Numerically stable Hermitian secular equation for the envelope-function approximation for superlattices

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A method is developed for implementing the coupled-band envelope-function-approximation (EFA) formalism for the calculation of the electronic structure of superlattices. The approach overcomes the difficulties in handling exponentially growing and decaying wave-function components, in particular, the so-called wing solutions, as is the case with existing secular equations. As importantly, the secular equation, which, in general, is general complex, is recast into a Hermitian form, which makes it easy to separate degenerate eigensolutions of the superlattice problem. Therefore, it is not necessary to first find a unitary transformation to eliminate the Kramers degeneracy of the starting $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian. In the case of the simple Kronig-Penney model, the present formalism recasts the characteristic equation into a form that directly exhibits its parentage to the underlying quantum-well problem. The present method can be used in conjunction with Burt's EFA formalism in the form of a coupled differential equation with piecewise-constant coefficients. The method is demonstrated on the example of the technologically important semiconducting $InAs/In_xGa_{1-x}Sb$ type-II superlattice. [S0163-1829(96)03340-1]

I. INTRODUCTION

The envelope-function approximation (EFA) continues to be a popular method for calculating the electronic structure of band-gap engineered materials such as quantum wells and superlattices.[1–3] However, the numerical implementation of the formalism suffers from two difficulties. First, the commonly used EFA secular equations[4–6] have difficulties in handling exponentially growing or decaying wave function components, especially the spurious evanescent solutions, sometimes called the ''wing solutions.''[7] A solution for handling such numerical problems for quantum wells was offered earlier.[8] In the case of nonperiodic semiconductor heterostructures, the mathematical problems caused by exponentially growing and decaying solutions are known to be acute in the transfer-matrix approach.[9,10] Ko and Inkson[11] were able to solve the problem through their scattering matrix approach.

Second, the superlattice secular equation is general complex, thus non-Hermitian.[4,5] In practice, this means that the secular determinant does not change sign at the root in the case of Kramers degeneracy, which makes it difficult to locate the eigenvalues of the superlattice problem. Such a degeneracy can be eliminated only if the bulk $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian can be exactly block diagonalized, which is difficult for higher-order Hamiltonians.[12]

In this paper the superlattice secular equation is recast in a form in which the evanescent solutions occur not in exponentials but inside hyperbolic tangents. Whereas for large arguments the exponentials lead to over and underflows, the hyperbolic tangents tend to ± 1. However, the problem of real spurious solutions, which lead to oscillatory behavior, is not addressed in this paper since such solutions more often cause physical but not mathematical problems. Next, for an N-band EFA problem, the secular equation is transformed into a $2N\times 2N$ Hermitian form, whose diagonalization produces N pairs of real eigenvalues. The product of distinct eigenvalues changes sign at the roots of the superlattice problem and Kramers degenerate solutions correspond to the two zero-diagonal elements of the secular matrix at the root. Therefore, it is not necessary to first find a unitary transformation to eliminate the Kramers degeneracy of the starting $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian.

In the case of the simple Kronig-Penney model,[13] a different characteristic equation is obtained, which, in the limit of very wide barriers, becomes the characteristic equation for a quantum well. The equation also furnishes convenient solutions for bands at the center and the edges of the Brillouin zone. In addition, the present method can be used in conjunction with Burt's EFA formalism[14] in the form of a coupled differential equation with piecewise-constant coefficients, as implemented by Foreman.[15] The method will be demonstrated on the example of the technologically important semiconducting $InAs/In_xGa_{1-x}Sb$ type-II superlattice.[16–18]

This paper is arranged as follows. Section II deals with the construction of the EFA secular equation based on Burt's boundary conditions.[14] Section III shows how the secular equation can be written in a form that does not lead to numerical instabilities. As a test of the formalism, it is shown that it reduces to the familiar Kronig-Penney equation in the case of a single band. However, even in this simple case, a different characteristic equation is derived and analyzed to obtain additional insights into band formation. Section IV shows how the secular equation can be made Hermitian by a simple matrix operation. In Sec. V, the formalism is applied to a sample calculation for an $InAs/In_xGa_{1-x}Sb$ superlattice. Conclusions are presented in Sec. VI.

II. THEORY

A. Notation

Let the superlattice consist of an infinite succession of material A of width $2a$ and material B of width $2b$. In a

superlattice, the total wave function for the Mth subband is an eigenstate of q and $\mathbf{k}_\parallel$, crystal momenta in the growth direction and parallel to the plane of the well, respectively. The total wave function is then given by[14]

$$\Psi_M(\mathbf{k}_\parallel q,\mathbf{r})=e^{i\mathbf{k}_\parallel\cdot\mathbf{r}}\sum_\nu F_\nu(M,\mathbf{k}_\parallel q,z)u_\nu(\mathbf{r}), \tag{1}$$

where $u_\nu(\mathbf{r})$ are a complete set of cell-periodic functions, which are required to be the same throughout the structure, independent of material composition,[14,15] and $F_\nu(M,\mathbf{k}_\parallel q,z)$ are the corresponding envelope-function amplitudes. Because the potential has the period $d=2a+2b$ in the growth direction, the Bloch condition requires that

$$F_\nu(M,\mathbf{k}_\parallel q,z+d)=e^{iqd}F_\nu(M,\mathbf{k}_\parallel q,z). \tag{2}$$

In arriving at an effective-mass equation, Burt first neglects the nonlocal parts of the exact EFA Schrödinger equation.[14] Next, he eliminates small envelope functions in favor of the larger ones, chosen to be N in number. This results in an N coupled-band formalism with a Hermitian $N\times N$ EFA Hamiltonian H whose formal structure is given by the following expansion in powers of d/dz:

$$H\left(\mathbf{k}_\parallel,-i\frac{d}{dz}\right)=\left(-i\frac{d}{dz}\right)H_2(\mathbf{k}_\parallel)\left(-i\frac{d}{dz}\right)+\frac{1}{2}\left[H_{1R}(\mathbf{k}_\parallel)\times\left(-i\frac{d}{dz}\right)+\left(-i\frac{d}{dz}\right)H_{1L}(\mathbf{k}_\parallel)\right]+H_0(\mathbf{k}_\parallel). \tag{3}$$

