^2/2m$ in H^2. For consistency, we "zero" these numbers when they appear in H^0 also.[18] The matrix H^2 now is diagonal with four zero-diagonal elements. In obvious notation, Eq. (8) can be written in blocked form as

$$\left[\begin{bmatrix}h & 0\\ 0 & 0\end{bmatrix}k^2+\begin{bmatrix}a & b\\ b^\dagger & c\end{bmatrix}k+\begin{bmatrix}\alpha & \beta\\ \beta^\dagger & \delta\end{bmatrix}\right]\begin{bmatrix}C^e\\ C^f\end{bmatrix}=0\ . \tag{11}$$

Equation (11) can be converted into a linear eigenvalue problem for k to give

$$\begin{bmatrix} 0 & 1 & 0 \\ -[h^{-1}(\alpha-bc^{-1}\beta^{\dagger})] & -[h^{-1}(a-bc^{-1}b^{\dagger})] & -[h^{-1}(\beta-bc^{-1}\delta)] \\ -c^{-1}\beta^{\dagger} & -c^{-1}b^{\dagger} & -c^{-1}\delta \end{bmatrix} \begin{bmatrix} C^e \\ kC^e \\ C^f \end{bmatrix} = k \begin{bmatrix} C^e \\ kC^e \\ C^f \end{bmatrix} . \tag{12}$$

For the case we consider, the blocks are 4×4, and thus the non-Hermitian matrix in Eq. (12) is 12×12. Thus there are 12 complex eigenvalues k for Eq. (12) and 12 corresponding eigenvectors. We refer to Eq. (12) as describing a 12-band model.

The additional four bands present in the 16-band model and not in the 12-band model describe states which are evanescent at all energies. They have rather large imaginary wave vectors and cannot be considered physically meaningful. These states do not contribute significantly to the description of the superlattice states.[19] The 12-band model provides a good description of the constitutent materials at small k and it is somewhat easier to handle numerically for the description of the superlattice.

In Fig. 1 we show the complex band structure of GaAs computed in the 16-band model. Calculations are done for two values of $\mathbf{k}_{\|}$: $\mathbf{k}_{\|}=0$ and $k_x=2\pi/10a_0$, $k_y=0$. As we will shortly show, if k is an eigenvalue k^*, $-k$ and $-k^*$ are also eigenvalues. In the figure only one of this set of eigenvalues is shown. For $\mathbf{k}$ in a [100] direction (i.e., $\mathbf{k}_{\|}=0$), the energy bands in the zinc-blende structure have a twofold "spin" degeneracy. For $\mathbf{k}$ in an arbitrary direction (i.e., $\mathbf{k}_{\|}\neq 0$), this degeneracy is broken.[20] However, on the energy scale of Fig. 1 the splitting is very small and we have not resolved it in this figure. Therefore each band in Fig. 1 corresponds to a twofold-degenerate pair of states. At a fixed energy there are 16 bands. Four bands are evanescent at all energies with large values of Im(k). At $\mathbf{k}_{\|}=0$, energy extrema occur at $k=0$ and the wave vectors are either pure real or pure imaginary. For the $\mathbf{k}_{\|}\neq 0$ case, the structure is somewhat more complicated. The valence-band extrema occur away from $k=$ and there are complex bands emanating from these extrema.

In Fig. 2 we show the complex band structure of GaAs computed in the 12-band model. The calculations are done for the same two values of $\mathbf{k}_{\|}$ as in Fig. 1. Except for the absence of the four everywhere evanescent states, the bands in the 12-band model are in fairly close agreement with those in the 16-band model.

The eigenvalues k and eigenvector C satisfy Eq. (7) in either model. Thus the eigenvalues k are determined by

$$\det(H^2k^2+H^1k+H^0)=0 . \tag{13}$$

Because the H matrices are Hermitian, if k satisfies Eq. (13) so does k^*. We thus have the important result that complex eigenvalues occur in pairs, k and k^*. That is evanescent states come in growing and decaying pairs with the same real part of k and imaginary parts of k with opposite signs. The right eigenvector associated with k^* is the conjugate of the left eigenvector associated with k. That is, if the row vector L_j satisfies

$$L_j(H^2k_j^2+H^1k_j+H^0)=0 , \tag{14a}$$

then taking the Hermitian adjoint gives

$$[H^2(k_j^*)^2+H^1k_j^*+H^0]L_j^{\dagger}=0 , \tag{14b}$$

and since C_{j^*} satisfies this same equation, to within a phase, one has

$$C_{j^*}=L_j^{\dagger} . \tag{15}$$

If the label j refers to the eigenvalue k_j, the label j^* is taken to refer to the eigenvalue $(k_j)^*$ [i.e., $k_{j^*}\equiv(k_j)^*$].

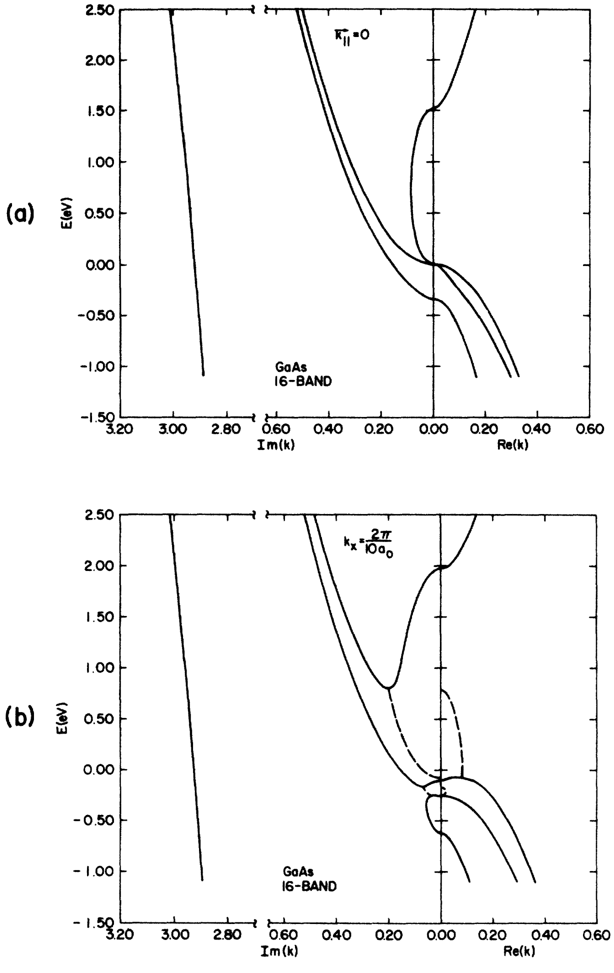
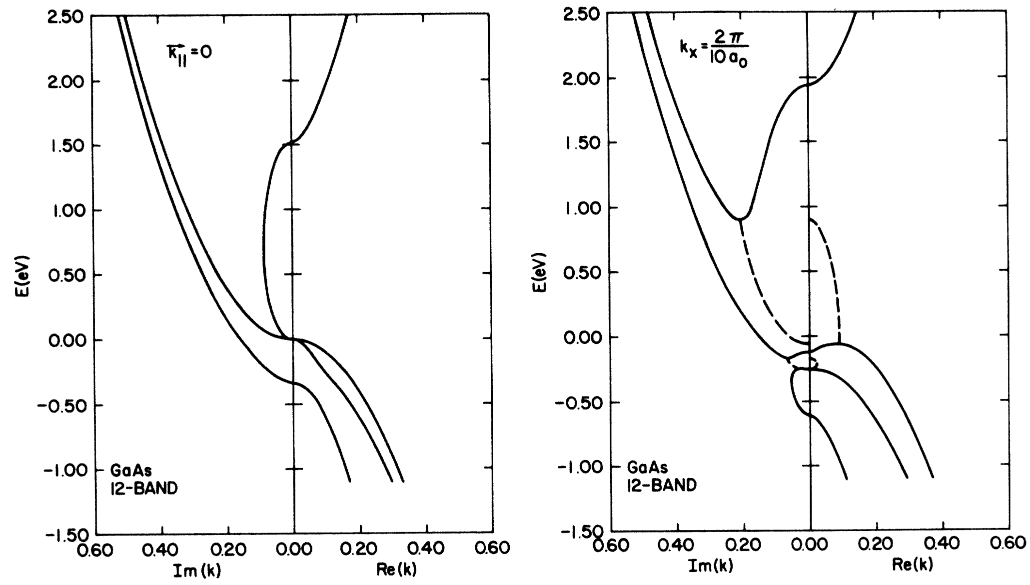


FIG. 1. Complex-k band structure of GaAs computed in the 16-band model. Energy as a function of k is shown for two values of $\mathbf{k}_{\|}$: $\mathbf{k}_{\|}=0$ (top panel) and $k_x=2\pi/10a_0$, $k_y=0$ (bottom panel). At a given energy, the purely real values of k are indicated by a solid line on the right-hand side of the figure and the purely imaginary values of k are indicated by a solid line on the left-hand side of the figure. Complex values of k are indicated by a dashed line, Re(k) on the right- and Im(k) on the left-hand side of the figure. The zero of energy is the valence-band maximum.



(a) (b)

FIG. 2. Complex-k band structure of GaAs computed in the 12-band model. Energy as a function of k is shown for the same values of $\mathbf{k}_{\parallel}$ as in Fig. 1. The curves have the same significance as in Fig. 1.

