Band theory of superlattices

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We present a first-principles theory of the band structure of lattice-matched superlattices. We formulate the one-electron problem of superlattices in the Bloch representation of one of the constituent materials. In this formulation, the symmetry breaking along the superlattice axis leads to partitioning and folding of the original homogeneous crystal Brillouin zone onto a thin region around the center of the zone. A single homogeneous crystal Bloch function becomes a multicomponent wave function. Each component represents a superlattice subband. We use Löwdin's theorem to derive series expressions for the subband energies and wave functions, and discuss the relation between these solutions and the eigenvalues and eigenfunctions corresponding to quantum-well models. We apply the general results to a superlattice composed of two different types of simple two-band model materials.

I. INTRODUCTION

Since it became possible to grow superlattice crystals in the early 1970s,[1] there have been several theoretical approaches to their band structure.[2–15] These approaches are generally based on some form of either the envelope function approximation[8–11] or the tight-binding approximation.[12–15] The early empirical results concerning absorption, luminescence, carrier transport, etc. in superlattices could be explained, at least qualitatively, by means of simple quantum wells and Kronig-Penney models.[2–7] Later experiments revealed the appearance of certain forbidden transitions.[16,17] To explain these, as well as subband energy dispersions, one needs to go to more sophisticated theories in which band mixing occurs.[10,11,18]

In Bastard's envelope function approach,[8–11] one generalizes Kane's theory[19] for the III-V semiconductor compounds to superlattices, and writes a Kane Hamiltonian for each type of material composing the superlattice. The solutions of these effective Hamiltonians are then joined across layer interfaces by means of boundary conditions which require continuity of wave functions and conservation of electron current densities. These calculations ultimately depend on the effective-mass concept. The effective mass of the electron is assumed to be position dependent along the superlattice axis (that is to say, along the direction which is vertical to the planes of the superlattice layers). The space dependence of the effective mass is not calculated, but is postulated to have a certain form; then the results are compared with empirical observations to the extent that this is possible.

Tight-binding calculations of superlattices can, in principle, be more accurate than calculations based on the envelope function approximation, but involve extensive and complex numerical computations. In a tight-binding calculation, one uses superpositions of large numbers of electronic orbitals to solve for the eigenvalues and eigenfunctions of a tight-binding Hamiltonian.[20] Band mixing can be directly incorporated into these computations and optical spectra of superlattices can be reproduced reasonably accurately.[18]

In this paper we develop a new one-electron theory of superlattices. We assume that the homogeneous crystal band structures of the composite materials are completely known, and derive a superlattice Hamiltonian which expresses all of the effects of symmetry breaking in terms of the quantities and parameters related to the homogeneous crystals of the composite materials and the superlattice geometry. We obtain series expressions for the superlattice subband energies and wave functions, which can be evaluated systematically with increasing accuracy. More importantly, the new formulation provides conceptual clarity and pliability for analytic manipulation.

Our formulation relies heavily on the properties of the momentum Bloch functions. It is well known that the Bloch functions of a homogeneous crystal can be written as

$$\psi_{n\mathbf{k}}(\mathbf{x})=\frac{1}{(\mathscr{V}_{c\ell})^{1/2}}\sum_{\mathbf{G}}\phi_n(\mathbf{k}-\mathbf{G})e^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{x}}\,, \tag{1}$$

where n is the band index, $\mathbf{k}$ is the electronic momentum confined to the Brillouin zone, G's are the reciprocal-lattice vectors, and ϕ_n is the momentum Bloch function. $\mathscr{V}_{c\ell}$ is the macroscopic volume of the sample, which we assume to be parallelepiped and set $\mathscr{V}_{c\ell}=\mathscr{L}_x\mathscr{L}_y\mathscr{L}_z$. Just as the set of the ordinary Bloch functions is complete, the set of the momentum Bloch functions is also complete. ϕ_n's obey the closure and orthogonality relations[21,22]

$$\sum_n \phi_n^*(\mathbf{k}-\mathbf{G})\phi_n(\mathbf{k}-\mathbf{G}')=\delta_{\mathbf{G}\mathbf{G}'}\,, \tag{2a}$$

$$\sum_{\mathbf{G}} \phi_n^*(\mathbf{k}-\mathbf{G})\phi_{n'}(\mathbf{k}-\mathbf{G})=\delta_{nn'}\,. \tag{2b}$$

One consequence of these relations is the fact that the crystal potential can be written as[22] (see also the Appendix)

$$V(\mathbf{x})=\sum_n E_n(0)\phi_n(0)\psi_{n0}^*(\mathbf{x})\,, \tag{3a}$$

where $E_n(\mathbf{k})$ is the band energy. Alternatively, if we define the Fourier expansion

$$V(\mathbf{x})=\sum_{\mathbf{G}} \mathscr{V}_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{x}} , \tag{3b}$$

then

$$\mathscr{V}_{\mathbf{G}}=\sum_{n} E_n(0)\phi_n(0)\phi_n^*(-\mathbf{G}) . \tag{3c}$$

We use these relations in Sec. II to express the matrix elements of the one-electron Hamiltonian of a superlattice in the Hilbert space representation defined by the Bloch functions of a homogeneous crystal. We start with a finite number of layers of one type of material embedded in a different type of material. In the limit of a superlattice, a fixed number of foldings of the homogeneous crystal Brillouin zone occurs, and a single homogeneous crystal band wave function becomes a many-component wave function. The different components correspond to superlattice subbands. In our formulation, the subband formation is intimately connected with the symmetry breaking along the superlattice axis and the corresponding foldings of the homogeneous crystal Brillouin zone. In Sec. II we obtain a superlattice Hamiltonian for the subbands and discuss its simplified form under certain assumptions.

In Sec. III we discuss the solutions of the superlattice Hamiltonian. We use Löwdin's theorem[23,24] to obtain series solutions for the energies and wave functions of the subbands. These expressions allow exploration of theoretical issues, as well as providing suitable expressions for numerical analysis. The results include band mixing in a natural way. There are no *ad hoc* assumptions concerning effective masses of the subbands. These can be obtained from the analytic expressions given for the subband energies. Actually, our formulation proves for the first time that the concept of effective mass can be defined for a superlattice, by providing explicit expressions for the subband energy dispersions. We discuss the relation between the superlattice subbands and the states of a quantum well. For an example, we apply our results to a superlattice composed of two-band-model materials.

In this paper we ignore spin-orbit coupling in order to keep the discussion simple. This is a serious shortcoming in view of the fact that present-day superlattices are composed of materials in which spin-orbit coupling is significant. We hope to return to this problem elsewhere.

II. FORMULATION IN MOMENTUM SPACE

Let us begin the discussion with two types of materials, A and B, whose homogeneous lattice structures match:

$$\mathbf{R}_A=\mathbf{R}_B=\mathbf{R} \text{ (lattice translation vectors)} , \tag{4a}$$

$$\mathbf{G}_A=\mathbf{G}_B=\mathbf{G} \text{ (reciprocal-lattice vectors)} . \tag{4b}$$

We assume that the Bloch functions of the homogeneous crystals of these materials are completely known:

$$H_{A,B}=\frac{\mathbf{p}^2}{2m}+V_{A,B}(\mathbf{x}) , \tag{5a}$$

$$\begin{aligned} &H_{A,B}\,|\,n\mathbf{k}\rangle_{A,B}=E_n^{A,B}(\mathbf{k})\,|\,n\mathbf{k}\rangle_{A,B} , \\ &\langle\,\mathbf{x}\,|\,n\mathbf{k}\rangle_{A,B}=\psi_{n\mathbf{k}}^{A,B}(\mathbf{x}) . \end{aligned} \tag{5b}$$

Consider now the geometry shown in Fig. 1. The layers of material A of width L_A are sandwiched in between the layers of material B of width L_B. We initially assume that a finite number $\mathscr{N}$ of A layers are embedded in B. At a later stage of the calculation we let $\mathscr{N}$ become infinite, making the composite structure a superlattice. Keeping $\mathscr{N}$ initially finite avoids some minor mathematical problems. We let the $\hat{\mathbf{z}}$ axis be vertical to the layers (the superlattice axis). We pick the origin of the coordinate system as symmetrically as possible for the convenience of evaluating certain sums later. If $\mathscr{N}$ is an odd integer, the origin is in the middle of an A layer as shown in Fig. 1(a). If $\mathscr{N}$ is even, the origin is in the middle of a B layer as shown in Fig. 1(b). In the superlattice limit, whether one starts with odd or even $\mathscr{N}$ does not matter; the results are independent of the initial configuration. We will choose our initial configuration to be the one shown in Fig. 1(a) with odd $\mathscr{N}$. The layers of A and B are assumed to have perfectly sharp plane interfaces.