In the conventional EFA,[3] the left and right coefficients are equal, so that

$$H_{1L}(\mathbf{k}_\parallel)=H_{1R}(\mathbf{k}_\parallel). \tag{4}$$

In Burt's formalism, however, the left and right coefficients only have to be Hermitian conjugates of one another,

$$[H_{1L}(\mathbf{k}_\parallel)]^\dagger=H_{1R}(\mathbf{k}_\parallel); \tag{5}$$

moreover, the exact meaning of the coefficients is different in conventional and Burt's formalisms.[14] The form of Eq. (3) is important when determining the connectivity of envelope function solutions at interfaces. Away from interfaces, one can combine the left and right coefficients in the Hamiltonian by forming

$$[H_{1L}(\mathbf{k}_\parallel)+H_{1R}(\mathbf{k}_\parallel)]/2\equiv H_1(\mathbf{k}_\parallel). \tag{6}$$

Because of the Hermiticity of the original $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian, the three $N\times N$ matrices H_0, H_1, and H_2 are Hermitian.[4] Boundary conditions require the continuity of envelope functions across interfaces as well as of a quantity obtained by integrating the Schrödinger equation across an interface, so that

$$F=F,$$

$$(iH_{1L}/2)F+H_2F'=(iH_{1L}/2)F+H_2F' \tag{7}$$

on both sides of an interface, where F are understood as N-column vectors. Note that the second condition uses $H_{1L}(\mathbf{k}_\parallel)$ rather than $H_1(\mathbf{k}_\parallel)$, as in conventional theory.

B. Construction of the envelope function

The N-column vector envelope function for the Mth band is the solution of the $N\times N$ coupled differential equation in each layer,[1–5]

$$\sum_{\nu=1}^{N}H_{\mu\nu}^{A,B}\left(\mathbf{k}_\parallel,-i\frac{d}{dz}\right)F_\nu^{A,B}(M,\mathbf{k}_\parallel q,z)=E_M(\mathbf{k}_\parallel q)F_\mu^{A,B}(M,\mathbf{k}_\parallel q,z), \tag{8}$$

where k_z has been replaced by the derivative in the z direction. By multiplying the original Hamiltonian by the inverse of the H_2 matrix, one can rewrite the original Hamiltonian equation in each layer of the heterostructure as

$$\frac{d^2F}{dz^2}+i(H_2)^{-1}H_1\frac{dF}{dz}-(H_2)^{-1}(H_0-E)F=0. \tag{9}$$

Augmenting the vector F with the vector F', it is possible to recast the EFA Schrödinger equation as a first-order differential equation

$$\begin{pmatrix}0 & I\\ H_2^{-1}(H_0-E) & -iH_2^{-1}H_1\end{pmatrix}\begin{pmatrix}F\\F'\end{pmatrix}=\frac{d}{dz}\begin{pmatrix}F\\F'\end{pmatrix}. \tag{10}$$

C. General solution

The solution of Eq. (10) is a superposition of functions of the form

$$\begin{pmatrix}F\\F'\end{pmatrix}=e^{ik_iz}\begin{pmatrix}C_i\\ik_iC_i\end{pmatrix}, \tag{11}$$

where C_i are N-column vectors for each $k_i(\mathbf{k}_\parallel,E)$. The exponents k are obtained by solving the $2N\times 2N$, complex, non-Hermitian eigenvalue problem[4,19]

$$\begin{pmatrix}-k & I\\ H_2^{-1}(H_0-E) & -H_2^{-1}H_1-k\end{pmatrix}\begin{pmatrix}C\\kC\end{pmatrix}=0. \tag{12}$$

The solution yields $2N$ linearly independent eigenvectors $C_i\equiv C(\mathbf{k}_\parallel,k_i)$ and $2N$ corresponding, complex eigenvalues k_i.

It is well known that, in the case of the 8×8 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian, the solutions for exponents $k_i(\mathbf{k}_\parallel,E)$ contain spurious solutions.[1,4,5,20] In the case of $GaAs/Al_xGa_{1-x}As$ and $InAs/In_xGa_{1-x}Sb$ heterojunctions, the spurious solutions can be large real (leading to propagating states) or imaginary numbers (resulting in evanescent states). Using a 2×2 model involving the conduction and light-hole bands, it can be shown that when $m_c^*m_L>0$ the spurious exponent is real and when $m_c^*m_L<0$ the spurious exponent is pure imaginary.[8] Solving analytically a 3×3 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian at $\mathbf{k}_\parallel=0$, involving the conduction, light-hole, and spin-orbit bands, exponents k are found to switch from real to imaginary depending on whether the quantity $1-8\gamma_2^2/(\gamma_1+2\gamma_2)\gamma_1$ is greater or smaller than zero.[8]

It is beyond the scope of this paper to discuss thoroughly the physical problems introduced by the spurious solutions or the possible means for their elimination. In this author's experience, spurious evanescent or oscillatory solutions make small contributions to the total wave function and even less to the calculated energies. Sometimes, one can convert

an oscillatory to an evanescent spurious solution by a small adjustment of the Luttinger parameters.