The fact that if k is an eigenvalue, k^* is also an eigenvalue, follows from the Hamiltonian being Hermitian and not from a spatial symmetry. For zinc-blende heterojunctions with a [100] growth direction (and, of course, also for the bulk material) a twofold rotation about the growth axis is a symmetry operator. Calling this operator R and the time-reversal operator T, it is useful to consider the operator RT. When operating on the plane wave $\exp[i(kz+\mathbf{k}_{\parallel}\cdot\mathbf{r}_{\parallel})]$, this operator gives $\exp[i(-k^*z+\mathbf{k}_{\parallel}\cdot\mathbf{r}_{\parallel})]$. Notice, in particular, that it does not change $\mathbf{k}_{\parallel}$. Let us define the state $U_{\gamma_d}(r)$ by

$$U_{\gamma_d}(r)\equiv(RT)U_d(r)\ . \tag{16}$$

For the case we consider, U_{γ_d} has the same spatial part as U_d, opposite spin, and is multiplied by a phase factor. For the first-order cell-periodic states, one finds

$$(RT)U_{d;k,\mathbf{k}_{\parallel}}=U_{\gamma_d;-k^*,\mathbf{k}_{\parallel}}\ . \tag{17}$$

Using the fact that RT commutes with the Hamiltonian, one finds that

$$\begin{aligned}(H^2_{dd'}k^2+H^{1l}_{dd'}k+H^{0l}_{dd'})\\ =[H^2_{\gamma_d\gamma_{d'}}(-k^*)^2+H^{1l}_{\gamma_d\gamma_{d'}}(-k^*)+H^{0l}_{\gamma_d\gamma_{d'}}]^*\ .\end{aligned} \tag{18}$$

Since the eigenvalues k can be found by setting the determinant of the matrix in Eq. (18) to zero, one sees that if k is an eigenvalue, $-k^*$ must also be an eigenvalue. The eigenvectors associated with the eigenvalues k and $-k^*$ are related by (to within a phase)

$$C_{d;k,\mathbf{k}_{\parallel}}=(C_{\gamma_d;-k^*,\mathbf{k}_{\parallel}})^*\ . \tag{19}$$

Combining with the previous result, we see that if k is an eigenvalue, k^*, $-k^*$, and $-k$ are also eigenvalues.

Orthogonality and completeness relations for the eigenvalue equation are particularly important. The orthogonality condition is found by considering two eigenvalues k_j and k_{i^*}, writing the two eigenvector equations, taking the Hermitian adjoint of the second equation, overlapping each equation with the other's eigenvector, and subtracting. This procedure gives

$$(k_j-k_i)\{\underline{C}^{\dagger}_{i^*}[\underline{H}^2(k_j+k_i)+\underline{H}^1]\underline{C}_j\}=\underline{0}\ . \tag{20}$$

Thus, k_j equals k_i, or else the vector product vanishes. The vector product has a simple physical interpretation. It is the z component of the current-density operator averaged over a unit cell,

$$\begin{aligned}\langle\psi^l_{i^*}\,|\,J_z(r)\,|\,\psi^l_j\rangle_A&\equiv J^l_{i^*j}\\ &=\frac{1}{\hbar\Omega}\underline{C}^{l\dagger}_{i^*}[\underline{H}^2(k^l_j+k^l_i)+\underline{H}^{1l}]\underline{C}^l_j\ ,\end{aligned} \tag{21}$$

where ψ^l_j is given in Eq. (5) and the subscript A implies an average over a unit cell. The orthogonality condition can then be written as

$$J^l_{i^*j}=J^l_{j^*j}\delta_{ij}\ . \tag{22}$$

(Notice the conjugation of the state vectors.)

The orthogonality condition takes the same form in the 16- and 12-band models. The completeness relations take somewhat different forms in the two models. The completeness relations will prove to be important in proving that our treatment of the interface leads to flux conservation and other important results. We will explicitly state the completeness relations in the 16-band model and also prove these results in this model. However, very similar arguments can be used to prove the same results in the 12-band model.

The derivation of the completeness relations proceeds in the usual way. An arbitrary 16-vector is expanded in terms of the eigenvectors of Eq. (10),

$$\begin{bmatrix} S_d \\ (KS)_d \end{bmatrix} = \sum_j B_j \begin{bmatrix} C_{dj} \\ k_j C_{dj} \end{bmatrix} . \tag{23}$$

The orthogonality relation is used to find B_j in terms of the components of the arbitrary vector. The result is substituted back into Eq. (23) and various possibilities for the vector are considered. As a result, one finds that the following relations are satisfied for all d and d'

$$0 = \sum_j \sum_{d_1} \frac{(C_{d_1 j^*})^* H^2_{d_1 d} C_{d'j}}{\Omega \hbar J_{j^* j}} , \tag{24a}$$

$$0 = \sum_j \sum_{d_1} \frac{(C_{d_1 j^*})^* H^1_{d_1 d} C_{d'j}}{\Omega \hbar J_{j^* j}} , \tag{24b}$$

$$0 = \sum_j \sum_{d_1} \frac{k_j^2 (C_{d_1 j^*})^* H^2_{d_1 d} C_{d'j} + k_j (C_{d_1 j^*})^* H^1_{d_1 d} C_{d'j}}{\Omega \hbar J_{j^* j}} , \tag{24c}$$

and

$$\delta_{dd'} = \sum_j \sum_{d_1} \frac{k_j (C_{d_1 j^*})^* H^2_{d_1 d} C_{d'j}}{\Omega \hbar J_{j^* j}} . \tag{24d}$$

Similar results are derived in the 12-band model using the same approach. The results in the 12-band model are somewhat longer to state.

III. INTERFACE DESCRIPTION

In the description of the individual materials making up a superlattice, there is an arbitrary energy zero. When describing an interface between two materials, the energy scales of the two materials must be the same. We include an offset energy between the valence-band maxima of the two materials.[21] We take this energy offset to be given empirically.

We describe the matching between bulk eigenstates of the individual materials to construct eigenstates of the interface using the z (interface normal) component of the current-density operator averaged over a unit cell. In analogy with Eq. (21), we define

$$\langle \psi^l_{i^*} | J_z(t) | \psi^{l'}_j \rangle_A = J^{ll'}_{i^* j} e^{i(k^{l'}_j - k^l_i)t} . \tag{25}$$

In Eq. (25), the interface is taken to include the origin of coordinates. For the interface a distance t from the origin, phase factors enter,

$$\langle \psi^l_{i^*} | J_z(t) | \psi^{l'}_j \rangle_A = J^{ll'}_{i^* j} e^{i(k^{l'}_j - k^l_i)t} \tag{26}$$

From this definition and Eq. (21), we see that

$$J^l_{j^* j'} = (J^l_{j' j^*})^* , \tag{27a}$$

$$J^{ll'}_{j^* j'} = (J^{l'l}_{j' j^*})^* . \tag{27b}$$

We expand an interface eigenstate Ψ with a given energy and $\mathbf{k}_{\parallel}$ in terms of the individual material bulk eigenstates (both Bloch and evanescent) with those values of ε and $\mathbf{k}_{\parallel}$,

$$\Psi(r) = \sum_j A_j \psi_j(r) + \sum_i B_i \phi_i(r) , \tag{28}$$

where A_j and B_i are expansion coefficients and ψ_j (ϕ_i) are the eigenstates in material a (b) at the given values of ε and $\mathbf{k}_{\parallel}$. In Eq. (28), the interface is assumed abrupt so that r is either in material a or b. The notation in Eq. (28) means that the sum on ψ is taken for r in material a and the sum on ϕ is taken for r in material b. We will show that the expansion coefficients A_j and B_i satisfy the relation

$$A_j = \sum_i \frac{1}{J^a_{j^* j}} J^{ab}_{j^* i} B_i , \tag{29}$$

where the interface was taken to contain the origin. This equation, together with boundary conditions to the left and to the right, provide a complete set of equations to describe a single interface.

It is clear that any argument applied to give Eq. (29) could equally well be applied in a different order to give

$$B_i = \sum_j \frac{1}{J^b_{i^* i}} J^{ba}_{i^* j} A_j . \tag{30}$$

For these relations to be consistent, it must be that

$$\sum_i \frac{1}{J^a_{j^* j}} J^{ab}_{j^* i} \frac{1}{J^b_{i^* i}} J^{ba}_{i^* j'} = \delta_{jj'} \tag{31a}$$

and

$$\sum_j \frac{1}{J^b_{i^* i}} J^{ba}_{i^* j} \frac{1}{J^a_{j^* j}} J^{ab}_{j^* i'} = \delta_{ii'} . \tag{31b}$$

These conditions imply flux conservation across the interface. To see this, note that flux conservation requires [see Eqs. (28) and (22)]

$$\sum_j (A_{j^*})^* J^a_{j^* j} A_j = \sum_i (B_{i^*})^* J^b_{i^* i} B_i . \tag{32}$$

Using Eq. (29) to eliminate A_j gives

$$\sum_{i,j} (B_{i^*})^* J^{ba}_{i^* j} \frac{1}{J^a_{j^* j}} J^{ab}_{j^* i} B_i = \sum_i (B_{i^*})^* J^b_{i^* i} B_i . \tag{33}$$

Equation (31b) then establishes the result. Using Eq. (30) to eliminate B_i, then Eq. (31a) will also establish the flux-conservation condition. It is easily seen that the phase factors which appear if the interface does not contain the origin of coordinates do not change the argument. We first show that Eq. (29) is valid and then use the completeness conditions of the single-material eigenvalue problem, Eqs. (24), to establish Eqs. (31).