The one-electron Hamiltonian of the composite crystal of Fig. 1(a) can be written as

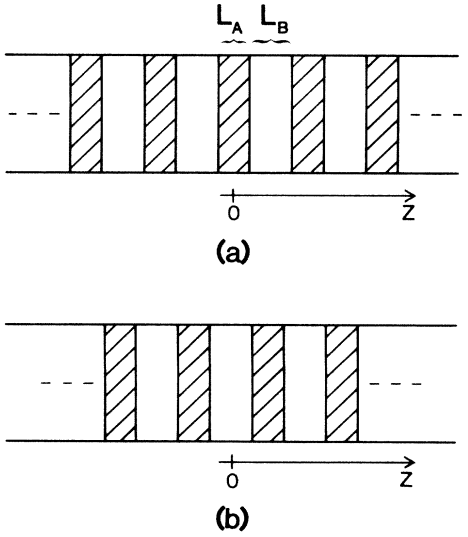

FIG. 1. Origin of the coordinates for odd (a) and even (b) $\mathscr{N}$.

$$H=\frac{\mathbf{p}^2}{2m}+V_B(\mathbf{x})+[V_A(\mathbf{x})-V_B(\mathbf{x})]\sum_{s=-(\mathcal{N}-1)/2}^{(\mathcal{N}-1)/2}[\Theta(z-sL+\tfrac{1}{2}L_A)-\Theta(z-sL-\tfrac{1}{2}L_A)]$$
$$=\frac{\mathbf{p}^2}{2m}+V_B(\mathbf{x})+H_{AW}(\mathbf{x}) , \tag{6}$$

where Θ's are the step functions, and L is the superlattice period along the superlattice axis:

$$L=L_A+L_B . \tag{7}$$

We now determine the matrix elements of this Hamiltonian in the representation defined by the Bloch functions of the B-type crystal. This is legitimate, since the set of the Bloch functions of a given homogeneous crystal is complete. First, consider the matrix elements of a step function. The step function $\Theta(z-z_0)$ can be written in the integral form

$$\Theta(z-z_0)=\frac{-i}{2\pi}\int_{-\infty}^{+\infty}dQ\frac{e^{iQ(z-z_0)}}{(Q-i\alpha)} , \tag{8}$$

where α is a positive infinitesimal quantity. Its matrix elements in the representation of the B-type Bloch functions become

$${}_B\langle n\mathbf{k}\,|\,\Theta(z-z_0)\,|\,n'\mathbf{k}'\rangle_B=\frac{-i}{2\pi}\int_{-\infty}^{+\infty}dQ\frac{e^{-iQz_0}}{(Q-i\alpha)}\int_{\mathcal{V}_{cl}}d\mathbf{x}\,\psi_{n\mathbf{k}}^{B*}(\mathbf{x})e^{i\mathbf{Q}\cdot\mathbf{x}}\psi_{n'\mathbf{k}'}^{B}(\mathbf{x}) , \tag{9}$$

where $\mathbf{Q}=\hat{\mathbf{z}}Q$. Using (1), one can perform the spatial integrations in (9):

$${}_B\langle n\mathbf{k}\,|\,\Theta(z-z_0)\,|\,n'\mathbf{k}'\rangle_B=\frac{-i(2\pi)^2}{\mathcal{L}_x\mathcal{L}_y\mathcal{L}_z}\int_{-\infty}^{+\infty}dQ\frac{e^{-iQz_0}}{(Q-i\alpha)}\sum_{\mathbf{G},\mathbf{G}'}\phi_n^{B*}(\mathbf{k}-\mathbf{G})\phi_{n'}^{B}(\mathbf{k}'-\mathbf{G})\delta(\mathbf{k}-\mathbf{G}-\mathbf{k}'+\mathbf{G}'-\mathbf{Q})$$
$$=-\frac{i}{\mathcal{L}_z}\sum_{\mathbf{G},\mathbf{G}'}\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}')\phi_n^{B*}(\mathbf{k}-\mathbf{G})\phi_{n'}^{B}(\mathbf{k}'-\mathbf{G}')$$
$$\times\int_{-\infty}^{+\infty}dQ\,\delta(k_z-G_z-k_z'+G_z'-Q)\frac{e^{-iQz_0}}{(Q-i\alpha)} , \tag{10}$$

where

$$\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}')=\frac{(2\pi)^2}{\mathcal{L}_x\mathcal{L}_y}\delta(k_x-G_x-k_x'+G_x')\delta(k_y-G_y-k_y'+G_y') . \tag{11}$$

Note that because $\mathbf{k}$ and $\mathbf{k}'$ are restricted to the Brillouin zone, the transverse δ function can be factorized as

$$\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}')=\delta_\perp(\mathbf{k},\mathbf{k}')\delta_{\perp\mathbf{G}\mathbf{G}'} . \tag{12}$$

Performing the integral over the δ function in (10), one finds

$${}_B\langle n\mathbf{k}\,|\,\Theta(z-z_0)\,|\,n'\mathbf{k}'\rangle_B=-\frac{i}{\mathcal{L}_z}\sum_{\mathbf{G},\mathbf{G}'}\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}')\phi_n^{B*}(\mathbf{k}-\mathbf{G})\phi_{n'}^{B}(\mathbf{k}'-\mathbf{G}')\frac{\exp[-i(k_z-G_z-k_z'+G_z')z_0]}{k_z-G_z-k_z'+G_z'-i\alpha} . \tag{13}$$

Using (13), the matrix elements of the sums of the step functions in the Hamiltonian become[25]

$${}_B\langle n\mathbf{k}\,|\sum_{s=-(\mathcal{N}-1)/2}^{(\mathcal{N}-1)/2}[\Theta(z-sL+\tfrac{1}{2}L_A)-\Theta(z-sL-\tfrac{1}{2}L_A)]\,|\,n'\mathbf{k}'\rangle_B$$
$$=\frac{2}{\mathcal{L}_z}\sum_{\mathbf{G},\mathbf{G}'}\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}')\phi_n^{B*}(\mathbf{k}-\mathbf{G})\phi_{n'}^{B}(\mathbf{k}'-\mathbf{G}')\frac{\sin[(k_z-k_z'-G_z+G_z')\frac{1}{2}L_A]}{(k_z-k_z'-G_z+G_z'-i\alpha)}\frac{\sin[\mathcal{N}L(k_z-k_z')/2]}{\sin[L(k_z-k_z')/2]} . \tag{14}$$

Let us define the function

$$\Delta(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}')=\frac{2}{\mathcal{L}_z}\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}')\frac{\sin[\frac{1}{2}L_A(k_z-k_z'-G_z+G_z')]}{(k_z-G_z-k_z'+G_z'-i\alpha)}\frac{\sin[\mathcal{N}L(k_z-k_z')/2]}{\sin[L(k_z-k_z')/2]} . \tag{15}$$

Equation (14) is then given by

$${}_B\langle n\mathbf{k}\,|\sum_{s=-(\mathcal{N}-1)/2}^{(\mathcal{N}-1)/2}[\Theta(z-sL+\tfrac{1}{2}L_A)-\Theta(z-sL-\tfrac{1}{2}L_A)]\,|\,n'\mathbf{k}'\rangle_B=\sum_{\mathbf{G},\mathbf{G}'}\phi_n^{B*}(\mathbf{k}-\mathbf{G})\phi_{n'}^{B}(\mathbf{k}'-\mathbf{G}')\Delta(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}') . \tag{16}$$

The folding of the Brillouin zone of the homogeneous crystal arises from the last factor in (15), which is just the Gegenbauer function:[26]

$$\mathcal{C}^{1}_{\mathcal{N}-1}[\cos(LK/2)]=\frac{\sin(\mathcal{N}LK/2)}{\sin(LK/2)},\quad K=k_z-k_z' . \tag{17}$$

This is an even, periodic function. Its period is $2\pi/L$, and its maxima are at

$$\frac{LK}{2}=\pi\ell , \tag{18}$$

where ℓ is equal to any integer. Let

$$K_\ell=\frac{2}{L}(\pi\ell+\delta),\quad \delta\ll 1 . \tag{19}$$

Then

$$\sin(LK_\ell/2)\simeq(-1)^\ell\delta , \tag{20a}$$

$$\sin(\mathcal{N}LK_\ell/2)\simeq(-1)^{\ell}\mathcal{N}\delta . \tag{20b}$$

Therefore,

$$\lim_{\delta\to 0}\frac{\sin(\mathcal{N}LK_\ell/2)}{\sin(LK_\ell/2)}=\mathcal{N}(-1)^{\ell(\mathcal{N}-1)}=\mathcal{N} . \tag{20c}$$

(Since $\mathcal{N}$ is odd and $\mathcal{N}-1$ is even.)