D. Properties of vectors $C(\mathbf{k}_\parallel,k_i)$ and exponents k_i

Equation (12) is equivalent to the non-Hermitian Hamiltonian[4]

$$H(\mathbf{k}_\parallel,k_i)C(\mathbf{k}_\parallel,k_i)=[H_2(\mathbf{k}_\parallel)k_i^2+H_1(\mathbf{k}_\parallel)k_i + H_0(\mathbf{k}_\parallel)]C(\mathbf{k}_\parallel,k_i)=EC(\mathbf{k}_\parallel,k_i). \tag{13}$$

Since $k_i(\mathbf{k}_\parallel,E)$ are in general complex, for each right eigenvector $C(\mathbf{k}_\parallel,k_i)$ there is a corresponding left eigenvector $L(\mathbf{k}_\parallel,k_i)$, which satisfies

$$L(\mathbf{k}_\parallel,k_i)H(\mathbf{k}_\parallel,k_i)=EL(\mathbf{k}_\parallel,k_i). \tag{14}$$

As shown by Smith and Mailhiot,[4] Eq. (12) has N pairs of doubly degenerate solutions. Also, if $k_i(\mathbf{k}_\parallel,E)$ is a solution, so are $-k_ik_i^*,-k_i^*$. The left- and right-hand eigenvectors satisfy the relation[4]

$$C_{i*}\equiv C(\mathbf{k}_\parallel,k_i^*)=L(\mathbf{k}_\parallel,k_i)^\dagger\equiv L_i^\dagger. \tag{15}$$

The orthogonality condition reads[4]

$$C_{j*}^\dagger[H_2(k_j+k_i)+H_1]C_i=J_{j*i}\delta_{ij}, \tag{16}$$

where J has the units of current density. The orthogonality relation becomes an orthonormality relation with the normalization of the eigenvectors

$$C_i\rightarrow C_i/\sqrt{J_{i*i}}, \tag{17}$$

$$L_i\rightarrow L_i/\sqrt{J_{i*i}}. \tag{18}$$

E. Wave-function expansion

The envelope wave function is a sum over all periods m of the superlattice,

$$F_\nu(M,\mathbf{k}_\parallel q,z) = \sum_m \sum_{i=1}^{2N} \begin{cases} c_i^{A,m}C_\nu^A(\mathbf{k}_\parallel,k_i)e^{ik_i^Az}, & md+b\leqslant z<md+b+2a \\ c_i^{B,m}C_\nu^B(\mathbf{k}_\parallel,k_i)e^{ik_i^Bz}, & md-b\leqslant z<md+b. \end{cases} \tag{19}$$

However, periodicity requires that

$$c_i^{A,m}(\mathbf{k}_\parallel q)=e^{i(q-k_i^A)md}c_i^{A,0}(\mathbf{k}_\parallel q), \qquad c_i^{B,m}(\mathbf{k}_\parallel q)=e^{i(q-k_i^B)md}c_i^{B,0}(\mathbf{k}_\parallel q) \tag{20}$$

in terms of the expansion coefficients for the zeroth period. From now on, $c_i^{A,B}$, without the superscript zero, will be used. The expansion coefficients also obey symmetry properties with respect to Brillouin-zone periodicity, mirror reflection symmetry, time reversal, inversion symmetry, and 180° rotation in the xy plane.

F. Burt's boundary conditions

Burt[14] has developed an exact envelope-function formalism that avoids *ad hoc* assumptions about the boundary conditions. In practical implementation of Burt's formalism (see, for example, Ref. 15), the effective-mass equation for the single- and coupled-band cases has the form of a differential equation with piecewise-constant coefficients. As implemented by Foreman, the boundary conditions require the continuity of

$$\begin{pmatrix} I & 0 \\ iH_{1L}/2 & H_2 \end{pmatrix}\begin{pmatrix} F \\ F' \end{pmatrix} \tag{21}$$

at each interface. For notational convenience, define a $2N\times 2N$ matrix

$$M=\begin{pmatrix} I & 0 \\ H_{1L}/2 & H_2 \end{pmatrix}\begin{pmatrix} C \\ CK \end{pmatrix}. \tag{22}$$

With this notation, the boundary conditions can be written compactly as

$$M_Ae^{iK_Ab}c^A=M_Be^{iK_Bb}c^B, \quad z=b \tag{23}$$

$$e^{-iqd}M_Ae^{iK_A(d-b)}c^A=M_Be^{-iK_Bb}c^B, \quad z=-b. \tag{24}$$

In constructing these equations, the following matrices are defined: a nonsquare $N\times 2N$ matrix

$$[C(\mathbf{k}_\parallel)]_{\nu i}\equiv C_\nu(\mathbf{k}_\parallel,k_i), \tag{25a}$$

a nonsquare $2N\times N$ matrix

$$[L(\mathbf{k}_\parallel)]_{i\nu}\equiv L_\nu(\mathbf{k}_\parallel,k_i), \tag{25b}$$

a diagonal $2N\times 2N$ matrix

$$[e^{iKb}]_{ij}\equiv\delta_{ij}e^{ik_ib}, \tag{26a}$$

and a diagonal $2N\times 2N$ matrix

$$K_{ij}\equiv k_i\delta_{ij}, \tag{26b}$$

Altogether, there are $4N$ equations in $4N$ unknowns c^A and c^B. At points of high symmetry (i.e., $q=0,\ \pm\pi/d$), these equations can be simplified further; in particular, solutions can be made eigenstates of parity, which reduces the size of the secular matrix to $N\times N$ only. With these definitions and normalizations [Eqs. (17) and (18)] the orthonormality condition [Eq. (16)] can be conveniently rewritten as

$$(L\ KL)\begin{pmatrix} H_1 & H_2 \\ H_2 & 0 \end{pmatrix}\begin{pmatrix} C \\ CK \end{pmatrix}=\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}. \tag{27}$$

Combining the two boundary conditions, one obtains the $2N\times 2N$ secular equation

$$\left\| \frac{[M_A e^{i2K_A a} M_A^{-1}][M_B e^{i2K_B b} M_B^{-1}] + [M_B e^{-i2K_B b} M_B^{-1}][M_A e^{-i2K_A a} M_A^{-1}]}{2} - \cos qd \right\| = 0. \tag{28}$$

The above matrix is not Hermitian, but can be made so, as will be shown in Sec. IV. It can also be reduced to a Kronig-Penney-like form.[13]

Diagonalizing Eq. (28), one finds that its eigenvalues are quadruply degenerate. The first double degeneracy is dictated by the invariance of the secular equation under the interchange $q \rightarrow -q$ and the second is the result of Kramers degeneracy.