To establish Eq. (29), we follow an argument presented in Ref. 22. Consider an abrupt interface at the $z=0$ plane. Let $\psi_j(r)$ be an eigenstate with ε and $\mathbf{k}_{\parallel}$ in material a to the left and let $\psi_j(r)$ drop rapidly but smoothly to zero for $z>0$. Likewise, let $\phi_i(r)$ be an eigenstate with ε and $\mathbf{k}_{\parallel}$ in material b on the right and let $\phi_i(r)$ go rapidly but smoothly to zero from $z<0$. Note that boundary conditions to the left and right of the interface are not specified. Expand the interface wave function as in Eq. (28). Let $|\zeta_\alpha\rangle$ be the (unknown) interface eigenstate which is equal to $\psi_\alpha(r)$ in material a. Overlapping the Schrödinger equation with $\langle\zeta_\alpha|$ gives

$$\sum_j \langle\zeta_\alpha|E-\varepsilon|\psi_j\rangle A_j+\sum_i\langle\zeta_\alpha|H-\varepsilon|\phi_i\rangle B_i=0\ . \tag{34}$$

Subtracting $\langle\psi_j^*|H-\varepsilon|\zeta_\alpha^*\rangle$ $(=0)$ from the coefficient of A_j gives

$$\langle\zeta_\alpha|H-\varepsilon|\psi_j\rangle=\frac{-\hbar^2}{2m}\int_S ds\,\hat{\mathbf{n}}\cdot(\zeta_\alpha^*\nabla\psi_j-\psi_j\nabla\zeta_\alpha^*)\ , \tag{35}$$

where S is a surface to the left of $z=0$ and $\hat{\mathbf{n}}$ is a unit outward normal to S. Because $\zeta_\alpha(r)=\psi_\alpha(r)$ for r to the left of the interface, one can replace ζ_α with ψ_α in Eq. (35). Because the surface integral in Eq. (35) has the same value for all surfaces everywhere to the left of the interface, it can be averaged over a unit cell to give

$$\langle\zeta_\alpha|H-\varepsilon|\psi_j\rangle=i\hbar a\langle\psi_\alpha|J_z|\psi_j\rangle_A\ , \tag{36}$$

where a is the area of the surface (z projection) integrated over.

In the same way, by subtracting $\langle\phi_i^*|H-\varepsilon|\zeta_\alpha^*\rangle$ $(=0)$ from the coefficient of B_i, one finds

$$\langle\zeta_\alpha|H-\varepsilon|\phi_i\rangle=\frac{-\hbar^2}{2m}\int_{S'} ds\,\hat{\mathbf{n}}\cdot(\zeta_\alpha^*\nabla\phi_i-\phi_i\nabla\zeta_\alpha^*)\ , \tag{37}$$

where S' is to the right of the interface and $\hat{\mathbf{n}}$ is a unit outward normal to S'. Taking S' to coincide with the interface, ζ_α can be replaced with ψ_α. One can then write

$$\langle\zeta_\alpha|H-\varepsilon|\phi_i\rangle=-i\hbar\int_{z=0} ds\langle\psi_\alpha|J_z(r)|\phi_i\rangle\ . \tag{38}$$

We next coarse-grain-average the current density over a unit cell to give

$$\langle\zeta_\alpha|H-\varepsilon|\phi_i\rangle\simeq-i\hbar a\langle\psi_\alpha|J_z(0)|\phi_j\rangle_A\ . \tag{39}$$

Substituting into Eq. (34), and using the definitions of Eqs. (21) and (25) and the orthogonalization condition of Eq. (22), gives the desired result stated in Eq. (29). This result can also be deduced following the variational argument of Ref. 23.

From Eq. (5), we see that the current-density operators can be written in the form

$$J_{j^*j'}^{ll'}=\sum_{d,d'}(C_{dj^*}^{l})^*C_{d'j'}^{l'}(\langle dk_{j^*}^{l}|J_z|d'k_{j'}^{l'}\rangle_A)\ , \tag{40a}$$

where

$$\langle r\,|dk_j^l\rangle=\frac{e^{i\mathbf{k}_j^l\cdot\mathbf{r}}}{\sqrt{N}}U_{dj}^l(r)\ . \tag{40b}$$

Through first order in the wave functions, we have

$$\begin{aligned}\langle dk_{j^*}^{l}|J_z|d'k_{j'}^{l'}\rangle_A=\frac{1}{\Omega m}\Bigg[&\frac{\hbar(k_j^l+k_{j'}^{l'})}{2}\delta_{dd'}+\langle U_d|p_\perp|U_{d'}\rangle\\&+\sum_\beta\Bigg[\frac{\langle U_d|p_\perp|U_\beta\rangle\langle U_\beta|\Delta V^{l'}+m^{-1}\hbar\mathbf{k}_{j'}^{l'}\cdot\mathbf{p}|U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}\\&+\frac{\langle U_d|\Delta V^{l}+m^{-1}\hbar\mathbf{k}_{j}^{l}\cdot\mathbf{p}|U_\beta\rangle\langle U_\beta|p_\perp|U_{d'}\rangle}{(\varepsilon_d+\varepsilon_{d'})/2-\varepsilon_\beta}\Bigg]\Bigg]\ .\end{aligned} \tag{41}$$

Detailed expressions for these matrices are derived in Appendix B. For the case $l=l'$, the result has already been stated in Eq. (21). For $l\neq l'$, we have

$$\langle dk_{j^*}^{a}|J_z|d'k_i^b\rangle=\frac{1}{\hbar\Omega}[H_{dd'}^2(k_j^a+k_i^b)+H_{dd'}^{1a}-\Delta_{dd'}]=\frac{1}{\hbar\Omega}[H_{dd'}^2(k_j^a+k_i^b)+H_{dd'}^{1b}+(\Delta_{d'd})^*]\ , \tag{42}$$

where $\Delta_{dd'}$ contains only first-order terms in ΔV [see Appendix B, Eqs. (B3)]. The matrix $\langle d'k_i^b|J_z|dk_{j^*}^a\rangle$ is found by taking the conjugate of Eq. (42).

Equations (31) are established by substituting Eq. (42) into those expressions and using the completeness relations for the 16-band model, Eqs. (24). After a straightforward but tedious calculation, one finds that these expressions are correct through first order.[24] That is, they are correct through the order to which the calculation was performed. In the 12-band model, the procedure and results are exactly the same as in the 16-band model. The completeness relations are somewhat more complicated and the calculation more tedious, but Eqs. (31) are also correct through first order (no additional approximations) in the 12-band model.

We next consider the relation of the matching condition expressed by Eqs. (29) and (30) to the smoothness of the state function of the interface. We use Eqs. (4) and (5) to rewrite the interface state function as

$$\Psi=\sum_{j,d}A_jC_{dj}^a\frac{e^{i\mathbf{k}_j^a\cdot\mathbf{r}}}{\sqrt{N}}U_d(r)+\sum_{j,d}\sum_\beta A_jC_{dj}^aW_{d\beta j}^a\frac{e^{i\mathbf{k}_j^a\cdot\mathbf{r}}}{\sqrt{N}}U_\beta(r)+\sum_{i,d}B_iC_{di}^b\frac{e^{i\mathbf{k}_i^b\cdot\mathbf{r}}}{\sqrt{N}}U_d(r)+\sum_{i,d}\sum_\beta B_iC_{di}^bW_{d\beta i}^b\frac{e^{i\mathbf{k}_i^b\cdot\mathbf{r}}}{\sqrt{N}}U_\beta(r)\ , \tag{43}$$

where $W^{l}_{d\beta j}$ is the matrix element in Eq. (4b) and A_j and B_i satisfy Eq. (29). Consider the functions

$$F^a_d(r)=\sum_j A_j C^a_{dj}\frac{e^{i\mathbf{k}^a_j\cdot\mathbf{r}}}{\sqrt{N}}\ , \tag{44a}$$

$$F^b_d(r)=\sum_i B_i C^b_{di}\frac{e^{i\mathbf{k}^b_i\cdot\mathbf{r}}}{\sqrt{N}}\ . \tag{44b}$$

These are "envelope" functions of the explicitly included cell-periodic functions $U_d(r)$. We show that in the 16-band model these functions are continuous and have continuous derivatives to zeroth order in the perturbation expansion.[25] To do this we write the matching condition (29) and substitute Eqs. (40) and (42) for $J^{ab}_{j^*i}$,

$$A_j=\sum_{d,d'}\sum_i\left[\frac{(C^a_{dj^*})^*[H^2_{dd'}(k^a_j+k^b_i)+H^{1a}_{dd'}-\Delta_{dd'}]C^b_{d'i}B_i}{\Omega\hbar J^a_{j^*j}}\right]\ . \tag{45}$$

Now drop $\Delta_{dd'}$ as being of higher order, multiply by $C^a_{d''j}$, and sum over j. Using the completeness relations (24), one finds

$$\sum_j C^a_{d''j}A_j=\sum_i C^b_{d''i}B_i\ . \tag{46}$$

Comparing with Eq. (44) and noting that the parallel components of $\mathbf{k}$ are the same for all cases, we see that Eq. (46) states that the envelope functions of the explicitly included states are continuous to zeroth order in the perturbation theory. In the same way, multiply Eq. (45) ($\Delta_{dd'}$ dropped) by $k^a_j C^a_{d''j}$ and sum over j. Using the completeness relations, one finds

$$\sum_j k^a_j C^a_{d''j}A_j=\sum_i k^b_i C^b_{d''i}B_i\ . \tag{47}$$

Comparing with Eq. (44), one sees that Eq. (47) states that the normal derivative of the explicitly considered states is continuous to zeroth order. In the 12-band model a similar argument shows continuity of the envelope functions to zeroth order, but the argument for continuous derivatives does not go through. Thus, we have seen that the matching condition given in Eq. (29) ensures flux conservation through first order in perturbation theory (the order to which the individual state functions are described) in both the 16- and 12-band models,[24] continuity of the normal derivative of the envelope function of the explicitly considered states to zeroth order in the 16-band model,[25] and continuity of the envelope function of the explicitly considered states to zeroth order in both the 16- and 12-band models.