We can now pass into the superlattice limit by letting $\mathcal{N}\to\infty$, $\mathcal{L}_z\to\infty$, but keeping the ratio

$$\rho=\frac{\mathcal{N}}{\mathcal{L}_z}=\text{const} , \tag{21}$$

which is the density of the A layers per unit length of the sample. In this limit, the Gegenbauer function becomes a series of δ functions located at $k_z-k_z'=2\pi\ell/L$. Thus, for a superlattice, Δ becomes

$$\Delta(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}')=\rho L_A\delta_\perp(\mathbf{k}-\mathbf{G},\mathbf{k}'-\mathbf{G}')\times\sum_\ell\delta(k_z,k_z'+2\pi\ell/L)\times\frac{\sin[\frac{1}{2}L_A(2\pi\ell/L-G_z+G_z')]}{[\frac{1}{2}L_A(2\pi\ell/L-G_z+G_z')]} . \tag{22}$$

Let us now consider the matrix elements of V_A-V_B. It follows from (1) and (3b) that

$${}_B\langle n\mathbf{k}\,|\,(V_A-V_B)\,|\,n'\mathbf{k}'\rangle_B=\int_{\mathcal{V}_{o\ell}}d\mathbf{x}\,\psi^{B*}_{n\mathbf{k}}(\mathbf{x})\sum_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{x}}(\mathcal{V}^A_{\mathbf{G}}-\mathcal{V}^B_{\mathbf{G}})\psi^B_{n\mathbf{k}'}(\mathbf{x}) . \tag{23}$$

Expressing the ordinary Bloch functions in terms of the momentum Bloch functions, one can do the space integral:

$$\sum_{\mathbf{G},\mathbf{G}',\mathbf{G}''}\phi^{B*}_n(\mathbf{k}-\mathbf{G})\phi^B_{n'}(\mathbf{k}'-\mathbf{G}')(\mathcal{V}^A_{\mathbf{G}''}-\mathcal{V}^B_{\mathbf{G}''})\frac{1}{\mathcal{V}_{o\ell}}\int_{\mathcal{V}_{o\ell}}d\mathbf{x}\,e^{-i(\mathbf{k}-\mathbf{G}-\mathbf{G}''-\mathbf{k}'+\mathbf{G}')\cdot\mathbf{x}}$$

$$=\delta(\mathbf{k},\mathbf{k}')\sum_{\mathbf{G},\mathbf{G}'}(\mathcal{V}^A_{\mathbf{G}'-\mathbf{G}}-\mathcal{V}^B_{\mathbf{G}'-\mathbf{G}})\phi^{B*}_n(\mathbf{k}-\mathbf{G})\phi^B_{n'}(\mathbf{k}'-\mathbf{G}'') . \tag{24}$$

Let us define the energy parameter

$$W(\mathbf{G})=\mathcal{V}^A_{\mathbf{G}}-\mathcal{V}^B_{\mathbf{G}}=\sum_n[E^A_n(0)\phi^A_n(0)\phi^{A*}_n(-\mathbf{G})-E^B_n(0)\phi^B_n(0)\phi^{B*}_n(-\mathbf{G})] . \tag{25}$$

The last line follows from (3c) and shows that W is related to the band offsets between the two materials. Equation (23) becomes

$${}_B\langle n\mathbf{k}\,|\,(V_A-V_B)\,|\,n'\mathbf{k}'\rangle_B=\delta(\mathbf{k},\mathbf{k}')\sum_{\mathbf{G},\mathbf{G}'}W(\mathbf{G}'-\mathbf{G})\phi^{B*}_n(\mathbf{k}-\mathbf{G})\phi^B_{n'}(\mathbf{k}-\mathbf{G}') . \tag{26}$$

Finally, inserting a complete set of states between (V_A-V_B) and the step functions in H_{AW}, we obtain

$${}_B\langle n\mathbf{k}\,|\,H\,|\,n'\mathbf{k}'\rangle_B=\delta_{nn'}\delta(\mathbf{k},\mathbf{k}')E^B_n(\mathbf{k})+{}_B\langle n\mathbf{k}\,|\,H_{AW}\,|\,n'\mathbf{k}'\rangle_B , \tag{27a}$$

$${}_B\langle n\mathbf{k}\,|\,H_{AW}\,|\,n'\mathbf{k}'\rangle_B=\sum_{\mathbf{G},\mathbf{G}',\mathbf{G}''}W(\mathbf{G}''-\mathbf{G}')\times\Delta(\mathbf{k}-\mathbf{G}'',\mathbf{k}'-\mathbf{G}')\times\phi^{B*}_n(\mathbf{k}-\mathbf{G})\phi^B_{n'}(\mathbf{k}'-\mathbf{G}') . \tag{27b}$$

Let us assume that the reciprocal lattice is a simple-cubic lattice with one of the principal directions along the $\hat{\mathbf{z}}$ axis. This is a minor simplifying assumption; the results are easily generalized for arbitrary lattice orientations. The reciprocal-lattice vectors G_z can then be written

$$G_z=\frac{2\pi}{a}M,\quad M=0,\pm1,\pm2,\ldots . \tag{28}$$

a is the fundamental lattice constant of the homogeneous crystals of A and B. We define

$$\ell_0=\frac{L}{a} , \tag{29}$$

which is equal to a positive integer. Using (22), the expression for the matrix element of H_{AW} can be more explicitly written as

$$ {}_B\langle n\mathbf{k}\,|\,H_{AW}\,|\,n'\mathbf{k}'\rangle_B=\rho L_A\sum_{\ell,M,\mathbf{G},\mathbf{G}'}\delta\left[\mathbf{k},\mathbf{k}'+\frac{2\pi\ell}{L}\hat{\mathbf{z}}\right]\frac{\sin[(\pi L_A/L)(\ell-\ell_0 M)]}{[(\pi L_A/L)(\ell-\ell_0 M)]} $$
$$ \times W(\mathbf{G}'-\mathbf{G})\phi_n^{B*}(\mathbf{k}-\mathbf{G})\phi_{n'}^B\left[\mathbf{k}-\mathbf{G}'-\frac{2\pi\ell}{L}\hat{\mathbf{z}}+\frac{2\pi M}{a}\hat{\mathbf{z}}\right]. \tag{30} $$

Next, consider a superlattice eigenstate $|\psi\rangle$. Since the set of B-type Bloch states is complete, one can write

$$ |\psi\rangle=\sum_{n,\mathbf{k}}a_n(\mathbf{k})\,|\,n\mathbf{k}\rangle_B\,. \tag{31} $$

Note that the sum over $\mathbf{k}$ is confined to the Brillouin zone of the homogeneous crystals. This important fact should be kept in mind; in the sums below, the argument of a_n must be confined to this Brillouin zone. The time-independent Schrödinger equation for $|\psi\rangle$ is

$$ H\,|\psi\rangle=\sum_{n',\mathbf{k}'}a_{n'}(\mathbf{k}')(H_B+H_{AW})\,|\,n'k'\rangle_B=\varepsilon\,|\,\psi\rangle\,. \tag{32} $$

Taking the scalar product with $|\,n\mathbf{k}\rangle_B$ and using (30), we find

$$ [\varepsilon-E_n^B(\mathbf{k})]a_n(\mathbf{k})-\sum_{\{\ell'\,|\,\mathbf{k}+(2\pi\ell'/L)\hat{\mathbf{z}}\in\mathrm{BZ}\}}\sum_{M=-\infty}^{+\infty}\rho L_A\frac{\sin[(\pi L_A/L)(\ell'+\ell_0 M)]}{[(\pi L_A/L)(\ell'+\ell_0 M)]} $$
$$ \times\sum_{\mathbf{G},\mathbf{G}'}W(\mathbf{G}'-\mathbf{G})\phi_n^{B*}(\mathbf{k}-\mathbf{G})\phi_{n'}^B\left[\mathbf{k}-\mathbf{G}'+\frac{2\pi M}{a}\hat{\mathbf{z}}+\frac{2\pi\ell'}{L}\hat{\mathbf{z}}\right]a_{n'}\left[\mathbf{k}+\frac{2\pi\ell'}{L}\hat{\mathbf{z}}\right]=0\,. \tag{33} $$

The condition on integers ℓ' makes this equation awkward to work with in its present form. It can be put into a more convenient form by separating $\mathbf{k}$ into two parts. Define

$$ \mathbf{k}=\boldsymbol{\kappa}+\frac{2\pi\ell}{L}\hat{\mathbf{z}} \tag{34a} $$

such that

$$ \begin{aligned} &k_x=\kappa_x\,,\\ &k_y=\kappa_y\,,\\ &-\frac{\pi}{L}<\kappa_z<\frac{\pi}{L}\,,\\ &\ell=0,\pm1,\pm2,\ldots,\pm(\ell_0-1)\,. \end{aligned} \tag{34b} $$

Equation (33) becomes

$$ \left[\varepsilon-E_n^B\left[\boldsymbol{\kappa}+\frac{2\pi\ell}{L}\hat{\mathbf{z}}\right]\right]a_n\left[\boldsymbol{\kappa}+\frac{2\pi\ell}{L}\hat{\mathbf{z}}\right]-\rho L_A\sum_{\ell'=-\ell_0+1}^{\ell_0-1}\sum_{M=-\infty}^{+\infty}\sum_{\mathbf{G},\mathbf{G}',n}\frac{\sin[(\pi L_A/L)(\ell-\ell'-\ell_0 M)]}{[(\pi L_A/L)(\ell-\ell'-\ell_0 M)]} $$
$$ \times W(\mathbf{G}'-\mathbf{G})\phi_n^B\left[\boldsymbol{\kappa}-\mathbf{G}+\frac{2\pi\ell}{L}\hat{\mathbf{z}}\right]\phi_{n'}^B\left[\boldsymbol{\kappa}-\mathbf{G}'+\frac{2\pi M}{a}\hat{\mathbf{z}}+\frac{2\pi\ell'}{L}\hat{\mathbf{z}}\right]a_{n'}\left[\boldsymbol{\kappa}+\frac{2\pi\ell'}{L}\hat{\mathbf{z}}\right]=0\,. \tag{35} $$