The transfer-matrix formalism of Ram-Mohan, Yoo, and Aggarwal[5] results in a secular equation that can be brought to the same algebraic form as the equation above, since both methods are based on wave-function matching at boundaries. However, because of the work of Smith and Mailhiot[4] and of the developments in this paper (Secs. II C and II D and Appendix A), the properties of the various components of the secular equation are better known for the present method.

In practice, however, the secular equation is dominated by the large exponentials of the wing solutions and of other large, complex exponents, making numerical computation impossible or inaccurate. Using a GaAs/$Al_{0.3}Ga_{0.7}As$ 50 Å/50 Å superlattice as an example (8×8 EFA calculation, with input parameters from Ref. 8), the diagonalization of the secular equation produced 4 very large and 12 very small eigenvalues, differing by at least 18 orders of magnitude. The search for roots of the secular equation was impossible and, as a result, an approach that eliminates the effect of the large exponential terms was sought. (However, this form can be useful in the absence of spurious solutions and large complex exponents and for the case of short period superlattices.)

G. Kronig-Penney test

In the case of a one-band model, it was checked that the secular equation properly reduces to the familiar Kronig-Penney model result. In fact, the secular matrix Eq. (28) is diagonal, with four equal roots, each equal to

$$\cos qd = \cos 2k_B b \ \cos 2k_A a - \frac{1}{2}\left(\frac{m_A k_B}{m_B k_A} + \frac{m_B k_A}{m_A k_B}\right) \times \sin 2k_B b \ \sin 2k_A a, \tag{29}$$

where $k_A = \sqrt{2m_A(E-V)/\hbar^2}$, $k_B = \sqrt{2m_B E/\hbar^2}$, and V is the height of the barrier. Interestingly, although a superlattice is a chain of quantum wells, the characteristic equation for bound states in a finite quantum well contains only tangents not sines or cosines.[1] This dilemma will be resolved in Sec. III.

III. ALTERNATIVE SECULAR EQUATION

Since the spurious wing solutions and other complex and other solutions of Eq. (12) lead to numerical over- and underflows in the computer code, the evaluation of superlattice eigenvalues and wave functions is unreliable or even impossible. The same is true in the transfer-matrix formalism of Ram-Mohan *et al.*[5,6] In order to overcome this shortcoming, an alternative form of the secular equation was sought. Such an approach was successful in the case of the quantum-well formalism of Ref. 8, where the spurious solutions were contained inside hyperbolic tangents, which asymptotically approach ± 1 as their argument goes to $\pm\infty$.

Therefore, the strategy is to eliminate the exponentials in Eq. (28) in favor of hyperbolic tangents. First, all four boundary conditions [Eqs. (23) and (24)] are rewritten in the form of a super $4N \times 4N$ secular equation

$$\begin{pmatrix} M_A e^{iK_A b} & -M_B e^{iK_B b} \\ e^{-iqd} M_A e^{iK_A(d-b)} & -M_B e^{-iK_B b} \end{pmatrix} \begin{pmatrix} c^A \\ c^B \end{pmatrix} = 0. \tag{30}$$

Through a series of elementary matrix transformations (factoring and row additions), Eq. (30) can be recast as

$$\begin{pmatrix} M_A \cos(K_A a - qd/2) & -M_B \cos K_B b \\ iM_A \sin(K_A a - qd/2) & iM_B \sin K_B b \end{pmatrix} \begin{pmatrix} e^{-iqd/2} e^{iK_A d/2} c^A \\ c^B \end{pmatrix} = 0. \tag{31}$$

Now, multiply row 1 on the left by $(iM_B \sin K_B b)(-M_B \cos K_B b)^{-1}$ and then subtract it from row 2, which annihilates the lower-right diagonal element, leaving

$$\begin{pmatrix} M_A \cos(K_A a - qd/2) & -M_B \cos K_B b \\ M_B \tan(K_B b) M_B^{-1} M_A \cos(K_A a - qd/2) + M_A \sin(K_A a - qd/2) & 0 \end{pmatrix} \begin{pmatrix} e^{-iqd/2} e^{iK_A d/2} c^A \\ c^B \end{pmatrix} = 0. \tag{32}$$

The determinant of Eq. (32) is of order $2N \times 2N$ only and is given by the product of the determinants of the two off-diagonal $2N \times 2N$ blocks

$$\| M_B \tan(K_B b) M_B^{-1} + M_A \tan(K_A a - qd/2) M_A^{-1} \| \times \| M_A \cos(K_A a - qd/2) \| \times \| M_B \cos(K_B b) \| = 0. \tag{33}$$

In the case of imaginary exponents, the cosine factors become hyperbolic cosines and are never zero, and so can be dropped, and the corresponding tangents become hyperbolic tangents, which are bounded by ± 1. So, unless one of the cosines becomes zero, the secular equation is given by

$$\| M_B \tan(K_B b) M_B^{-1} + M_A \tan(K_A a - qd/2) M_A^{-1} \| = 0; \tag{34}$$

several other variants of Eq. (34) are possible. For real exponents, the cosine factors in Eq. (33) should be retained to remove the singularities due to the tangents. The cosines do not, however, alter the solutions of the secular equation. Equation (34) represents the alternative form that is the subject of this paper.