We have noted previously that the interface problem has a symmetry operator which does not change $\mathbf{k}_{\parallel}$. This operator consists of a twofold rotation about the z axis and time reversal (RT). We have seen that if ψ_j is a single-material eigenstate with normal wave vector k_j, then $(RT)\psi_j$ is also a single-material eigenstate with normal wave vector $-k^*_j$. Let us define the label γ_j by

$$\psi_{\gamma_j}=(RT)\psi_j\ . \tag{48}$$

(ψ_{γ_j} is an eigenstate with the same ε and $\mathbf{k}_{\parallel}$ as ψ_j and has normal wave vector $-k^*_j$.) One then has

$$J^{ll'}_{j^*i}=-(J^{ll'}_{\gamma_{j^*}\gamma_i})^*\ . \tag{49}$$

This symmetry condition is of use in describing superlattice solutions.

IV. SUPERLATTICE EIGENVALUE EQUATION

We label the superlattice cycles $\ldots,-1,0,1,\ldots$ and define the superlattice wave functions as piecewise sums

$$\Psi_\eta(r)=\sum_c[\Psi^\eta_{a,c}(r)+\Psi^\eta_{b,c}(r)]\ , \tag{50a}$$

where η is the superlattice quantum numbers and the notation means that

$$\Psi_\eta(r)=\Psi^\eta_{a,0}(r) \tag{50b}$$

for r in material a and the zeroth superlattice cycle, etc. Because of the superlattice translational symmetry, the superlattice wave function must satisfy

$$\Psi_\eta(r+D)=e^{i\mathbf{Q}_\eta\cdot\mathbf{D}}\Psi_\eta(r)\ , \tag{51}$$

where $\mathbf{D}$ is any superlattice translation vector and $\mathbf{Q}_\eta$ is the superlattice wave vector. For a superlattice of two zinc-blende structure materials grown along the [100] direction and having M_a layers of material a and N_b layers of material b, the primitive superlattice translation vectors are

$$\boldsymbol{\alpha}=\begin{cases}(M_a+N_b)\dfrac{a_0}{2}\hat{\mathbf{z}}, & M_a+N_b=\text{even}\\[2ex](M_a+N_b)\dfrac{a_0}{2}\hat{\mathbf{z}}+\dfrac{a_0}{2}\hat{\mathbf{x}}, & M_a+N_b=\text{odd}\end{cases} \tag{52a}$$

$$\boldsymbol{\beta}=\frac{a_0}{2}(\hat{\mathbf{x}}+\hat{\mathbf{y}})\ , \tag{52b}$$

$$\boldsymbol{\gamma}=\frac{a_0}{2}(\hat{\mathbf{x}}-\hat{\mathbf{y}})\ , \tag{52c}$$

where a_0 is the lattice constant. From Eqs. (51) and (52), we have

$$\Psi^\eta_{a,n}(r+n\alpha)=e^{in\boldsymbol{\alpha}\cdot\mathbf{Q}_\eta}\Psi^\eta_{a,0}(r) \tag{53a}$$

and

$$\Psi^\eta_{b,n}(r+n\alpha)=e^{in\boldsymbol{\alpha}\cdot\mathbf{Q}_\eta}\Psi^\eta_{b,0}(r)\ . \tag{53b}$$

We now expand $\Psi_{a,n}(r)$ and $\Psi_{b,n}(r)$ in terms of the eigenstates of the individual materials with a given energy ε and parallel wave-vector component $\mathbf{k}_{\parallel}$,

$$\Psi^{\eta}_{a,n}(r)=\sum_{j} A^{n}_{j;\eta}\psi_j(r)\ , \tag{54a}$$

$$\Psi^{\eta}_{b,n}(r)=\sum_{i} B^{n}_{i;\eta}\phi_i(r)\ . \tag{54b}$$

By the symmetry property of Eqs. (53),

$$A^{n}_{j;\eta}=A_{j;\eta}e^{i(\mathbf{Q}_{\eta}-\mathbf{k}^{a}_{j})\cdot\mathbf{a}n} \tag{55a}$$

and

$$B^{n}_{i;\eta}=B_{i;\eta}e^{i(\mathbf{Q}_{\eta}-\mathbf{k}^{b}_{i})\cdot\mathbf{a}n}\ . \tag{55b}$$

The interface-matching condition applied to the $(a,n;b,n)$ interface[26] requires

$$A^{n}_{j;\eta}e^{i\mathbf{k}^{a}_{j}\cdot\mathbf{a}n}=\sum_{i}\frac{J^{ab}_{j^{*}i}}{J^{a}_{j^{*}j}}B^{n}_{i,\eta}e^{i\mathbf{k}^{b}_{i}\cdot\mathbf{a}n}\ . \tag{56}$$

Using Eqs. (55), all these conditions are satisfied if

$$A_{j,\eta}=\sum_{i}\frac{J^{ab}_{j^{*}i}}{J^{a}_{j^{*}j}}B_{i,\eta}\ . \tag{57}$$

In the same way, the interface-matching condition is applied to the $(b,n;a,n+1)$ interface to give

$$A^{n+1}_{j;\eta}(e^{i\mathbf{k}^{a}_{j}\cdot\mathbf{a}n}e^{ik^{a}_{j}b})=\sum_{i}\frac{J^{ab}_{j^{*}i}}{J^{a}_{j^{*}j}}B^{n}_{i;\eta}(e^{i\mathbf{k}^{b}_{i}\cdot\mathbf{a}n}e^{ik^{b}_{i}b})\ , \tag{58}$$

where b is the layer thickness of material b. Substituting the symmetry condition of Eqs. (55), all these equations are satisfied if

$$A_{j;\eta}(e^{i\mathbf{Q}_{\eta}\cdot\mathbf{a}}e^{-ik^{a}_{j}a}e^{-i\mathbf{k}^{a}_{j}\cdot\mathbf{a}_{\parallel}})=\sum_{i}\frac{J^{ab}_{j^{*}i}}{J^{a}_{j^{*}j}}B_{i;\eta}e^{ik^{b}_{i}b}\ , \tag{59}$$

where a is the layer thickness of material a. Since $\mathbf{Q}_{\eta}$ and $\mathbf{k}^{a}_{j}$ (all j) have the same parallel component, we have

$$A_{j;\eta}e^{iQ_{\eta}(a+b)}e^{-ik^{a}_{j}a}=\sum_{i}\frac{J^{ab}_{j^{*}i}}{J^{a}_{j^{*}j}}B_{i;\eta}e^{ik^{b}_{i}b}\ . \tag{60}$$

Equations (57) and (60) are our basic result. They can be converted to an eigenvalue equation by eliminating $B_{j;\eta}$ in Eq. (60),

$$\sum_{j'}M_{jj'}A_{j';\eta}=e^{iQ_{\eta}(a+b)}A_{jn}\ , \tag{61a}$$

$$M_{jj'}=\sum_{i}e^{ik^{a}_{j}a}\frac{1}{J^{a}_{j^{*}j}}J^{ab}_{j^{*}i}e^{ik^{b}_{i}b}\frac{1}{J^{b}_{i^{*}i}}J^{ba}_{i^{*}j'}\ . \tag{61b}$$

The eigenvalue equation Eqs. (61) is solved for the eigenvalue $\exp[iQ_{\eta}(a+b)]$ and the eigenvector $A_{j;\eta}$. The expansion coefficients in material b are then found from Eq. (57). Clearly, an equivalent result can be obtained by eliminating $A_{j;\eta}$.