Note that both ℓ and ℓ' vary over the integers in the interval

$$ -\ell_0+1\le\ell,\ell'\le\ell_0-1\,. \tag{36} $$

One can therefore introduce $2\ell_0-1$ dimensional spinors (that is to say, column vectors) for each a_n. Define

$$ a_{n\ell}(\boldsymbol{\kappa})=a_n\left[\boldsymbol{\kappa}+\frac{2\pi\ell}{L}\hat{\mathbf{z}}\right], \tag{37a} $$

$$ E_{n\ell}^B(\boldsymbol{\kappa})=E_n^B\left[\boldsymbol{\kappa}+\frac{2\pi\ell}{L}\hat{\mathbf{z}}\right], \tag{37b} $$

$$ V_{n\ell;n'\ell'}(\boldsymbol{\kappa})=\rho L_A\sum_{M=-\infty}^{+\infty}\frac{\sin[(\pi L_A/L)(\ell-\ell'-\ell_0 M)]}{[(\pi L_A/L)(\ell-\ell'-\ell_0 M)]} $$
$$ \times\sum_{\mathbf{G},\mathbf{G}'}W(\mathbf{G}'-\mathbf{G})\phi_n^B\left[\boldsymbol{\kappa}-\mathbf{G}+\frac{2\pi\ell}{L}\hat{\mathbf{z}}\right]\phi_{n'}^B\left[\boldsymbol{\kappa}-\mathbf{G}+\frac{2\pi M}{a}\hat{\mathbf{z}}+\frac{2\pi\ell'}{L}\hat{\mathbf{z}}\right]. \tag{37c} $$

Equation (35) becomes

$$[\varepsilon - E^B_{n\ell}(\kappa)]a_{n\ell}(\kappa) - \sum_{n',l'} V_{n\ell;n'\ell'}(\kappa)a_{n'\ell'}(\kappa) = 0 \ . \tag{38}$$

Let

$$\alpha_n(\kappa) = \begin{bmatrix} a_{n\ell_0-1}(\kappa) \\ a_{n\ell_0-2}(\kappa) \\ \vdots \\ a_{n-\ell_0+1}(\kappa) \end{bmatrix} , \tag{39a}$$

$$\mathscr{E}^B_n(\kappa) = \begin{bmatrix} E^B_{n\ell_0-1}(\kappa) & & & 0 \\ & E^B_{n\ell_0-2}(\kappa) & & \\ & & \ddots & \\ 0 & & & E^B_{n-\ell_0+1}(\kappa) \end{bmatrix} , \tag{39b}$$

and

$$[\mathscr{V}_{nn'}(\kappa)]_{\ell\ell'} = V_{n\ell;n'\ell'}(\kappa) \ . \tag{39c}$$

Equation (38) can be written in terms of the $2\ell_0-1$ component spinors α_n and $(2\ell_0-1)\times(2\ell_0-1)$ matrices $\mathscr{V}_{nn'}$ as

$$\sum_{n'}[\mathscr{E}^B_n(\kappa)\delta_{nn'} + \mathscr{V}_{nn'}(\kappa)]\alpha_{n'}(\kappa) = \varepsilon\alpha_n(\kappa) \ . \tag{40}$$

This is just a more compact notation.

Equation (38), either in expanded or compact form, is the fundamental equation of this paper. It shows that a given band of the homogeneous crystal splits into $2\ell_0-1$ components in the superlattice. These components are the superlattice subbands, and as we shall see below, there is a correspondence between them and the bound states of quantum wells. The splitting arises entirely from the symmetry breaking along the $\hat{\mathbf{z}}$ axis. The original Brillouin zone of the homogeneous crystal is partitioned into $2\ell_0-1$ sections. The central piece for $-\pi/L < \kappa_z < \pi/L$ becomes the new Brillouin zone for the superlattice. The subbands of a band n arise from the folding of the original E_n onto the superlattice Brillouin zone. Furthermore, the Hamiltonian which determines the subband energies and subband states (in the representation of $\{|n\mathbf{k}\rangle_B\}$) becomes a supermatrix given by

$$\mathscr{H}^{\rm SL}_{n\ell;n'\ell'}(\kappa) = E^B_{n\ell}(\kappa)\delta_{nn'}\delta_{\ell\ell'} + V_{n\ell;n'\ell'}(\kappa) \ . \tag{41}$$

We should note that $\kappa_z = \pm\pi/L$ represent identical points in the superlattice Brillouin zone, since they are related by the momentum $2\pi\hat{\mathbf{z}}/L$. One needs to include only one end in the superlattice Brillouin zone, for example $\kappa_z = +\pi/L$.

Before we discuss the solutions of (38), a few remarks about $W(\mathbf{G})$ are in order. It is clear from the defining equation (25) that $W(\mathbf{G})$ is related to the band offsets of the A and B materials. Its maximum value is expected to be at $\mathbf{G}=0$ because of the weighting factors of the momentum Bloch functions, which are expected to be an order of magnitude smaller at the values of momenta outside the homogeneous crystal Brillouin zone than at finite $\mathbf{k}$'s inside the zone.[27] $W(0)$ is simply given by the spatial average of the potential difference over a macroscopic volume:

$$W(0) = \frac{1}{\mathscr{V}_{o\ell}} \int_{\mathscr{V}_{o\ell}} d\mathbf{x}[V_A(\mathbf{x}) - V_B(\mathbf{x})] \ . \tag{42}$$

It is therefore related to the difference between the electron affinities of the two materials.

The fact that $W(0)$ is the largest value permits one to approximate $W(\mathbf{G})$ by $\delta_{\mathbf{G}0}W(0)$, and to derive an approximate form of $V_{n\ell;n'\ell'}$ which is free of explicit reference to the momentum Bloch functions. To obtain this form, consider the matrix element of the position operator in a homogeneous crystal:

$$\int_{\rm crystal} d\mathbf{x}\, \psi^*_{n\mathbf{k}}\mathbf{x}\psi_{n'\mathbf{k}'} = -i\delta_{nn'}\frac{\partial}{\partial\mathbf{k}'}\delta(\mathbf{k},\mathbf{k}') + \delta(\mathbf{k},\mathbf{k}')\mathbf{X}_{nn'}(\mathbf{k}) \ , \tag{43}$$

where

$$\mathbf{X}_{nn'}(\mathbf{k}) = \sum_n \phi^*_n(\mathbf{k}-\mathbf{G})\left[i\frac{\partial}{\partial\mathbf{k}}\right]\phi_{n'}(\mathbf{k}-\mathbf{G}) \ . \tag{44}$$

The diagonal elements of $\mathbf{X}$ can be set equal to zero, since they are gauge dependent.[28] The off-diagonal elements of $\mathbf{X}$ are given by

$$\mathbf{X}_{nn'}(\mathbf{k}) = \frac{-i\hbar\mathbf{p}_{nn'}(\mathbf{k})}{m_e[E_n(\mathbf{k}) - E_{n'}(\mathbf{k})]} \ , \tag{45}$$

where $\mathbf{p}_{nn'}$ are the matrix elements of the momentum operator, m_e is the bare electronic mass. Note that $\mathbf{X}$ is periodic in the reciprocal-lattice space:

$$\mathbf{X}(\mathbf{k}+\mathbf{G}) = \mathbf{X}(\mathbf{k}) \ . \tag{46}$$

Using the closure property (2a), one can convert (44) into a set of differential equations for the momentum Bloch functions:

$$\frac{\partial}{\partial\mathbf{k}}\phi_n(\mathbf{k}-\mathbf{G}) = -i\sum_{n'}\phi_{n'}(\mathbf{k}-\mathbf{G})\mathbf{X}_{n'n}(\mathbf{k}) \ . \tag{47}$$

Consider a fixed $\mathbf{k}_0$ and a small neighborhood around $\mathbf{k}_0$. Assume that $\mathbf{X}$ can be taken constant in this neighborhood. For this neighborhood Eq. (47) becomes

$$\frac{\partial}{\partial\mathbf{k}}\phi_n(\mathbf{k}+\mathbf{k}_0-\mathbf{G}) = -i\sum_{n'}\phi_{n'}(\mathbf{k}+\mathbf{k}_0-\mathbf{G})\mathbf{X}_{n'n}(\mathbf{k}_0) \ . \tag{48}$$

Since $\mathbf{X}$ is Hermitian, there exists a unitary matrix $U(\mathbf{k}_0)$ which diagonalizes $\mathbf{X}$:

$$U(\mathbf{k}_0)\mathbf{X}(\mathbf{k}_0)U^\dagger(\mathbf{k}_0) = \mathbf{X}^D(\mathbf{k}_0) \ . \tag{49}$$

One can write (48) in matrix notation as

$$\frac{\partial}{\partial\mathbf{k}}(\phi^T U^\dagger) = -i(\phi^T U^\dagger)\mathbf{X}^D \ , \tag{50}$$

where $\phi^T = (\phi_1, \phi_2, \ldots)$. Equation (50) is readily solved in the neighborhood of $\mathbf{k}_0$:

$$\phi^T(\mathbf{k})U^\dagger = \phi^T(\mathbf{k}=0)U^\dagger e^{-i\mathbf{k}\cdot\mathbf{X}^D} \ . \tag{51}$$