A. Wave functions

Once a root of Eq. (34) is located, the corresponding wave function can be found. Using Eq. (32), one obtains the $2N \times 2N$ equation

$$[M_B \tan(K_B b) M_B^{-1} M_A \cos(K_A a - qd/2) + M_A \sin(K_A a - qd/2)][e^{-iqd/2} e^{iK_A d/2} c^A] = 0. \tag{35}$$

Factoring out $M_A \cos(K_A a - qd/2)$, one obtains

$$[M_B \tan(K_B b) M_B^{-1} + M_A \tan(K_A a - qd/2) M_A^{-1}] \chi = 0,$$
$$\chi = M_A \cos(K_A a - qd/2) e^{iK_A d/2} e^{-iqd/2} c^A. \tag{36}$$

The c^B coefficients can be found by back substitution into Eq. (32)

$$\chi = M_B \cos(K_B b) c^B. \tag{37}$$

Once the expansion coefficients are found, the corresponding wave function can be normalized and its band character (conduction electron, heavy hole, light hole, or spin orbit) examined. In normalizing the wave function, to avoid numerical problems, it is better to deal with

$$A \equiv e^{-iqd/2} e^{iK_A d/2} \cos(K_A a - qd/2) c^A = M_A^{-1} \chi,$$
$$B \equiv \cos(K_B b) c^B = M_B^{-1} \chi. \tag{38}$$

B. Relation to previous work

The secular equation used in this work [Eq. (36)], involves terms of the form

$$\sum_{P=1}^{2N} \sum_{j=1}^{2N} [M_{Qj} \tan k_j a M_{jP}^{-1}] \chi_P . \tag{39}$$

Here P and Q denote band indices and the expansion coefficient χ_P is subscripted with band indices as well. This is in contrast to the original problem [Eqs. (23) and (24)] in which the expansion coefficients $c_i^{A,B}$ were subscripted with exponents k_i. The latter situation is the one encountered in the work of Smith and Mailhiot,[4] whereas the former is used in the formalism of Ram-Mohan, Yoo, and Aggarwal.[5] However, none of the these approaches, including Eqs. (28) and (34), yields Hermitian secular matrices.

C. Single-band test case

As an illustration, one can use a single-band model of a superlattice. Equation (34) leads to the secular equation for a single band ($N=2$ with two spins)

$$\begin{pmatrix} A_1 & 0 & \frac{2m_A}{\hbar^2 k_A} A_2 + \frac{2m_B}{\hbar^2 k_B} A_3 & 0 \\ 0 & A_1 & 0 & \frac{2m_A}{\hbar^2 k_A} A_2 + \frac{2m_B}{\hbar^2 k_B} A_3 \\ \frac{\hbar^2 k_A}{2m_A} A_2 + \frac{\hbar^2 k_B}{2m_B} A_3 & 0 & A_1 & 0 \\ 0 & \frac{\hbar^2 k_A}{2m_A} A_2 + \frac{\hbar^2 k_B}{2m_B} A_3 & 0 & A_1 \end{pmatrix}, \tag{40}$$

where

$$A_1 = [\tan(k_A a - qd/2) - \tan(k_A a + qd/2)]/2,$$
$$A_2 = [\tan(k_A a + qd/2) + \tan(k_A a - qd/2)]/2,$$
$$A_3 = \tan k_B b, \tag{41}$$

and other symbols have the same meaning as before. Observe that Eq. (40) is non-Hermitian; however, *as will be proved more generally later*, if one interchanges the first two columns (rows) with the last two columns (rows), the secular equation does become Hermitian.

In this simple case, one can decouple the up- and down-spin solutions by performing additional row and column interchanges and obtain two identical 2×2 blocks of the form

$$\begin{pmatrix} \frac{2m_A}{\hbar^2 k_A} A_2 + \frac{2m_B}{\hbar^2 k_B} A_3 & A_1 \\ A_1 & \frac{\hbar^2 k_A}{2m_A} A_2 + \frac{\hbar^2 k_B}{2m_B} A_3 \end{pmatrix}. \tag{42}$$

Setting the determinant to zero, one obtains an eigenvalue equation *with tangents only*

$$(A^+ + \alpha B)(A^- + B/\alpha) + (A^- + \alpha B)(A^+ + B/\alpha) = 0, \tag{43}$$

where $A^+ = \tan(k_A a + qd/2)$, $A^- = \tan(k_A a - qd/2)$, $B = \tan k_B b$, and $\alpha = m_A k_B / m_B k_A$. It is this tangents-only form that makes the present derivation more akin to the underlying quantum-well problem. Except near the tangent discontinuities (removable by multiplication by cosines), the present superlattice equation can be shown by trigonometric identi-

ties to be equivalent to the standard Kronig-Penney equation [Eq. (29)]. Equation (43) can be made more symmetric in A and B.

One immediate benefit of the present secular equation is that it is simple to obtain the conditions for band extrema at $q=0, \pm\pi/d$. These conditions are not apparent from the standard Kronig-Penney equation. In fact, the standard Kronig-Penney equation for these wave vectors is obtained by first constructing even- and odd-parity wave functions.[2] However, in the present formalism, Eq. (43) immediately yields the eigenvalue conditions

$$q=0, \quad \tan k_B b=\beta \tanh\kappa_A a \xrightarrow[a\to\infty]{} \beta,$$

$$q=\pm\pi/d, \quad \tan k_B b=\beta \coth\kappa_A a \xrightarrow[a\to\infty]{} \beta, \tag{44}$$

for even-parity bands and

$$q=0, \quad \tan k_B b=-\tanh\kappa_A a/\beta \xrightarrow[a\to\infty]{} -1/\beta,$$

$$q=\pm\pi/d, \quad \tan k_B b=-\coth\kappa_A a/\beta \xrightarrow[a\to\infty]{} -1/\beta, \tag{45}$$

for odd-parity bands, where $\beta\equiv(m_B\kappa_A)/(m_A k_B)$ and $k_A=i\kappa_A$ for $E\leqslant V$.