We consider some features of this eigenvalue equation. It is useful to define an adjoint operator (denoted by superscript tilde, or overtilde) by

$$[\tilde{A}]_{jj'}=(A_{(j')^{*}j^{*}})^{*}\ . \tag{62}$$

This operator is similar to the usual Hermitian adjoint, except each evanescent state is interchanged with its conjugate state. It is easy to verify that

$$([\tilde{A}])^{\sim}=A\ , \tag{63a}$$

$$(A+B)^{\sim}=\tilde{A}+\tilde{B}\ , \tag{63b}$$

$$(AB)^{\sim}=\tilde{B}\ \tilde{A}\ , \tag{63c}$$

$$(cA)^{\sim}=C^{*}\tilde{A}\ , \tag{63d}$$

where c is a scalar. We also define the diagonal matrix

$$J_{jj'}=J^{a}_{j^{*}j'}\ . \tag{64a}$$

It is easy to verify

$$\tilde{J}=J\ . \tag{64b}$$

Using Eq. (31), one finds

$$M^{-1}=J^{-1}\tilde{M}J\ , \tag{65}$$

where M is given by Eq. (61b). Let Q_{η} and $A_{j;\eta}$ satisfy Eq. (61a) and let $L_{j\eta}$ be the left eigenvector associated with Q_{η}; that is, $L_{j\eta}$ solves

$$L_{j\eta}M_{jj'}=e^{iQ_{\eta}(a+b)}L_{j'\eta}\ . \tag{66}$$

Taking the adjoint operator of this equation and using Eq. (65) gives

$$M_{jj'}\left[\frac{1}{J_{j'j'}}\tilde{L}_{\eta j'}\right]=e^{iQ^{*}_{\eta}(a+b)}\left[\frac{1}{J_{jj}}\tilde{L}_{\eta j}\right]\ . \tag{67}$$

If Q_{η} is a solution to the eigenvalue equation with right and left eigenvectors A_{η} and $L_{\eta'}$, then Q^{*}_{η} is also a solution with right and left eigenvectors,[27]

$$\left[\frac{1}{J}\tilde{L}_{\eta}\right]\ \text{and}\ (\tilde{A}_{\eta}J)\ .$$

Using this result, the orthogonality and completeness relations for the eigenvalue equation are found in the usual way

$$\sum_{j}\left[\frac{(A_{j^{*}(Q')^{*}})^{*}J^{a}_{j^{*}j}A_{jQ}}{\sum_{j}(A_{j^{*}Q^{*}})^{*}J^{a}_{j^{*}j}A_{jQ}}\right]=\delta_{QQ'}\ , \tag{68a}$$

$$\sum_{Q}\left[\frac{(A_{j^{*}Q^{*}})^{*}J^{a}_{j^{*}j}A_{j'Q}}{\sum_{j}(A_{j^{*}Q^{*}})^{*}J^{a}_{j^{*}j}A_{jQ}}\right]=\delta_{jj'}\ . \tag{68b}$$

The analogous relations for B and J^{b} are also valid, as is easily verified by using Eq. (57) to eliminate A in terms of B and then using Eqs. (31).

The inverse relation Eq. (65) can be used to cast the eigenvalue equation into an equivalent form which can be more convenient numerically. Taking the inverse of Eq. (61a) and using Eq. (65) gives

$$\left[\frac{M+J^{-1}\tilde{M}J}{2}\right]_{jj'}A_{j',\eta}=\cos[Q_{\eta}(a+b)]A_{j,\eta}\ , \tag{69a}$$

$$\left[\frac{M-J^{-1}\tilde{M}J}{2i}\right]_{jj'}A_{j',\eta}=\sin[Q_\eta(a+b)]A_{j,\eta}\ . \tag{69b}$$

For the particular case of [100] growth of zinc-blende materials, the symmetry operator (RT) also implies conditions on the values of Q_η. From Eq. (49), we see that

$$M_{jj'}=(M_{\gamma_j;\gamma_{j'}})^*\ , \tag{70}$$

so that the eigenvalue equation can be written as

$$M_{jj'}A_{\gamma_{j'}\eta}=e^{-iQ_\eta^*(a+b)}A^*_{\gamma_j\eta}\ . \tag{71}$$

Thus, if Q_η is a solution with eigenvector $A_{j\eta}$, $-Q_\eta^*$ is a solution with eigenvector $(A_{\gamma_j\eta})^*$. Combining with a previous result, we see that if Q_η is a solution Q_η^*, $-Q_\eta^*$ and $-Q_\eta$ are also solutions.

The normalization conditions on the expansion coefficients A and B are derived in Appendix C. Here we state the result as

$$\begin{aligned}\int \Psi_\eta^*\Psi_\eta d^3r&=1\\ &=\sum_{j^*,j'}(A_{j^*\eta})^*N^a_{j^*j'}A_{j'\eta}\\ &\quad+\sum_{i^*,i'}(B_{i^*\eta})^*N^b_{i^*i'}B_{i'\eta}\ ,\end{aligned} \tag{72a}$$

where

$$N^a_{j^*j'}=\sum_{d,d'}(C^a_{dj^*})^*P^a_{dd'}(k^a_j,k^a_{j'})C^a_{d'j'}\ , \tag{72b}$$

$$N^b_{i^*i'}=\sum_{d,d'}(C^b_{di^*})^*P^b_{dd'}(k^b_i,k^b_{i'})C^b_{d'i'}\ , \tag{72c}$$

and P are spin-diagonal matrices given by

$$\begin{aligned}P^a_{dd'}(k^a_j,k^a_{j'})&=\frac{-i}{a+b}\left[\frac{1-e^{-i(k^a_{j'}-k^a_j)a}}{k^a_{j'}-k^a_j}\right]\\ &\quad\times[\delta_{dd'}+(k^a_{j'}-k^a_j)S_{dd'}]\ ,\end{aligned} \tag{73a}$$

$$\begin{aligned}P^b_{dd'}(k^b_i,k^b_{i'})&=\frac{-i}{a+b}\left[\frac{e^{i(k^b_{i'}-k^b_i)b}-1}{k^b_{i'}-k^b_i}\right]\\ &\quad\times[\delta_{dd'}+(k^b_{i'}-k^b_i)S_{dd'}]\ .\end{aligned} \tag{73b}$$

Here, $S_{dd'}$ is given by

$$S_{dd'}=\sum_{\mathbf{G},\mathbf{G}'}\frac{R^*_{dG}R_{d'G'}}{G'_\perp-G_\perp}\delta_{\mathbf{G}^*_\parallel\mathbf{G}_\parallel}(1-\delta_{G'_\perp G_\perp})\ . \tag{73c}$$

The P matrices satisfy the condition

$$P_{dd'}(k_j,k_{j'})=[P_{d'd}(k^*_{j'},k^*_j)]^*\ , \tag{74}$$

which ensures that the normalization integral is real.

We have considered a superlattice consisting of alternating layers of two materials. The approach here can equally well describe superlattices in which the repeat cycle consists of more than two layers. In Appendix D we briefly describe this case.

V. SYNOPSIS

We have presented a theory of the electronic structure of semiconductor superlattices based on the $\mathbf{k}\cdot\mathbf{p}$ formalism. An empirical pseudopotential calculation, using averaged pseudopotential form factors for the constituent materials, is performed to provide a basis set for the zone-center Bloch states. Including spin, eight zone-center Bloch states are treated explicitly and a larger number (46, as actually implemented) are included in Löwdin perturbation theory.[12] The perturbation interaction is the $m^{-1}\mathbf{k}\cdot\mathbf{p}$ operator and ΔV the difference between the given material and the averaged pseudopotential. Perturbation theory is done to first order for wave functions and to second order for energies. The spin-orbit interaction and stress interaction, due to possible lattice mismatch, are taken between the explicitly included states. Using this description of the individual materials, Bloch and evanescent states are found by solving a non-Hermitian eigenvalue problem. Two forms of the theory are considered: a 16-band model and a 12-band model. The additional four bands which appear in the 16-band model are evanescent at all energies and have very large imaginary wave vectors.

States in the two materials are joined at the interfaces using results derived about the normal component of the current-density operator. This interface description ensures flux conservation through the order in perturbation theory at which wave functions are calculated in both 16- and 12-band models.[24] The envelope functions of the explicitly included zone-center states are continuous to zeroth order in the perturbation for both 16- and 12-band models,[25] and the normal derivative is continuous to zeroth order in the perturbation in the 16-band model.[25]

The superlattice translational symmetry is used to derive an eigenvalue equation for the superlattice-normal wave-vector component and wave function. A result concerning the possible values of the superlattice-normal wave-vector component is used to cast the eigenvalue equation into a computationally simpler form. The final form of the theory consists of a non-Hermitian 12×12 (or 16×16) eigenvalue equation for the normal component of the superlattice wave vector for fixed energy and the parallel component of superlattice wave vector. The superlattice wave function is determined in terms of spatially varying functions, multiplying the zone-center functions determined by the pseudopotential calculation.

In this paper we have presented the formal results of our theory. In the following paper,[10] the numerical implementation of these results are described.

Note added in proof. One can show the terms proportional to $S_{dd'}$ vanish in the normalization integral when the sums on j^* and j' (i^* and i') are performed.

ACKNOWLEDGMENTS

The authors thank T. C. McGill for valuable discussions in the early stages of this work. The work of one of us (D.L.S.) has been financially supported by the U.S. Defense Advanced Research Projects Agency and Los

Alamos National Laboratory Internal Supporting Research.

APPENDIX A: EVALUATION OF THE HAMILTONIAN MATRICES

In this appendix we present the explicit form of the matrices $H^2_{dd'}$, $H^{ll}_{dd'}$, and $H^{0l}_{dd'}$ defined in Eqs. (9). We consider the case of zinc-blende semiconductors with k in the z direction and $\mathbf{k}_{\parallel}$ in the (x,y) plane. Spins are quantized in the z direction.