Multiplying both sides of (51) by U from the right, we find

$$\phi_n(\mathbf{k}+\mathbf{k}_0-\mathbf{G})=\sum_{n'}\phi_{n'}(\mathbf{k}_0-\mathbf{G})(e^{-i\mathbf{k}\cdot\mathbf{X}(\mathbf{k}_0)})_{n'n} . \quad (52)$$

We can use (52) to express the momentum Bloch functions in $V_{n\ell;n'\ell'}$ [Eq. (37c)] in terms of the matrix elements of the operator $\mathbf{X}$. Suppose that ℓ_0 is sufficiently large such that, in each section of the partitioned homogeneous crystal Brillouin zone, we can take $\mathbf{X}^B$ to be constant in the $\hat{\mathbf{z}}$ direction. In other words, we replace the continuous operator X_z^B with a piecewise constant operator. Define the matrix operators

$$D^{\pm|\ell|}_{nn'}(\kappa)=\left\{\prod_{j=0}^{|\ell|-1}\exp\left[\mp i\frac{2\pi}{L}X_z^B\left[\kappa\pm\frac{2\pi j}{L}\hat{\mathbf{z}}\right]\right]\right\}_{nn'} \quad (53a)$$

for finite integer ℓ, and

$$D^0_{nn'}=\delta_{nn'} . \quad (53b)$$

It follows from (52) then that

$$\phi_n^{B*}\left[\kappa-\mathbf{G}+\frac{2\pi\ell}{L}\hat{\mathbf{z}}\right]=\sum_{n'}[D^{\ell\dagger}(\kappa)]_{nn'}\phi_{n'}^{B*}(\kappa-\mathbf{G}) , \quad (54a)$$

$$\phi_n^B\left[\kappa-\mathbf{G}'+\frac{2\pi\ell'}{L}\hat{\mathbf{z}}+\frac{2\pi M}{a}\hat{\mathbf{z}}\right]=\sum_{n'n''}\phi_{n''}^B(\kappa-\mathbf{G})\{[D^{\ell_0}(\kappa)]^M\}_{n''n'}D^{\ell'}_{n'n}(\kappa) . \quad (54b)$$

In (54b), D^{ℓ_0} is multiplied by itself M times. Thus $V_{n\ell;n'\ell'}$ can be approximated by

$$V_{n\ell;n'\ell'}(\kappa)=\rho L_A\sum_{M=-\infty}^{\infty}\frac{\sin[(\pi L_A/L)(\ell-\ell'-\ell_0M)]}{\sin[(\pi L_A/L)(\ell-\ell'-\ell_0M)]}\sum_{\mathbf{G},\mathbf{G}',n'',n'''}W(\mathbf{G}'-\mathbf{G})D^{\ell\dagger}_{nn''}(\kappa)\phi^{B*}_{n''}(\kappa-\mathbf{G})\phi^B_{n'''}(\kappa-\mathbf{G}')$$
$$\times[(D^{\ell_0}(\kappa)^MD^{\ell'}(\kappa)]_{n'''n'} . \quad (55)$$

Replacing the band offset factor $W(\mathbf{G}'-\mathbf{G})$ by $W(0)\delta_{\mathbf{G}\mathbf{G}'}$ and using (2c), we find

$$V_{n\ell;n'\ell'}(\kappa)=\rho L_AW(0)\sum_{M=-\infty}^{+\infty}\frac{\sin[(\pi L_A/L)(\ell-\ell'-\ell_0M)]}{[(\pi L_A/L)(\ell-\ell'-\ell_0M)]}\{D^{\ell\dagger}(\kappa)[D^{\ell_0}(\kappa)]^MD^{\ell'}(\kappa)\}_{nn'} . \quad (56)$$

Because of the sine factor, the most important contribution comes from the $M=0$ term. Taking just this term, $V_{n\ell;n'\ell'}$ is further simplified to

$$V_{n\ell;n'\ell'}(\kappa)=\rho L_AW(0)[D^{\ell\dagger}(\kappa)D^{\ell'}(\kappa)]_{nn'}\times\frac{\sin[(\pi L_A/L)(\ell-\ell')]}{[(\pi L_A/L)(\ell-\ell')]} . \quad (57)$$

Expressions (56) and (57) have no direct reference to the momentum Bloch functions. Instead they express $V_{n\ell;n'\ell'}$ essentially in terms of momentum matrix elements and energy-band separations which are directly determinable from measurements of radiative transitions in homogeneous crystals.

III. SUBBANDS AND SUBBAND ENERGIES

When the folding of the homogeneous crystal Brillouin zone is taken into account, a superlattice wave function becomes

$$\psi(\mathbf{x})=\sum_{n,\ell,\kappa}a_{n\ell}(\kappa)\psi^B_{n\kappa+(2\pi\ell/L)\hat{\mathbf{z}}}(\mathbf{x}) , \quad (58)$$

which is obtained from (31). It is obvious from the superlattice Hamiltonian (41) that its eigenvalues can be designated by $\varepsilon_{n\ell}(\kappa)$; the corresponding eigenfunction is given by

$$\psi_{n\ell\kappa}(\mathbf{x})=\sum_{n',\ell'}a^{(n\ell)}_{n'\ell'}(\kappa)\psi^B_{n'\kappa+(2\pi\ell'/L)\hat{\mathbf{z}}}(\mathbf{x}) . \quad (59)$$

Other indices may be used if the eigenvalue is degenerate.

To discuss the diagonalization of the superlattice Hamiltonian, we can make use of Löwdin's theorem,[23,24] which is concerned with the determination of a small number of eigenvalues and eigenvectors of a Hermitian matrix without diagonalizing the entire matrix. Given a Hermitian matrix U, its basis states can be separated into two sets S and R. Define

$$U^S_{mm'}(E)=U_{mm'}+\sum_{r\in R}\frac{U'_{mr}U'_{rm}}{E-U_{rr}}+\sum_{r_1,r_2\in R}\frac{U'_{mr_1}U'_{r_1r_2}U'_{r_2m_1}}{(E-U_{r_1r_1})(E-U_{r_2r_2})}+\cdots , \quad (60)$$

where $U'_{mm'}=(1-\delta_{mm'})U_{mm'}$. If the matrix M is such that $M_{ss'}=U^S_{ss'}$ for $s,s'\in S$, then the theorem states that the eigenvalues of U corresponding to the set S are the roots of the equation $\det(M-E)=0$. Furthermore, if E_s is a solution of this equation and if $\underset{\sim}{\xi}^{(s)}$ is the corresponding eigenvector, then it is given by

$$\xi_m^{(s)}=\begin{cases}\eta_s\mu_m^{(s)} & \text{if } m\in S\ ,\\ \eta_s\displaystyle\sum_{s'\in S}\frac{U^S_{ms'}(E_s)}{E_{ss}-U_{mm}}\mu_{s'}^{(s)} & \text{if } m\in R\ ,\end{cases} \tag{61a}$$

where

$$\eta_s=\left[1+\sum_{s',s''\in S}\sum_{r\in R}\mu_{s'}^{(s)}\mu_{s''}^{*(s)}\frac{U^{S*}_{rs'}(E_s)U^S_{rs''}(E_s)}{(E_s-U_{rr})^2}\right]^{-1/2} \tag{61b}$$

The theorem yields the method of approximation, which is used, for example, in Kane's theory of III-V semiconductor compounds.[19] The standard Schrödinger perturbation theory[29] is a special case of this more general method.

To proceed, we define

$$\mathscr{H}^D_{n\ell}=\mathscr{H}^{\rm SL}_{n\ell;n\ell}\ , \tag{62}$$

$$V'_{n\ell;n'\ell'}=(1-\delta_{nn'}\delta_{\ell\ell'})V_{n\ell;n'\ell'}\ . \tag{63}$$

We further define the matrix function $\mathscr{Z}_{n\ell;n'\ell'}(E)$ in terms of the infinite series

$$\mathscr{Z}_{n\ell;n'\ell'}(E)=\mathscr{H}^{\rm SL}_{n\ell,n'\ell'}+\sum_{n_1,\ell_1}{}'\frac{V'_{n\ell;n_1\ell_1}V'_{n_1\ell_1;n'\ell'}}{(E-\mathscr{H}^D_{n_1\ell_1})}+\sum_{n_1,\ell_1,n_2,\ell_2}{}'\frac{V'_{n\ell;n_1\ell_1}V'_{n_1\ell_1;n_2\ell_2}V'_{n_2\ell_2;n'\ell'}}{(E-\mathscr{H}^D_{n_1\ell_1})(E-\mathscr{H}^D_{n_2\ell_2})}+\cdots\ , \tag{64}$$

where the primes over the summation signs mean that the sums exclude the $n\ell$ terms. Consider an eigenvalue of (38) which is not degenerate. In Löwdin's method, it is given by the solution of the equation

$$\varepsilon_{n\ell}(\kappa)=\mathscr{Z}_{n\ell;n\ell}(\varepsilon_{n\ell}(\kappa))\ . \tag{65}$$

The solution of this equation must be such that

$$\lim_{W\to 0}\varepsilon_{n\ell}(\kappa)=E^B_{n\ell}(\kappa)\ . \tag{66}$$

In the Schrödinger perturbation theory, the same nondegenerate eigenvalue is given by

$$\varepsilon_{n\ell}(\kappa)=\mathscr{Z}_{n\ell;n\ell}(\mathscr{H}^D_{n\ell})\equiv\overline{\mathscr{Z}}_{n\ell;n\ell}\ . \tag{67}$$