Unlike in the present treatment, Eqs. (44) and (45) are not immediately derivable from the Kronig-Penney model.[2] In particular, in the limit of infinite barriers $a\to\infty$, the hyperbolic tangents and cotangents approach unity and the conditions for the even- and odd-parity bands immediately become the standard conditions for the even- and odd-parity levels of an isolated quantum well.[1,2]

As importantly, for states below the top of the well and wide barriers, Eq. (43) (multiplied by cosines to remove discontinuities in the tangents, if necessary) leads to secular determinants on the order of unity, while the Kronig-Penney model Eq. (29) can lead to numbers on the order of 10^{16} and larger. In the case of multiband EFA, especially in the presence of the so-called wing solutions, the numerical overflows in the standard formulation Eq. (28) can be even more severe.

IV. HERMITICITY

Here it will be shown that a simple column (row) interchange can render the present secular equation [either Eq. (28) or (34)] Hermitian. The theorem to be proved is as follows.

Theorem. Interchanging the first N columns (or rows) and the last N columns (or rows) of secular equation [Eqs. (34)] results in a Hermitian matrix.

Proof. The proof proceeds as follows. Define a unitary matrix T

$$T=\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}=T^{-1}=T^{\dagger} \tag{46}$$

of order $2N\times 2N$, where the unit matrices are of order $N\times N$. When premultiplying a matrix, T interchanges the first and last N rows; when postmultiplying a matrix, T interchanges the first and last N columns.

Next, consider the form of the two terms comprising Eq. (34), i.e.,

$$\Omega\equiv M \tan Ka(M^{-1}), \tag{47}$$

where $\Omega_{PR}\equiv\Sigma_k M_{Pk}\tan ka M^{-1}_{kR}$ and P,R are band indices. The equation for the inverse M^{-1} is developed in the Appendix, Eq. (A5). To explore Hermiticity, it is necessary to deal with the Hermitian adjoint of Ω, whose elements are

$$\Omega^*_{RP}\equiv\sum_k (M^{-1}_{k*R})^*\tan ka(M_{Pk*})^*. \tag{48}$$

However, from (A1), (A5), and (15),

$$(M_{Pk*})^*\Rightarrow\begin{pmatrix} I & 0 \\ H^*_{1L}/2 & H^*_2 \end{pmatrix}\begin{pmatrix} C^*_{k*} \\ kC^*_{k*} \end{pmatrix}$$

$$=(L_k\ kL_k)\begin{pmatrix} I & H_{1R}/2 \\ 0 & H_2 \end{pmatrix}\Rightarrow(M^{-1}T)_{kP}. \tag{49}$$

Similarly, using the equation for the inverse [Eq. (A5)]

$$(M^{-1}_{k*Q})^*\Rightarrow(L^*_{k*}\ kL^*_{k*})\begin{pmatrix} H^*_{1R}/2 & I \\ H^*_2 & 0 \end{pmatrix}$$

$$=\begin{pmatrix} H_{1L}/2 & H_2 \\ I & 0 \end{pmatrix}\begin{pmatrix} C_k \\ kC_k \end{pmatrix}\Rightarrow(TM)_{Qk}. \tag{50}$$

Inserting Eqs. (49) and (50) into Eq. (48), one finds that

$$\Omega^{\dagger}=T\Omega T, \tag{51}$$

so that $(\Omega T)^{\dagger}=T\Omega^{\dagger}=T^2\Omega T=\Omega T$. Therefore, although Ω is not Hermitian, matrices ΩT and $T\Omega$, obtained by interchanging the first and last N columns or rows, respectively, of the original matrix Ω, are Hermitian. These developments were anticipated in the discussion of the secular equation for the single-band case Eq. (40). Finally, following the lines of the present derivation, one can also show that the original superlattice secular equation [Eq. (28)] can be made Hermitian by the same row and column interchange.

A. Properties of the secular equation

Given an operator Ω that is not Hermitian but obeys the condition $\Omega^{\dagger}=T\Omega T$ so that ΩT and $T\Omega$ are Hermitian, several theorems can be proved.

(i) If λ_i is an eigenvalue of Ω, then λ_i^* is an eigenvalues of $\Omega^{\dagger}$ (standard result from linear algebra[21]).

(ii) The eigenvalues of Ω come in complex-conjugate pairs.

Proof. If λ is an eigenvalue of Ω, then $\det(\Omega-\lambda I)=0$. From the general relation

$$0=\det(\Omega-\lambda I)^{\dagger}=\det(\Omega^{\dagger}-\lambda^* I)=\det(T\Omega T-\lambda^* I)$$

$$=\det T(\Omega-\lambda^* I)T=\det(\Omega-\lambda^* I), \tag{52}$$

so that both λ and λ^* are eigenvalues of Ω. By contrast, the eigenvalues of ΩT and $T\Omega$ are real.

(iii) If φ_i is an eigenvector of Ω with eigenvalue λ_i, then $T\varphi_i$ is an eigenvector of $\Omega^{\dagger}$ with the same eigenvalue.

Proof. Let φ_i satisfy the eigenvalue equation $\Omega\varphi_i=\lambda_i\varphi_i$. Multiplying by T, one obtains $T\Omega\varphi_i=\lambda_i T\varphi_i$. But, $T\Omega=\Omega^\dagger T$, so that $\Omega^\dagger(T\varphi_i)=\lambda_i(T\varphi_i)$.

(iv) Hermitian operators ΩT and $T\Omega$ have the same eigenvalues and their eigenvectors differ only by row interchange.

Proof. If μ_i is an eigenvalue of ΩT and ξ_i the corresponding eigenvector, then $(\Omega T)\xi_i=\mu_i\xi_i$. Therefore,

$$T(\Omega T)\xi_i=\mu_i T\xi_i, \quad (T\Omega)(T\xi_i)=\mu_i(T\xi_i), \tag{53}$$

so that $T\xi_i$ is the corresponding eigenvector of $T\Omega$ with the same eigenvalue μ_i. In effect, the problem can be made Hermitian by either row or column interchange.