We first note that except for the contribution of $H^l_{\text{s.o.}}$ to H^{0l}, the matrices are spin diagonal and independent. We label the eight basis states by $|S\rangle, |X\rangle, |Y\rangle, |Z\rangle$ combined with a spinor $\uparrow$ and $\downarrow$, where $|S\rangle$ corresponds to the Γ_1 conduction-band spatial state and $|X\rangle, |Y\rangle, |Z\rangle$ to the three components of the Γ_{15} valence-band spatial state.

The general form for the matrices are given in Eq. (9), the matrix H^2 is spin diagonal and independent. The nonzero matrix elements, in obvious notation, are

$$(S\,|\,S)=A'+\frac{\hbar^2}{2m}\;, \tag{A1a}$$

$$(X\,|\,X)=(Y\,|\,Y)=M+\frac{\hbar^2}{2m}\;, \tag{A1b}$$

$$(Z\,|\,Z)=L'+\frac{\hbar^2}{2m}\;, \tag{A1c}$$

where[28]

$$A'=\left[\frac{\hbar}{m}\right]^2\sum_{j\in\Gamma_{15}}\frac{|\langle S\,|P_z|\,U_j\rangle|^2}{\varepsilon_c-\varepsilon_j}\;, \tag{A1d}$$

$$M=H_1+H_2\;, \tag{A1e}$$

$$H_1=\left[\frac{\hbar}{m}\right]^2\sum_{j\in\Gamma_{15}}\frac{|\langle X\,|P_y|\,U_j\rangle|^2}{\varepsilon_v-\varepsilon_j}\;, \tag{A1f}$$

$$H_2=\left[\frac{\hbar}{m}\right]^2\sum_{j\in\Gamma_{25}}\frac{|\langle X\,|P_y|\,U_j\rangle|^2}{\varepsilon_v-\varepsilon_j}\;, \tag{A1g}$$

$$L'=F'+2G\;, \tag{A1h}$$

$$G=\frac{1}{2}\left[\frac{\hbar}{m}\right]^2\sum_{j\in\Gamma_{12}}\frac{|\langle z\,|P_z|\,U_j\rangle|^2}{\varepsilon_v-\varepsilon_j}\;, \tag{A1i}$$

and

$$F'=\left[\frac{\hbar}{m}\right]^2\sum_{j\in\Gamma_{1}}\frac{|\langle z\,|P_z|\,U_j\rangle|^2}{\varepsilon_v-\varepsilon_j}\;. \tag{A1j}$$

The explicitly treated states are not included in the sums on states which appear. The zone-center eigenstates and eigenvalues of the reference pseudopotential Hamiltonian are used to calculate the constants which appear in H^2. Note that H^2 is the same for each material.

The matrices H^{ll} are also spin diagonal and independent. The nonzero matrix elements are

$$(S\,|\,X)=(X\,|\,S)=Bk_y\;, \tag{A2a}$$

$$(S\,|\,Y)=(Y\,|\,S)=Bk_x\;, \tag{A2b}$$

$$(S\,|\,Z)=-(Z\,|\,S)=iP^l\;, \tag{A2c}$$

$$(X\,|\,Z)=(Z\,|\,X)=N'k_x\;, \tag{A2d}$$

$$(Y\,|\,Z)=(Z\,|\,Y)=N'k_y\;, \tag{A2e}$$

where[28]

$$N'=F'-G+H_1-H_2 \tag{A2f}$$

and

$$B=2\left[\frac{\hbar}{m}\right]^2\sum_{j\in\Gamma_{15}}\left[\frac{\langle S\,|P_x|\,U_j\rangle\langle U_j\,|P_y|\,Z\rangle}{(\varepsilon_c+\varepsilon_v)/2-\varepsilon_j}\right]. \tag{A2g}$$

The results for the various materials differ by the value of the constant P^l, which is given by

$$P^l=P+\Delta P^l\;, \tag{A3a}$$

where

$$P=\left[\frac{-i\hbar}{m}\right]\langle S\,|P_z|\,Z\rangle\;, \tag{A3b}$$

$$\Delta P^l=\left[\frac{-i\hbar}{m}\right]\left[\sum_{j\in\Gamma_{15}}\left[\frac{\langle S\,|P_z|\,U_j\rangle\langle U_j\,|\Delta V^l|\,Z\rangle}{(\varepsilon_c+\varepsilon_v)/2-\varepsilon_j}\right]+\sum_{j\in\Gamma_1}\left[\frac{\langle S\,|\Delta V^l|\,U_j\rangle\langle U_j\,|P_z|\,Z\rangle}{(\varepsilon_c+\varepsilon_v)/2-\varepsilon_j}\right]\right]. \tag{A3c}$$

It is convenient to write H^{0l} as the sum of three terms

$$H^{0l}=H^{0l}_{\text{s.o.}}+H^{0l}_{\text{st}}+H^{0l}_{R}\;, \tag{A4}$$

where $H^{0l}_{\text{s.o.}}$ is the spin-orbit contribution, H^{0l}_{st} is the stress contribution,, and H^{0l}_{R} are the other contributions. The form of $H^{0l}_{\text{s.o.}}$ is well known,[28] the nonzero matrix elements are

$$(X\uparrow|\,Z\downarrow)=-(Z\uparrow|\,X\downarrow)=-(X\downarrow|\,Z\uparrow)=(Z\downarrow|\,X\uparrow)=\frac{\Delta^l}{3}\;, \tag{A5a}$$

and

$$\begin{aligned}(Z\uparrow|\,Y\downarrow)&=-(Y\uparrow|\,Z\downarrow)=(Z\downarrow|\,Y\uparrow)\\&=-(Y\downarrow|\,Z\uparrow)=(Y\uparrow|\,Z\uparrow)\\&=-(X\uparrow|\,Y\uparrow)=-(Y\downarrow|\,X\downarrow)\\&=(X\downarrow|\,Y\downarrow)=\frac{i\Delta^l}{3}\;,\end{aligned} \tag{A5b}$$

where Δ^l is the spin-orbit—interaction parameter in material l, which we determine empirically.

For a superlattice made of two zinc-blende-structure materials, and a [100] growth axis, only diagonal strain components are introduced (i.e., $\varepsilon_{xy}=0$, etc.) by lattice mismatch. The diagonal components are[29]

$$\varepsilon^l_{zz}=-\left[\frac{2C^l_{12}}{C^l_{11}}\right]\varepsilon^l_{xx}\;, \tag{A6a}$$

$$\varepsilon_{xx}^a=\varepsilon_{yy}^a=\frac{-\Delta a_0}{a_0}\left[\frac{G^b b}{G^a a+G^b b}\right], \tag{A6b}$$

$$\varepsilon_{xx}^b=\varepsilon_{yy}^b=\frac{\Delta a_0}{a_0}\left[\frac{G^a a}{G^a a+G^b b}\right], \tag{A6c}$$

where

$$\Delta a_0=a_0^a-a_0^b\,, \tag{A6d}$$

$$a_0=\frac{a_0^a+a_0^b}{2}\,, \tag{A6e}$$

$$G^l=2\left[C_{11}^l+C_{12}^l-\frac{2(C_{12}^l)^2}{C_{11}^l}\right], \tag{A6f}$$

and a_0 refers to a lattice constant and the C's are the elastic constants. We neglect the spin dependence of the stress interaction as small. Then, $H_{\rm st}^{0l}$ is spin diagonal and independent with nonzero matrix elements,[30]

$$(S\,|\,S)=c^l(2\varepsilon_{xx}^l+\varepsilon_{zz}^l)\,, \tag{A7a}$$

$$(X\,|\,X)=(Y\,|\,Y)=(l^l+m^l)\varepsilon_{xx}^l+m^l\varepsilon_{zz}^l\,, \tag{A7b}$$

$$(Z\,|\,Z)=2m^l\varepsilon_{xx}^l+l^l\varepsilon_{zz}^l\,, \tag{A7c}$$

where c, l, and m are deformation-potential constants. We determine the deformation-potential constants and the elastic constants empirically.