In the following discussion we will set an overbar on $\mathscr{Z}$ whenever E is replaced by $\mathscr{H}^D$. Let us now consider the eigenstate corresponding to $\varepsilon_{n\ell}$. Define

$$a^{(n\ell)}_{n'\ell'}=\begin{cases}\eta_{n\ell} & \text{if } n=n',\ \ell=\ell'\ ,\\ \eta_{n\ell}\dfrac{\mathscr{Z}_{n'\ell';n\ell}(\varepsilon_{n\ell})}{(\varepsilon_{n\ell}-\mathscr{H}^D_{n'\ell'})} & \text{if } n\neq n',\ \text{or } \ell\neq\ell',\ \text{or both}\ ,\end{cases} \tag{68a}$$

$$\eta_{n\ell}=\left[1+\sum_{n'\ell'}{}'\frac{\mathscr{Z}^*_{n'\ell';n\ell}(\varepsilon_{n\ell})\mathscr{Z}_{n'\ell';n\ell}(\varepsilon_{n\ell})}{(\varepsilon_{n\ell}-\mathscr{H}^D_{n'\ell'})^2}\right]^{-1/2}\ . \tag{68b}$$

The nondegenerate eigenstate corresponding to $\varepsilon_{n\ell}$ is then given by

$$\psi_{n\ell\kappa}(\mathbf{x})=\eta_{n\ell}\left[\psi^B_{n\kappa+(2\pi\ell/L)\hat{\mathbf{z}}}(\mathbf{x})+\sum_{n'\ell'}{}'\frac{\mathscr{Z}_{n'\ell';n\ell}(\varepsilon_{n\ell})\psi^B_{n'\kappa+(2\pi\ell'/L)}(\mathbf{x})}{(\varepsilon_{n\ell}-\mathscr{H}^D_{n'\ell'})}\right]\ . \tag{69}$$

It is more common that there are degeneracies, because of the band structure of constituent homogeneous crystals. An important instance of this is the degeneracy between the $-|\ell|$ and $|\ell|$ components for finite ℓ. Consider a homogeneous crystal band n that is parabolic:

$$\begin{aligned}E^B_n(\kappa+(2\pi\ell/L)\hat{\mathbf{z}})&=E^B_n(0)+\frac{\hbar^2}{2m_{Bn}}\left[\kappa+\frac{2\pi\ell}{L}\hat{\mathbf{z}}\right]^2\\&=E^B_n(0)+\frac{\hbar^2\kappa^2}{2m_{Bn}}+\frac{2\pi^2\hbar^2\ell^2}{m_{Bn}L^2}\\&\quad+\frac{2\pi\ell\hbar^2}{m_{Bn}L}\hat{\mathbf{z}}\cdot\kappa\ ,\end{aligned} \tag{70}$$

where m_{Bn} is the effective mass of the band n of the B-type material. One can see from this expression that the leading term in the subband energy becomes degenerate for $\pm\ell$ and $\kappa_z=0$ as $W\to 0$. The degeneracy also shows itself by the divergence of the series for $\overline{\mathscr{Z}}$ obtained from (64). Thus, the two subbands $n\pm|\ell|$ are strongly coupled and must be separated from the other subbands. We again define a $\mathscr{Z}$ matrix as in (64), except that this time the sums exclude both $n\pm|\ell|$. This prevents the divergence of $\overline{\mathscr{Z}}$. We further define a 2×2 matrix $M_{n|\ell|}$:

$$M_{n|\ell|}=\begin{bmatrix}\mathscr{Z}_{n|\ell|;n|\ell|} & \mathscr{Z}_{n|\ell|;n-|\ell|}\\ \mathscr{Z}_{n-|\ell|;n|\ell|} & \mathscr{Z}_{n-|\ell|;n-|\ell|}\end{bmatrix}. \tag{71}$$

The eigenvalues are the solutions of the equation

$$\det(M_{n|\ell|}-E)=0\ . \tag{72}$$

This is an extremely complex algebraic equation which cannot be handled without further simplification. To a good approximation, one can replace $\mathscr{Z}$'s by $\overline{\mathscr{Z}}$'s in (71). Designate the resulting matrix by $\overline{M}_{n|\ell|}$. With $M_{n|\ell|}$ replaced by $\overline{M}_{n|\ell|}$ in (72), one has a much simpler quadratic equation to solve. The two eigenvalues are

$$\begin{aligned}\varepsilon^{\pm}_{n|\ell|}(\kappa)=&\tfrac{1}{2}(\overline{\mathscr{Z}}_{n|\ell|;n|\ell|}+\overline{\mathscr{Z}}_{n-|\ell|;n-|\ell|})\\&\pm\tfrac{1}{2}[(\overline{\mathscr{Z}}_{n|\ell|;n|\ell|}-\overline{\mathscr{Z}}_{n-|\ell|;n-|\ell|})^2\\&+4\overline{\mathscr{Z}}_{n|\ell|;n-|\ell|}\overline{\mathscr{Z}}_{n-|\ell|;n|\ell|}]^{1/2}\ .\end{aligned} \tag{73}$$

The normalized eigenvectors of $\overline{M}_{n|\ell|}$ corresponding to $\varepsilon^{\pm}_{n|\ell|}$,

$$\begin{aligned}&\overline{M}_{n|\ell|}u^{(n|\ell|\pm)}=\varepsilon^{\pm}_{n|\ell|}u^{(n|\ell|\pm)}\ ,\\&u^{(n|\ell|\pm)}=\begin{bmatrix}u^{(n|\ell|\pm)}_{|\ell|}\\u^{(n|\ell|\pm)}_{-|\ell|}\end{bmatrix}\ ,\end{aligned} \tag{74}$$

are also readily obtained:

$$u^{(n|\ell|+)}_{|\ell|}=\overline{\mathscr{Z}}_{n|\ell|;n-|\ell|}(|\varepsilon^{+}_{n|\ell|}-\overline{\mathscr{Z}}_{n|\ell|;n|\ell|}|^2+|\overline{\mathscr{Z}}_{n|\ell|;n-|\ell|}|^2)^{-1/2}\ , \tag{75a}$$

$$u^{(n|\ell|+)}_{-|\ell|}=(\varepsilon^{+}_{n|\ell|}-\overline{\mathscr{Z}}_{n|\ell|;b|\ell|})(|\varepsilon^{+}_{n|\ell|}-\overline{\mathscr{Z}}_{n|\ell|;n|\ell|}|^2+|\overline{\mathscr{Z}}_{n|\ell|;n-|\ell|}|^2)^{-1/2}\ , \tag{75b}$$

$$u^{(n|\ell|-)}_{|\ell|}=(\varepsilon^{-}_{n|\ell|}-\overline{\mathscr{Z}}_{n-|\ell|;n-|\ell|})(|\varepsilon^{-}_{n|\ell|}-\overline{\mathscr{Z}}_{n-|\ell|;n-|\ell|}|^2+|\overline{\mathscr{Z}}_{n-|\ell|;n|\ell|}|^2)^{-1/2}\ , \tag{75c}$$

$$u^{(n|\ell|-)}_{-|\ell|}=\overline{\mathscr{Z}}_{n-|\ell|;n|\ell|}(|\varepsilon^{-}_{n|\ell|}\overline{\mathscr{Z}}_{n-|\ell|;n-|\ell|}|^2+|\overline{\mathscr{Z}}_{n-|\ell|;n|\ell|}|^2)^{-1/2}\ . \tag{75d}$$

The coefficients of the expansion in (59) become

$$a^{(n|\ell|\pm)}_{n|\ell|}=\eta_{n|\ell|\pm}u^{(n|\ell|\pm)}_{|\ell|}\ , \tag{76a}$$

$$a^{(n|\ell|\pm)}_{n-|\ell|}=\eta_{n|\ell|\pm}u^{(n|\ell|\pm)}_{-|\ell|}\ , \tag{76b}$$

$$a^{(n|\ell|\pm)}_{n'\ell'}=\eta_{n|\ell|\pm}\sum_{\ell''=\pm|\ell|}\frac{\mathscr{Z}_{n'\ell';n\ell''}(\varepsilon^{\pm}_{n|\ell|})u^{(n|\ell|\pm)}_{\ell''}}{(\varepsilon^{\pm}_{n|\ell|}-\mathscr{H}^{D}_{n'\ell'})}\quad\text{for } n'\neq n \text{ and/or } \ell'\neq\pm|\ell|\ , \tag{76c}$$

where $\eta_{n|\ell|\pm}$ is the normalization constant:

$$\eta_{n|\ell|\pm}=\left[1+\sum_{n_1\ell_1}{}'\sum_{\ell',\ell''=\pm|\ell|}\frac{u^{(n|\ell|\pm)*}_{\ell'}u^{(n|\ell|\pm)}_{\ell''}}{(\varepsilon^{\pm}_{n|\ell|}-\mathscr{H}^{D}_{n_1\ell_1})^2}\mathscr{Z}^{*}_{n_1\ell_1;n\ell'}(\varepsilon^{\pm}_{n|\ell|})\mathscr{Z}_{n_1\ell_1;n\ell''}(\varepsilon^{\pm}_{n|\ell|})\right]^{-1/2}\ . \tag{76d}$$