(v) The determinants of ΩT and Ω are equal to within a sign since $\det T=(-1)^N$. In practice, because of spin multiplicity, N is even. However, N could be odd if the Kramers degeneracy is eliminated beforehand by block diagonalizing the starting bulk Hamiltonian (e.g., as in the case of the 6×6 Hamiltonian for the heavy-, light-, and spin-orbit-hole manifolds). In fact, it is easy to show that

$$\det(\Omega^\dagger\Omega)=\prod_i \lambda_i^*\lambda_i=\det(\Omega^\dagger TT\Omega)=\det(T\Omega)^2=\prod_i \mu_i^2, \tag{54}$$

so that for each real root μ_i there is one (λ_i,λ_i^*) pair; however, $\lambda_i^*\lambda_i\neq\mu_i^2$.

The practical implication of these theorems has to do with the multiplicity of eigenvalues and their reality. In the case of the time-reversal and inversion symmetries, each solution in the superlattice at a given $(\mathbf{k}_\parallel q)$ is doubly degenerate. Therefore, each root of the Hermitian secular equation will be at least a double root. As a result, the product of distinct eigenvalues of the Hermitian matrix furnishes a real secular determinant that changes sign at the roots of the problem.

However, by theorem (v), to each such real root, there will correspond a pair of complex-conjugate roots of the original, non-Hermitian secular equation. If the complex-conjugate roots happen to be real [as is the case for the single-band case of Eq. (28)], then such roots will occur as real quadruplets. The zeros of the corresponding secular determinant are not easily identified, as it does not change sign at the roots of the problem. Finally, note that the reformulated secular equation [Eq. (34)] is not invariant under the interchange $q\rightarrow -q$, so no additional degeneracies ensue as a result.

B. Comparisons

The secular equation of Smith and Mailhiot[5] for superlattices is non-Hermitian as it yields complex eigenvalues that come in conjugate pairs. Therefore, the zeros of their determinant are not located as easily as those of the Hermitian matrix derived above. In the case of the transfer matrix formalism of Ram-Mohan, Yoo, and Aggarwal,[5] their secular equation leads to a general complex matrix, which is also less convenient for locating the zeros of the determinant, especially in the case of degenerate roots. As importantly, both Smith and Mailhiot[4] as well as Ram-Mohan, Yoo, and Aggarwal[5] report grave difficulties in handling imaginary exponents, a problem that the present formalism avoids by recasting the secular equation in terms of tangents. Since the present formalism and that of Ram-Mohan, Yoo, and Aggarwal are related via a similarity transformation, the latter should obey the relations derived in the present paper.

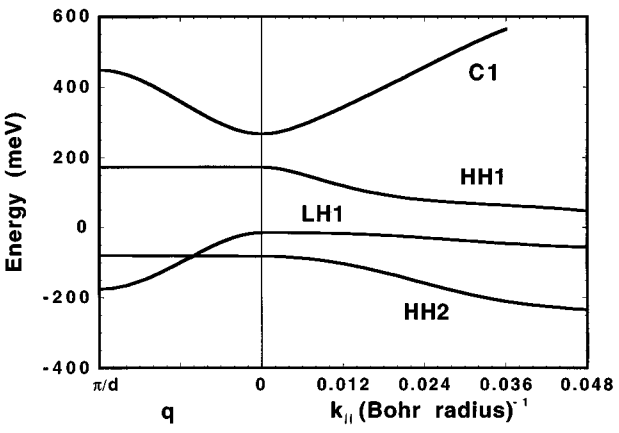

FIG. 1. Band dispersions for a 30 Å/30 Å $InAs/In_{0.3}Ga_{0.7}Sb$ superlattice calculated using the method developed in this paper.

V. APPLICATION TO $InAs/In_xGa_{1-x}Sb$ SUPERLATTICES

In this section an $InAs/In_xGa_{1-x}Sb$ superlattice is used as an example to demonstrate the utility of the calculational scheme developed here. A fuller discussion of the system is left for a separate paper.

The calculation involves an 8×8 EFA Hamiltonian and the standard EFA boundary conditions.[1–3] (Observe that in the 8×8 case, the conduction band is included explicitly, so that the valence-band coupling to the first conduction band is not included in the Luttinger parameters γ'. It is this coupling that is the main source of the discrepancy discovered by Foreman[15] between the conventional and Burt 6×6 EFA-formalisms.) The superlattice is chosen to have 30-Å InAs layers and 30-Å $In_xGa_{1-x}Sb$ layers with $x=0.30$ M indium content. The superlattice is free standing and oriented in the [001] direction. The material input parameters are the same as those used earlier[22,23] (mainly from Refs. 24 and 25). Strain effects are treated using the Bir-Picus deformation-potential theory.[26] The secular equation is in the tangent form Eq. (34) and is made Hermitian via column interchange (Sec. IV). Spurious exponents on the order of 2 inverse Bohr radii were found in diagonalizing Eq. (12), leading to exponentials on the order of $10^{\pm49}$ in Eq. (28).

The accuracy of the eigenvalue determination was checked against a separate code for $q=0$ and π/d. These two cases possess more symmetry than at a general q, which allows one to halve the size of the secular determinant and to implement numerical techniques for avoiding overflows that are similar to those used for quantum wells.[8] Both $InAs/In_xGa_{1-x}Sb$ and $GaAs/Al_xGa_{1-x}As$ superlattices were examined. The eigenvalues obtained in these test cases were identical to within the machine accuracy when compared to those obtained from the more general code tested here.

Figure 1 shows the calculated band dispersions for the $InAs/In_xGa_{1-x}Sb$ superlattice. The chosen example is a semiconducting superlattice, with a gap in midinfrared. Its design is not optimized for any particular use. The example

is included here only to demonstrate that the scheme developed here is eminently workable and possesses many useful properties. In particular, an eigenvalue search is trivial because of the Hermiticity of the secular equation, because the secular determinants are on the order of unity, and because they change sign at each root.