The matrix H_R^{0l} is spin diagonal and independent; its nonzero matrix elements are

$$(S\,|\,S)=(\varepsilon_c+\Delta\varepsilon_c^l-\varepsilon)+\left[A'+\frac{\hbar^2}{2m}\right]k_\parallel^2\,, \tag{A8a}$$

$$(X\,|\,X)=(\varepsilon_v+\Delta\varepsilon_v^l-\varepsilon)+L'k_x^2+Mk_y^2+\frac{\hbar^2}{2m}k_\parallel^2\,, \tag{A8b}$$

$$(Y\,|\,Y)=(\varepsilon_v+\Delta\varepsilon_v^l-\varepsilon)+L'k_y^2+Mk_x^2+\frac{\hbar^2}{2m}k_\parallel^2\,, \tag{A8c}$$

$$(Z\,|\,Z)=(\varepsilon_v+\Delta\varepsilon_v^l-\varepsilon)+\left[M+\frac{\hbar^2}{2m}\right]k_\parallel^2\,, \tag{A8d}$$

$$(S\,|\,X)=-(X\,|\,S)=iP^lk_x\,, \tag{A8e}$$

$$(S\,|\,Y)=-(Y\,|\,S)=iP^lk_y\,, \tag{A8f}$$

$$(S\,|\,Z)=(Z\,|\,S)=Bk_xk_y\,, \tag{A8g}$$

$$(X\,|\,Y)=(Y\,|\,X)=N'k_xk_y\,, \tag{A8h}$$

where

$$\Delta\varepsilon_c^l=\langle S\,|\,\Delta V^l\,|\,S\rangle+\sum_{j\in\Gamma_1}\frac{|\langle S\,|\,\Delta V^l\,|\,U_j\rangle|^2}{\varepsilon_c-\varepsilon_j}\,, \tag{A8i}$$

$$\Delta\varepsilon_v^l=\langle X\,|\,\Delta V^l\,|\,X\rangle+\sum_{j\in\Gamma_{15}}\frac{|\langle X\,|\,\Delta V^l\,|\,U_j\rangle|^2}{\varepsilon_v-\varepsilon_j}\,. \tag{A8j}$$

APPENDIX B: EVALUATION OF THE CURRENT-DENSITY MATRICES

In this appendix we present explicit forms for the current density matrices

$$\langle dk_{j*}^l\,|\,J_z\,|\,d'k_{j'}^{l'}\rangle_A\,.$$

These matrices are spin diagonal and independent. The general form is given in Eq. (41). For the case $l=l'$, a straightforward calculation shows

$$\langle dk_{j*}^l\,|\,J_z\,|\,d'k_{j'}^l\rangle=\frac{1}{\Omega\hbar}[H_{dd'}^2(k_j^l+k_{j'}^l)+H_{dd'}^{1l}]\,. \tag{B1}$$

For the case $l\neq l'$, we find

$$\begin{aligned}\langle dk_{j*}^a\,|\,J_z\,|\,d'k_i^b\rangle&=\frac{1}{\Omega\hbar}[H_{dd'}^2(k_j^a+k_i^b)+H_{dd'}^{1a}-\Delta_{dd'}]\\&=\frac{1}{\Omega\hbar}[H_{dd'}^2(k_j^a+k_i^b)+H_{dd'}^{1b}+\Delta_{d'd}^*]\,,\end{aligned} \tag{B2}$$

where $\Delta_{dd'}$ is a non-Hermitian spin-diagonal and independent matrix. The nonzero matrix elements of $\Delta_{dd'}$ are

$$(S\,|\,Z)=i\left[\frac{-i\hbar}{m}\right]\left[2\sum_{j\in\Gamma_{15}}\frac{\langle S\,|\,P_z\,|\,U_j\rangle\langle U_j\,|\,\Delta V^a\,|\,Z\rangle}{(\varepsilon_c+\varepsilon_v)/2-\varepsilon_j}\right], \tag{B3a}$$

$$\begin{aligned}(Z\,|\,S)=&-i\left[\frac{-i\hbar}{m}\right]\\&\times\left[2\sum_{j\in\Gamma_1}\frac{\langle S\,|\,\Delta V^a\,|\,U_j\rangle\langle U_j\,|\,P_z\,|\,Z\rangle}{(\varepsilon_c+\varepsilon_v)/2-\varepsilon_j}\right],\end{aligned} \tag{B3b}$$

$$\begin{aligned}(X\,|\,Y)&=(Y\,|\,X)\\&=-i\left[\frac{-i\hbar}{m}\right]\\&\quad\times\left[2\sum_{j\in\Gamma_{15}}\frac{\langle X\,|\,\Delta V^a\,|\,U_j\rangle\langle U_j\,|\,P_z\,|\,Y\rangle}{\varepsilon_v-\varepsilon_j}\right],\end{aligned} \tag{B3c}$$

where we have used $\Delta V^a=-\Delta V^b$.

APPENDIX C: WAVE-FUNCTION NORMALIZATION

In this appendix we evaluate the superlattice wave-function normalization integral

$$\int\Psi_\eta^*\Psi_\eta d^3r$$

for the case that Q_η is real (i.e., for superlattice Bloch states). Substituting the expanded form of the superlattice wave function as given by Eqs. (54), (50), and (5) into the normalization integral, we immediately find that it is given by Eqs. (72), where

$$\begin{aligned}P_{dd'}^a(k_j^a,k_{j'}^a)=&\frac{1}{N_b+M_a}\\&\times\int_{\omega^a}d^3r[e^{i(\mathbf{k}_{j'}^a-\mathbf{k}_j^a)\cdot\mathbf{r}}(U_{dj*}^a)^*(U_{d'j'}^a)]\,,\end{aligned} \tag{C1a}$$

$$P_{dd'}(k_i^b,k_{i'}^b)=\frac{1}{N_b+M_a}\times\int_{\omega^b}d^3r[e^{i(\mathbf{k}_{i'}^b-\mathbf{k}_i^b)\cdot\mathbf{r}}(U^b_{di*})^*(U^b_{d'i'})]\ , \quad \text{(C1b)}$$

where the ω^a and ω^b are the regions in material a and b of the superlattice unit cell, respectively. A spin overlap is assumed in Eqs. (C1), so the P matrices are spin diagonal and independent.

We consider explicitly the matrix P^a; the matrix P^b is evaluated in an analogous way. The periodic part of the Bloch functions are written to first order as in Eqs. (4) and zone-center basis functions are expanded in plane waves as in Eq. (2) to give (to first order)

$$P^a_{dd'}(k_j^a,k_{j'}^a)=\left[\frac{1}{N_b+M_a}\right]\frac{1}{\Omega}\int_{\omega^a}d^3r\sum_{\mathbf{G},\mathbf{G}'}e^{i(\mathbf{k}_{j'}^a-\mathbf{k}_j^a+\mathbf{G}'-\mathbf{G})\cdot\mathbf{r}}\left[R^*_{d\mathbf{G}}R_{d\mathbf{G}'}+\sum_{\beta}(R^*_{d\mathbf{G}}R_{\beta\mathbf{G}'}W^a_{d'\beta j'}+R^*_{\beta\mathbf{G}}R_{d'\mathbf{G}'}W^a_{b\beta j})\right]. \quad \text{(C2)}$$

Evaluation of the integral gives

$$\frac{1}{\Omega(N_b+M_a)}\int_{\omega^a}e^{i(\mathbf{k}_{j'}^a-\mathbf{k}_j^a+\mathbf{G}'-\mathbf{G})\cdot\mathbf{r}}d^3r=\left[\frac{-i}{a+b}\right]\delta_{\mathbf{G}'_{\parallel};\mathbf{G}_{\parallel}}\frac{1-e^{-i(k_{j'}^a-k_j^a)a}}{(k_{j'}^a-k_j^a)+(G'_{\perp}-G_{\perp})}\ . \quad \text{(C3)}$$

For $G'_{\perp}\neq G_{\perp}$, $G'_{\perp}-G_{\perp}\gg k_{j'}^a-k_j^a$ and the denominator of Eq. (C3) is expanded to first order. This expansion is consistent with the first-order calculation in the $m^{-1}\mathbf{k}\cdot\mathbf{p}$ operator. Keeping terms to first order and noting the orthogonality of the periodic basis functions gives Eq. (73a). The result for P^b follows in exactly the same way, only the integration range is different.

APPENDIX D: MULTILAYER SUPERLATTICES

The formal structure presented here can be used to describe superlattices whose repeat cycle consists of more than two material layers. Let the superlattice wave function be written as

$$\Psi_\eta=\sum_l(\Psi^\eta_{1;l}+\Psi^\eta_{2;l}+\cdots+\Psi^\eta_{r;l})\ , \quad \text{(D1)}$$

where l labels the repeat cycle and the first subscript labels the layer in the cycle. The piecewise functions are expanded as

$$\Psi^\eta_{p,l}=\sum_{j_p}A^{p,l}_{j_p;\eta}\psi^p_{j_p}(r)\ , \quad \text{(D2)}$$

where j_p labels the Bloch and evanescent states with fixed ε and $\mathbf{k}_{\parallel}$ in material p. By the superlattice symmetry,

$$A^{p,l}_{j_p;\eta}=A^p_{j_p;\eta}e^{i(\mathbf{Q}_\eta-\mathbf{k}^p_{j_p})\cdot l\boldsymbol{\alpha}}\ , \quad \text{(D3)}$$

where $\boldsymbol{\alpha}$ is the superlattice translation vector which translates one repeat cycle.