The prime in the first sum means that $n_1\ell_1$ cannot be equal to $n\pm\ell$. From (76a)—(76c), one obtains the new subband states

$$\begin{aligned}\psi_{n|\ell|\kappa\pm}(\mathbf{x})=\eta_{n|\ell|\pm}\Bigg[&u^{(n|\ell|\pm)}_{|\ell|}\psi^{B}_{n\kappa+(2\pi|\ell|/L)\hat{\mathbf{z}}}(\mathbf{x})+u^{(n|\ell|\pm)}_{-|\ell|}\psi^{B}_{n\kappa-(2\pi|\ell|/L)\hat{\mathbf{z}}}(\mathbf{x})\\&+\sum_{n',\ell'}{}'\left[\frac{\mathscr{Z}_{n'\ell';n|\ell|}(\varepsilon^{\pm}_{n|\ell|})u^{(n|\ell|\pm)}_{|\ell|}+\mathscr{Z}_{n'\ell';n-|\ell|}(\varepsilon^{\pm}_{n|\ell|})u^{(n|\ell|\pm)}_{-|\ell|}}{(\varepsilon^{\pm}_{n|\ell|}-\mathscr{H}^{D}_{n'\ell'})}\right]\psi^{B}_{n'\kappa+(2\pi\ell'/L)\hat{\mathbf{z}}}(\mathbf{x})\Bigg]\ .\end{aligned} \tag{77}$$

If there are further degeneracies, they show up by making the present expression for $\overline{\mathscr{Z}}$ blow up. The above discussion makes it clear how to handle this problem. These degenerate states are also excluded from the sums in (64), and new matrices M are defined. If there are other states degenerate with $n\pm|\ell|$, then the dimension of M in (71) is increased to include these states. If the new degenerate states form a separate group among themselves, a new matrix M is defined and diagonalized just for these states.

The above discussion is based upon the matrix functions $\mathscr{Z}$ and $\overline{\mathscr{Z}}$, and therefore on whether the infinite series in their definitions are well defined and convergent. It is clear that for the series for $\overline{\mathscr{Z}}$ to be convergent, the matrix elements of V' must be such that

$$\left|\frac{V'_{n'\ell';n''\ell''}}{\mathscr{H}^{D}_{n\ell}-\mathscr{H}^{D}_{n'\ell'}}\right|<1\ . \tag{78}$$

If the series for $\overline{\mathscr{Z}}$ is slowly convergent, or not convergent at all for some states, one needs to use $\mathscr{Z}(E)$ for arbitrary energy E, and solve complex algebraic equations of the same type as (72).

The preceding discussion has been rather abstract. Let us consider a superlattice crystal composed of two-band materials, and apply the preceding formulas to this extremely simple case. What we mean by the two-band model is that we assume that the position operator in (47) has nonvanishing matrix elements just for two bands, one conduction and one valence band. We further assume

that it is a constant independent of momentum. Its $\hat{z}$ component can be written in terms of the Pauli matrix σ_y as

$$X_z^B=\frac{P_{Bcv}^z}{m_e(E_c^B-E_v^B)}\sigma_y \ . \tag{79}$$

Let us also define

$$\xi=\frac{2\pi P_{Bcv}^z}{m_e L(E_c^B-E_v^B)} \ . \tag{80}$$

From (53a),

$$D^{\ell\dagger}D^{\ell'}=\exp\left[-\frac{2\pi i}{L}(\ell-\ell')X_z^B\right] \tag{81a}$$

and

$$\exp\left[-\frac{2\pi i}{L}(\ell-\ell')X_z^B\right]=\begin{bmatrix}\cos[\xi(\ell-\ell')] & -\sin[\xi(\ell-\ell')]\\ \sin[\xi(\ell-\ell')] & \cos[\xi(\ell-\ell')]\end{bmatrix} \ . \tag{81b}$$

Thus, from (57) we find

$$V_{c\ell;c\ell'}=V_{v\ell;v\ell'}=\rho L_A W(0)\cos[\xi(\ell-\ell')]\times\frac{\sin[(\pi L_A/L)(\ell-\ell')]}{[(\pi L_A/L)(\ell-\ell')]} \ . \tag{82a}$$

$$V_{c\ell;v\ell'}=-V_{v\ell;c\ell'}=-\rho L_A W(0)\sin[\xi(\ell-\ell')]\times\frac{\sin[(\pi L_A/L)(\ell-\ell')]}{[(\pi L_A/L)(\ell-\ell')]} \ . \tag{82b}$$

Consider now the nondegenerate $\varepsilon_{c0}(\kappa)$ and $\varepsilon_{v0}(\kappa)$. From (64), (67), and (82), we find

$$\varepsilon_{c0}(\kappa)=E_{c0}^B(\kappa)+\rho L_A W(0)+\sum_{\ell}\frac{(1-\delta_{\ell 0})\rho^2 L_A^2 W^2(0)\cos^2(\ell\xi)\sin^2(\pi L_A/L)}{[E_{c0}^B(\kappa)-E_{c\ell}^B(\kappa)](\pi L_A\ell/L)^2}-\sum_{\ell}\frac{(1-\delta_{\ell 0})\rho^2 L_A^2 W^2(0)\sin^2(\ell\xi)\sin^2(\pi L_A\ell/L)}{[E_{c0}^B(\kappa)-E_{v0}^B(\kappa)](\pi L_A\ell/L)^2}+\cdots \ . \tag{83}$$

Interchanging c with v yields $\varepsilon_{v0}(\kappa)$.

For finite ℓ, we use (73). Let us take just the leading terms in $\mathscr{T}$. For parabolic $n=c$:

$$\mathscr{T}_{c\pm|\ell|;c\pm|\ell|}\simeq E_c^B(0)+\rho L_A W(0)+\frac{\hbar^2\kappa^2}{2m_{Bc}}+\frac{2\pi^2\hbar^2\ell^2}{m_{Bc}L^2}\pm\frac{2\pi|\ell|\hbar^2\kappa_z}{m_{Bc}L} \ , \tag{84a}$$

$$\mathscr{T}_{c\pm|\ell|;c\mp|\ell|}\simeq-\rho L_A W(0)\cos(2\ell\xi)\frac{\sin(2\pi\ell L_A/L)}{(2\pi\ell L_A/L)} \ . \tag{84b}$$

Thus

$$\varepsilon_{c|\ell}^{\pm}(\kappa)=E_c^B(0)+\rho L_A W(0)+\frac{\hbar^2\kappa^2}{2m_{Bc}}+\frac{2\pi^2\hbar^2\ell^2}{m_{Bc}L^2}\pm\left[\left[\frac{2\pi^2\hbar^2\ell\kappa_z}{m_{Bc}L}\right]^2+\rho^2L_A^2W^2(0)\cos^2(2\ell\xi)\frac{\sin^2(2\pi\ell L_A/L)}{(2\pi\ell L_A/L)^2}\right]^{1/2} \ . \tag{85}$$

For the convenience of writing the vectors $u^{(c|\ell|\pm)}$, define

$$v_\ell=\frac{2\pi|\ell|\hbar}{m_{Bc}L} \ , \tag{86a}$$

$$\tilde{W}=\rho L_A W(0) \ , \tag{86b}$$

$$S_\ell=\frac{\sin(2\pi\ell L_A/L)}{2\pi\ell L_A/L)} \ , \tag{86c}$$

$$C_\ell=\cos(2\ell\xi) \ . \tag{86d}$$

The vectors $u^{(c|\ell|\pm)}$ are then given by

$$u_{|\ell|}^{(c|\ell|\pm)}=\frac{-\tilde{W}C_\ell S_\ell}{[\tilde{W}^2C_\ell^2S_\ell^2+|-\hbar v_\ell\kappa_z+(\hbar^2v_\ell^2\kappa_z^2+\tilde{W}^2C_\ell^2S_\ell^2)^{1/2}|^2]^{1/2}} \ , \tag{87a}$$

$$u_{-|\ell|}^{(c|\ell|+)}=\frac{-\hbar v_\ell\kappa_z+(\hbar^2v_\ell^2\kappa_z^2+\tilde{W}^2C_\ell^2S_\ell^2)^{1/2}}{[\tilde{W}^2C_\ell^2S_\ell^2+|-\hbar v_\ell\kappa_z+(\hbar^2v_\ell^2\kappa_z^2+\tilde{W}^2C_\ell^2S_\ell^2)^{1/2}|^2]^{1/2}} \ , \tag{87b}$$

$$u_{|\ell|}^{(c|\ell|-)}=-u_{-|\ell|}^{(c|\ell|+)} \ , \tag{87c}$$

$$u_{-|\ell|}^{(c|\ell|-)}=u_{|\ell|}^{(c|\ell|+)} \ . \tag{87d}$$

Similar expressions are found for $\varepsilon_{v|\ell|}^{\pm}$ and $u^{(v|\ell|\pm)}$.