VI. CONCLUSION

In this paper an alternative form of the EFA secular equation for superlattices was developed. The present secular equation avoids troublesome exponentials in favor of well-behaved hyperbolic tangents whenever wave function exponents are imaginary. As a result, the method has no difficulties in handling evanescent wave function components, in particular the so-called wing solutions, which often render the calculation impossible. The present method does not address the issue of spurious oscillatory solutions because they do not lead to over- and underflows, although they may lead to physical problems.

As importantly, the generally complex secular equation is made Hermitian by a simple interchange of rows or columns. Its diagonalization produces N pairs of real eigenvalues. At a root, two of the eigenvalues are zero and the corresponding eigenvectors are associated with the Kramers degenerate wave functions for the superlattice. Roots are easily identified since the secular determinant obtained by multiplying distinct eigenvalues changes sign at the roots. Therefore, it is not necessary to first find a unitary transformation to eliminate the Kramers degeneracy of the starting $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian.

When applied to the case of a carrier in a single parabolic band (i.e., the simple Kronig-Penney model), the present formalism results in a secular equation with tangents rather than sines and cosines. The present form is more closely related to the underlying quantum-well problem. In addition, the present method was shown to be applicable to Burt's EFA formalism as implemented by Foreman. Finally, the method was demonstrated by the example of the technologically important semiconducting $InAs/In_xGa_{1-x}Sb$ type-II superlattice.

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APPENDIX: INVERSE OF MATRIX M

1. Left inverse

The matrix M is given by

$$M=\begin{pmatrix} I & 0 \\ H_{1L}/2 & H_2 \end{pmatrix}\begin{pmatrix} C \\ CK \end{pmatrix}, \tag{A1}$$

so that its left inverse is given by

$$M^{-1}=\begin{pmatrix} C \\ CK \end{pmatrix}^{-1}\begin{pmatrix} I & 0 \\ -H_2^{-1}H_{1L}/2 & H_2^{-1} \end{pmatrix}. \tag{A2}$$

From the orthonormality relation [Eq. (27)]

$$(L\ KL)\begin{pmatrix} H_1 & H_2 \\ H_2 & 0 \end{pmatrix}\begin{pmatrix} C \\ CK \end{pmatrix}=\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}, \tag{A3}$$

one finds that

$$\begin{pmatrix} C \\ CK \end{pmatrix}^{-1}=(L\ KL)\begin{pmatrix} H_1 & H_2 \\ H_2 & 0 \end{pmatrix}, \tag{A4}$$

so that

$$M^{-1}=(L\ KL)\begin{pmatrix} H_{1R}/2 & I \\ H_2 & 0 \end{pmatrix}. \tag{A5}$$

Verifying, one finds that

$$\begin{aligned} M^{-1}M&=(L\ KL)\begin{pmatrix} H_{1R}/2 & I \\ H_2 & 0 \end{pmatrix}\begin{pmatrix} I & 0 \\ H_{1L}/2 & H_2 \end{pmatrix}\begin{pmatrix} C \\ CK \end{pmatrix} \\ &=(L\ KL)\begin{pmatrix} H_1 & H_2 \\ H_2 & 0 \end{pmatrix}\begin{pmatrix} C \\ CK \end{pmatrix}=\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \end{aligned} \tag{A6}$$

is the left inverse, so that

$$\sum_{L=1}^{2N} M_{jL}^{-1}M_{Li}=\delta_{ij}, \tag{A7}$$

where the sum proceeds of the band indices L and the Kronecker delta is with respect to exponents k_i.

2. Right inverse

From matrix algebra, it is known that the left inverse of a matrix is also its right inverse.[27] Nevertheless, in our case, it is instructive to prove this fact based on orthogonality relations. Forming the required product, one obtains

$$\begin{pmatrix} I & 0 \\ H_{1L/2} & H_2 \end{pmatrix}\begin{pmatrix} C \\ CK \end{pmatrix}(L\ KL)\begin{pmatrix} H_{1R}/2 & I \\ H_2 & 0 \end{pmatrix}\equiv\begin{pmatrix} \Pi_1 & \Pi_2 \\ \Pi_3 & \Pi_4 \end{pmatrix}. \tag{A8}$$

Explicitly,

$$(\Pi_2)_{nm}=\sum_j C_{nj}L_{jm}=0, \tag{A9}$$

which is implicit in identities (24a) and (24b) of Smith and Mailhiot;[4]

$$\begin{aligned} (\Pi_1)_{nm}=(\Pi_4)^*_{mn}&=\sum_{j,p} C_{nj}L_{jp}[(H_{1R}/2)_{pm}+k_j(H_2)_{pm}] \\ &=\delta_{nm}, \end{aligned} \tag{A10}$$

from (A9) and identities (24b) and (24d) of Smith and Mailhiot;[4] and

$$\begin{aligned} (\Pi_3)_{nm}=\sum_{p,r}\sum_j\ &[(H_{1L}/2)_{np}+k_j(H_2)_{np}]C_{pj}L_{jr}[(H_{1R}/2)_{rm} \\ &+k_j(H_2)_{rm}]=0, \end{aligned} \tag{A11}$$

from (A9) and identities (24b) and (24c) of Smith and Mailhiot.[4] Therefore, Eq. (A5) is both the left and the right inverse of matrix M.

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$$\begin{pmatrix} -iH_2^{-1}H_1/2 & H_2^{-1} \\ (H_0-E)-H_1H_2^{-1}H_1/4 & -iH_1H_2^{-1}/2 \end{pmatrix} \begin{pmatrix} F \\ H_2F'+iH_1F/2 \end{pmatrix} \equiv \frac{d}{dz}\begin{pmatrix} F \\ H_2F'+iH_1F/2 \end{pmatrix}.$$

The present formalism is related to the above by a similarity transformation.

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