To be consistent with the treatment in the text, we take the origin of coordinates to lie on the (1,0;2,0) interface. Applying the interface-matching condition [Eq. (29)] at the $(i,l;i+1,l)$ $(1\leq i\leq r-1)$ interfaces gives

$$A^{i+1}_{j\eta}=\sum_{j'}\frac{J^{i+1,i}_{j*j'}}{J^{i+1}_{j*j}}e^{-i(k_j^{i+1}-k_{j'}^i)d_i}A^i_{j'\eta}\ , \quad \text{(D4)}$$

where d_i is the normal distance between the origin and the $(i,0;i+1,0)$ interface. Applying the interface-matching condition at the $(r,l-1;1,l)$ interfaces gives

$$A^1_{j\eta}e^{iQ_\eta d}=\sum_{j'}\frac{J^{1,r}_{j*j'}}{J^1_{j*j}}e^{ik_j^1a_1}e^{ik^r_{j'}(d-a_1)}A^r_{j'}\ , \quad \text{(D5)}$$

where d is the thickness of the repeat cycle and a_i is the thickness of the ith layer (i.e., $\sum_{i=1}^r a_i=d$ and $\sum_{i=2}^l a_i=d_l$). These equations can be combined to form an eigenvalue equation,

$$A^1_{j\eta}e^{iQ_\eta d}=\sum_{j'}\left[\sum_{l,l',\ldots,l''}e^{ik_j^1a_1}\frac{J^{1,r}_{j*l}}{J^1_{j*j}}e^{ik_l^ra_r}\frac{J^{r,r-1}_{l*l'}}{J^r_{l*l}}\times\cdots\times e^{ik^2_{l''}a_2}\frac{J^{2,1}_{(l'')*j'}}{J^2_{(l'')*,l}}\right]A^1_{j'h}\ . \quad \text{(D6)}$$

This eigenvalue equation can be solved to find A^1 and Q_η. The remaining expansion coefficients can then be found from Eq. (D4). We also note that this formulation can be used to approximate continuously varying potentials (e.g., graded interfaces, band bending) by dividing the spatially varying region into a series of steps.

APPENDIX E: COMPARISON WITH PREVIOUS k·p MODELS

In this appendix we show that our results can be reduced to those of White and Sham,[6] and Bastard,[7,8] if only special cases are considered and a series of approximations are made. Starting with our results, we only consider the $\mathbf{k}_{\parallel}=0$ case, drop all first-order terms of the $\Delta V+m^{-1}\mathbf{k}\cdot\mathbf{p}$ operator in the wave functions so that states outside of the eight explicitly considered ones do not enter, drop the stress interaction, switch to a Kramers basis, and take the spin-orbit interaction to be very large so as to drop the split-off band states.

Taking the spin-orbit interaction to be very large reduces the Hamiltonian matrix to 6×6. Neglecting the effect of higher-energy states mixed in by the $\Delta V+m^{-1}\mathbf{k}\cdot\mathbf{p}$ operator and taking $\mathbf{k}_{\parallel}=0$ decouples the $|\frac{3}{2}\pm\frac{3}{2}\rangle$ states in the Kramers basis from the other states. These states correspond to the heavy-hole band for $\mathbf{k}_{\parallel}=0$. With the approximations described above, these states are dispersionless. These approximations are not appropriate for a description of the heavy-hole band. Dropping these states, the Hamiltonian is 4×4. It is block diagonal in two identical 2×2 blocks describing electron and light-hole states with a z component of "angular momentum" of $+\frac{1}{2}$ and $-\frac{1}{2}$. The $+\frac{1}{2}$ matrix elements of the Hamiltonian for material l are

$$(S\uparrow|S\uparrow)=\varepsilon_c+\Delta\varepsilon_c^l-\varepsilon\ , \tag{E1a}$$

$$(S\uparrow|\tfrac{3}{2}\,\tfrac{1}{2})=-(\tfrac{3}{2}\,\tfrac{1}{2}|S\uparrow)=iP\frac{2}{\sqrt{6}}k\ , \tag{E1b}$$

$$(\tfrac{3}{2}\,\tfrac{1}{2}|\tfrac{3}{2}\,\tfrac{1}{2})=\varepsilon_v+\Delta\varepsilon_v^l+\frac{\Delta^l}{3}-\varepsilon\ , \tag{E1c}$$

where only the first-order term [Eqs. (A8i) and (A8j)] is kept in $\Delta\varepsilon_c^l$ and $\Delta\varepsilon_v^l$. Only the lowest-order term is kept in the calculation of the momentum matrix element p. It must be the same for the two materials. The current-density matrix elements $\langle dk|J_z|d'k'\rangle$ become the same for all material combinations and are independent of k and k' because of the neglect of higher-energy states mixed in by the $\Delta V+m^{-1}\mathbf{k}\cdot\mathbf{p}$ interaction. The nonzero matrix elements of this operator are ($+\frac{1}{2}$ states)

$$(S\uparrow|\tfrac{3}{2}\,\tfrac{1}{2})=-(\tfrac{3}{2}\,\tfrac{1}{2}|S\uparrow)=iP\frac{2}{\sqrt{6}}\ . \tag{E2}$$

It is a straightforward matter to determine k and eigenfunctions for the two materials from the 2×2 Hamiltonian matrices, construct the current matrices of Eq. (40a) from these eigenfunctions, construct the 2×2 final matrix of Eqs. (61), and find the superlattice dispersion relations from the eigenvalues of this matrix. In this way one finds

$$\cos[Q(a+b)]=\cos(k^a a)\cos(k^b b)-\frac{1}{2}\left[\frac{\beta^a}{\beta^b}+\frac{\beta^b}{\beta^a}\right]\sin(k^a a)\sin(k^b b)\ , \tag{E3a}$$

where

$$\beta^l=\frac{k^l}{\varepsilon-(\varepsilon_v+\Delta^l\varepsilon_v+\Delta^l/3)}\ . \tag{E3b}$$

This is exactly the form reported by Bastard [Ref. 8, Eq. (11)]. It is equivalent to the form reported by White and Sham [Ref. 6, Eq. (6)], as is easily verified using a series of trigonometric identities.

---

[1] See, for example, L. Esaki, in *Proceedings of the 17th International Conference on the Physics of Semiconductors*, edited by J. D. Chadi and W. A. Harrison (Springer-Verlag, New York, 1984), p. 473.

[2] See, for example, N. Holonyak, Jr., R. M. Kolbas, R. D. Dupuis, and P. D. Dapkus, IEEE J. Quantum Electron. **QE-16**, 170 (1980).

[3] D. A. B. Miller, D. S. Chemla, T. C. Damen, A. C. Gossard, W. Wiegmann, T. H. Wood, and C. A. Burrus, Appl. Phys. Lett. **45**, 13 (1984).

[4] D. S. Chemla, D. A. B. Miller, P. W. Smith, A. C. Gossard, and W. Wiegmann, IEEE J. Quantum Electron **QE-20**, 265 (1984).

[5] D. L. Smith, T. C. McGill, and J. N. Schulman, Appl. Phys. Lett. **43**, 180 (1983).

[6] S. R. White and L. J. Sham, Phys. Rev. Lett. **47**, 879 (1981).

[7] G. Bastard, Phys. Rev. B **24**, 5693 (1981).

[8] G. Bastard, Phys. Rev. B **25**, 7584 (1982).

[9] M. Altarelli, Phys. Rev. B **28**, 842 (1983).

[10] C. Mailhiot and D. L. Smith, Phys. Rev. B **33-I**, 8360 (1986), following paper.

[11] M. L. Cohen and T. K. Bergstresser, Phys. Rev. **141**, 789 (1966).

[12] P. O. Löwdin, J. Chem. Phys. **19**, 1396 (1951).

[13] C. Mailhiot, T. C. McGill, and D. L. Smith, J. Vac. Sci. Technol. B **2**, 371 (1984).

[14] G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-two Point Groups* (MIT Press, Cambridge, Mass., 1963).

[15] That is, we neglect k dependence of the spin-orbit and stress interactions and terms proportional to $\Delta V^l H^l_{\text{s.o.}}$ and $\Delta V^l H^l_{\text{st}}$.

[16] Y. C. Chang and J. N. Schulman, Phys. Rev. B **25**, 3975 (1982).

[17] Although the dropped terms in H^2 are smaller than the retained terms, the justification for neglecting them is primarily the way they enter the calculation.

[18] One could retain these terms in H^0. It improves, slightly, the bands as a function of $\mathbf{k}_{\parallel}$.

[19] Their coupling to physically significant states at the interfaces is very small.

[20] See, for example, E. O. Kane, J. Phys. Chem. Solids **1**, 249 (1957).

[21] See, for example, H. Kroemer, in *Proceedings of the NATO Advanced Study Institute on Molecular Beam Epitaxy and Heterostructures, Erice, Sicily, 1983*, edited by L. L. Chang and K. Ploog (Nijhoff, Leyden, 1985), p. 331.

[22] J. Bardeen, Phys. Rev. Lett. **6**, 57 (1961).

[23] H. Schlosser and P. M. Marcus, Phys. Rev. **131**, 2529 (1963).

[24] Residual terms are of order $(\Delta_{dd'})^2$; that is, second order in ΔV.

[25] Residual terms are of order $\Delta_{dd'}$; that is, first order in ΔV.

[26] We use the notation $(a,n;b,m)$ to indicate the interface between material a in the nth superlattice cycle and material b in the mth superlattice cycle.

[27] For any periodic system described by a Hermitian Hamiltonian, if Q is a wave vector at a given energy, Q^* must also be a

wave vector at this energy. A superlattice can be described by a Hermitian Hamiltonian and thus it must have this property. Therefore, it is important to show that our description of the superlattice, which is not directly based on a superlattice Hamiltonian, correctly describes this feature of the superlattice electronic structure.

[28] E. O. Kane, in *Semiconductors and Semimetals,* edited by R. K. Willardson and A. C. Beer (Academic, New York, 1966), Vol. 1, p. 75.

[29] G. C. Osbourn, J. Appl. Phys. **53**, 1586 (1982).

[30] See, for example, G. L. Bir and G. E. Pikus, *Symmetry and Strain-Induced Effects in Semiconductors* (Wiley, New York, 1974).