Consider $\varepsilon_{c|\ell|}^{\pm}$ given by (85). The first two terms define the position of the energy band, taking into account the band offsets between the two materials. The third term gives mainly the dispersion in the transverse directions. The fourth term comes from the folding of the Brillouin zone and describes the partial localization of the electron. For $L_A=L_B=L/2$, this term becomes

$$\frac{2\pi^2\hbar^2\ell^2}{m_{Bc}L^2}=\frac{\hbar^2}{2m_{Bc}}\left[\frac{\pi\ell}{L_A}\right]^2 . \tag{88}$$

This is identical to the standard expression for a rectangular well of width L_A (for an infinitely deep well).

The same relation can be discerned in the subband wave function (77). In the limit that $\kappa_z\to 0$, Eqs. (87a)—(87d) yield

$$u_{\pm|\ell|}^{(c|\ell|+)}\to\mp\frac{1}{\sqrt{2}} , \tag{89a}$$

$$u_{\pm|\ell|}^{(c|\ell|-)}\to-\frac{1}{\sqrt{2}} . \tag{89b}$$

Thus for small κ_z, the first two terms in (77) are proportional to

$$u_{|\ell|}^{(c|\ell|+)}\psi^B_{c\kappa+(2\pi|\ell|/L)\hat{\mathbf{z}}}(\mathbf{x})+u_{-|\ell|}^{(c|\ell|+)}\psi^B_{c\kappa-(2\pi|\ell|/L)\hat{\mathbf{z}}}(\mathbf{x})$$
$$\sim\sum_{\mathbf{G}}e^{i(\mathbf{k}_\perp-\mathbf{G})\cdot\mathbf{x}}\left[\frac{-1}{\sqrt{2}}\exp\left[i\frac{2\pi|\ell|z}{L}\right]\phi_c^B\left[\mathbf{k}_\perp-\frac{2\pi|\ell|\hat{\mathbf{z}}}{L}-\mathbf{G}\right]+\frac{1}{\sqrt{2}}\exp\left[-i\frac{2\pi|\ell|z}{L}\right]\phi_c^B\left[\mathbf{k}_\perp+\frac{2\pi|\ell|\hat{\mathbf{z}}}{L}-\mathbf{G}\right]\right] . \tag{90}$$

If we neglect the ℓ-dependent terms in the arguments of the momentum Bloch functions, then Eq. (90) is approximately

$$-i\sqrt{2}\sin(2\pi|\ell|z/L)\psi^B_{c\mathbf{k}_\perp}(\mathbf{x}) . \tag{91a}$$

Similarly

$$u_{|\ell|}^{(c|\ell|-)}\psi^B_{c\kappa+(2\pi|\ell|/L)\hat{\mathbf{z}}}(\mathbf{x})+u_{-|\ell|}^{(c|\ell|-)}\psi^B_{c\kappa-(2\pi|\ell|/L)\hat{\mathbf{z}}}(\mathbf{x})\sim-i\sqrt{2}\cos(2\pi|\ell|z/L)\psi^B_{c\mathbf{k}_\perp}(\mathbf{x}) . \tag{91b}$$

Equations (91a) and (91b) are instructive in showing the connection between $\psi_{c\kappa|\ell|\pm}$ and odd and even parity rectangular potential-well states.

We should point out one major difference between our theory and the quantum-well model. In a potential-well problem, even and odd eigenstates correspond to different quantum numbers $|\ell|$. In the above expressions, however, they correspond to the same integer $|\ell|$. Evenness and oddness for the superlattice subbands appear to be associated with another quantum number which can take on only two values, plus or minus (or 1,2). Clearly, in the present theory the assignment of quantum numbers to the superlattice spectrum differs from the assignments based on quantum-well states.

The above comparisons with the quantum-well model depend heavily on the fact that the homogeneous crystal bands are parabolic. If they are not parabolic, it is much harder to make comparisons. For some narrow-gap semiconductors, conduction and valence bands can be approximated with linear dispersion relations.[30] For example, let

$$E_c^B(\mathbf{k})=E_c^B(0)+|\alpha\cdot\mathbf{k}| . \tag{92a}$$

The folded conduction-band energy then becomes

$$E_{c\ell}^B(\kappa)=E_c^B(0)+|\boldsymbol{\alpha}\cdot\boldsymbol{\kappa}+2\pi\ell\alpha_z/L| . \tag{92b}$$

Using (73), (84), and (86b)—(86d), we find

$$\varepsilon_{c|\ell|}^{\pm}(\kappa)=E_c^B(0)+\tfrac{1}{2}(|\boldsymbol{\alpha}\cdot\boldsymbol{\kappa}+2\pi\ell\alpha_z/L|+|\boldsymbol{\alpha}\cdot\boldsymbol{\kappa}-2\pi\ell\alpha_z/L|)$$
$$\pm[\tfrac{1}{4}(|\boldsymbol{\alpha}\cdot\boldsymbol{\kappa}+2\pi\ell\alpha_z/L|-|\boldsymbol{\alpha}\cdot\boldsymbol{\kappa}-2\pi\ell\alpha_z/L|)^2+\tilde{W}^2C_\ell^2S_\ell^2]^{1/2} . \tag{92c}$$

The dependence on $|\ell|$ here is quite different than in (88).

Let us return to Eq. (85) again. The last term, which is a square root, makes the subbands nonparabolic in the $\hat{\mathbf{z}}$ direction. In the x,y directions they are still parabolic. Because of nonparabolicity, one must be careful in assigning an effective mass for a subband. The effective mass can be quite different for $\kappa_z=0$ and κ_z finite for nonparabolic bands. For $\ell\neq 0$, we find from (85) that the effective masses as $\kappa_z\to 0$ are given by

$$\frac{1}{m_{c|\ell|}^{\pm}}=\frac{1}{\hbar^2}\left[\frac{\partial^2\varepsilon_{c|\ell|}^{\pm}}{\partial\kappa_z^2}\right]_{\kappa=0}=\frac{1}{m_{Bc}}\left[1\pm\frac{4\pi^2\hbar^2\ell^2}{m_{Bc}L^2\rho L_A|W(0)\cos2\xi\ell|}\left|\frac{(2\pi\ell L_A/L)}{\sin(2\pi\ell L_A/L)}\right|\right] . \tag{93}$$

For $\ell=0$, we use (83):

$$\frac{1}{m_{c0}}=\frac{1}{m_{Bc}}\left[1-\frac{2m_{Bc}^2L^8\rho^2W^2(0)}{\pi^6\hbar^4}\sum_{\ell=1}^{\ell_0-1}\frac{1}{\ell^8}\cos^2(\ell\xi)\sin^2\left[\frac{\pi\ell L_A}{L}\right]\pm\cdots\right]. \tag{94}$$

Note that

$$\frac{m_{c0}}{m_{Bc}}>1,\quad \frac{m_{c|\ell|}^-}{m_{Bc}}>1,\quad \frac{m_{c|\ell|}^+}{m_{Bc}}<1. \tag{95}$$

For large ℓ, the difference of $m_{c|\ell|}^{\pm}/m_{Bc}$ from unity becomes more pronounced.

A final comment concerns band mixing. Even with the lowest-order approximation for $\overline{\mathscr{H}}$, as in (84), band mixing occurs throughout the formulas. In the subband energies, band mixing is associated with the parameter ξ. If ξ is zero or some multiple of π, then band mixing does not occur [the matrix (81b) becomes $\pm$ identity]. In the subband wave functions given by (77), the last set of terms under the summation sign represents the band-mixing terms. These terms are responsible for the modification of the selection rules for radiative transitions.

Note added. We recently became aware that M. Jaros and his collaborators[31] have also used momentum Bloch functions in their numerical pseudopotential calculations of superlattice state energies.

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APPENDIX

The Schrödinger equation for the momentum Bloch function of the band n can be written as

$$\frac{\hbar^2\mathbf{k}^2}{2m}\phi_n(\mathbf{k})=E_n(\mathbf{k})\phi_n(\mathbf{k})-\sum_{\mathbf{G}'}\mathscr{V}_{G'}\phi_n(\mathbf{k}-\mathbf{G}'). \tag{A1}$$

Multiplying (A1) with $\phi_n(\mathbf{k}-\mathbf{G})$, summing over the bands, and using (2a), one finds

$$\mathscr{V}_{\mathbf{G}}=\sum_n E_n(\mathbf{k})\phi_n^*(\mathbf{k}-\mathbf{G})\phi_n(\mathbf{k})-\frac{\hbar^2\mathbf{k}}{2m}\delta_{\mathbf{G},0}. \tag{A2}$$

The $\mathbf{k}$ dependence of E_n's and ϕ_n's must be such that the right-hand side is independent of $\mathbf{k}$, since the left-hand side is. Setting $\mathbf{k}=\mathbf{0}$, one obtains (3c). Setting $u_{n\mathbf{k}}(\mathbf{x})=e^{i\mathbf{k}\cdot\mathbf{x}}\psi_{n\mathbf{k}}(\mathbf{x})$, one has, from (1) and (A2),

$$V(\mathbf{x})=-\frac{\hbar^2\mathbf{k}^2}{2m}+\sum_n E_n(\mathbf{k})\phi_n(\mathbf{k})u_{n\mathbf{k}}^*(\mathbf{x}). \tag{A3}$$

Again, the $\mathbf{k}$ dependence must cancel out in the overall expression on the right-hand side. Setting $\mathbf{k}=\mathbf{0}$, one finds (3a).

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