Operator ordering and interface-band mixing in the Kane-like Hamiltonian of lattice-matched semiconductor superlattices with abrupt interfaces

P. C. Klipstein*
Semiconductor Devices, P.O. Box 2250, Haifa 31021, Israel
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A Kane-like envelope function Hamiltonian is derived for the Γ_{15} valence and Γ_1 conduction states of lattice-matched, semiconductor superlattice structures, with metallurgically abrupt interfaces. The local microscopic potential is treated as a weak perturbation on that of a reference crystal and is expressed in terms of a one-dimensional profile function, $G(z)$, which modulates the difference between the potentials of the well and barrier materials. In contrast to many previous treatments, all terms up to order $\ell=2$ in $\delta\bar{V}\cdot(\bar{k}a)^{\ell}$ are included, where $\delta\bar{V}$ is the typical band offset, $\hbar\bar{k}$ is the average momentum modulus of the envelope function, and a is the bulk lattice parameter. Far from the interfaces, the Hamiltonian is identical to the familiar bulk Kane Hamiltonian, with the standard bulk parameters. However, the operator ordering in the valence band is revised from the commonly used Burt scheme. An operator ordering scheme has also been derived for the linear-k P terms that couple conduction and valence states. Expressions have been derived for the δ functionlike, and derivative of a δ functionlike, interface terms. These are off-diagonal and diagonal, respectively, in common atom superlattices like GaAs/$Al_xGa_{1-x}As$, where the antisymmetric contribution to $G'(z)$ is expected to be small. For superlattices with no common atom, additional interface terms are introduced. If the difference in the spin-orbit splitting energy for the two superlattice materials is comparable with the valence-band offset, then relativistic corrections can introduce many more, weak interface contributions. Part of the relativistic interface matrix has been derived, which includes the most significant terms. Finally, a scheme is proposed for reducing the number of independent Luttinger parameters required, when using the Hamiltonian to fit experimental spectral data.

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I. INTRODUCTION

More than 50 years after the development of the Kane model for band structure in bulk semiconductors,[1–3] its extension to semiconductor superlattices and microstructures is still not firmly established. Although $\mathbf{k}\cdot\mathbf{p}$ methods have been applied widely to semiconductor heterostructures for many years[4] and even though the results obtained often compare favorably with experiment, no consistent set of rules has yet been agreed for the correct operator ordering or for which significant interface potentials should be included. Even the widely implemented, and intuitively obvious, piecewise use of the bulk material parameters is still not rigorously justified. Generally, a Kane-like or Luttinger-like Hamiltonian is used in a piecewise fashion and a variety of approaches have been followed for the interface boundary conditions. In one widely used approach, operators are "symmetrized" before integration of the Hamiltonian across an interface. The symmetrization procedure is often justified on the basis of probability flux conservation or similar arguments, which unfortunately can yield ambiguous results. For example, the perfectly symmetric second derivative operators in Baraff and Gershoni[5] and their asymmetric counterparts in Dallen and Stavrinou[6] are both consistent with flux conservation. In this work it will be shown that neither procedure is correct.

In the early 1990s, Burt[7] provided important insights into how to treat the interface region properly. His approach has been extended more recently by several authors including Takhtamirov and Volkov[8–10] and Foreman.[11,12] Burt's basic idea was to introduce a bulk reference crystal whose Bloch functions are used as the basis states. This leads to spatially independent momentum matrix elements and envelope function continuity at any interface is a natural consequence. The difference between the real and reference Hamiltonians, $\delta V(\boldsymbol{r})$, is a spatially dependent perturbation and this introduces extra terms into the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian, many of which are suppressed on symmetry grounds, except near an interface. The most important contribution of Burt's approach was to introduce an explicit δ-functionlike interface term which can mix different bands at a zone-center or zone-edge symmetry point, such as Γ or X.[11] This term depends on the microscopic structure of the interface and was shown to take the simple form: $\langle n|\delta V|n'\rangle|_{z_i}=\Omega_{nn'}\delta(z-z_i)$, where the matrix element is evaluated over the volume of a bulk unit cell centered on the interface at z_i, and $|n\rangle$ and $|n'\rangle$ are states of different symmetry, such as the zone-center Γ_{15x} and Γ_{15y} valence states or the Γ_{15z} valence and Γ_1 conduction states. Foreman calculated theoretical estimates for the mixing strength in these cases as well as in a few others at an abrupt GaAs/AlAs (001) interface and came up with typical magnitudes in the range $\Omega_{nn'}=0.1-0.7$ eV Å.[11]

Burt also proposed a scheme for the ordering of the differential operators in the envelope function approximation[7,13] which has become quite widely adopted.[14–20] Unfortunately his treatment results in material parameters such as effective-mass components which are energy dependent and which also depend on the choice of the reference crystal. If piecewise bulk parameters are used instead, the difference between these parameters and the energy-dependent ones leads to errors comparable with those obtained using the same virtual-crystal average parameter values throughout, in which case the operator ordering becomes irrelevant. The use

of the local bulk parameters with the proposed operator ordering is therefore not really justified.

In the 1997 paper by Volkov and Takhtamirov[8] the basic difficulties were presented of constructing a 6×6 envelope function Hamiltonian for the Γ_{15} valence states, or an 8×8 Hamiltonian which also includes the Γ_1 conduction states, in which bulk piecewise parameters can be used. They pointed out in several works,[9,10] which were reviewed by Foreman,[12] that in order to achieve this, it is necessary to keep all terms up to order $\ell=2$ in $\delta\bar{V}\cdot(\bar{k}a)^{\ell}$, where $\delta\bar{V}$ is a typical band offset, $\hbar\bar{k}$ is the average momentum modulus of the solution, and a is the bulk lattice parameter. In subsequent discussions of the Γ_{15} valence band, Takhtamirov and Volkov acknowledged the complexity of deriving a fully consistent 6×6 or 8×8 Hamiltonian, and so considered only the simplest delta-functionlike interface-band mixing discussed above, which is of order $\ell=1$. They did not consider other forms of interface-band mixing, including that due to the correct operator ordering associated with the bulk parameters, which has contributions of order $\ell=1$ and $\ell=2$.[10] This paper tries to address exactly these issues in a lattice-matched superlattice grown along [001] with metallurgically abrupt interfaces. The aim is to end up with a relatively simple Hamiltonian which essentially preserves the familiar Kane form and in which many of the material parameters are the same Kane parameters. The main differences with the bulk form are the operator ordering and the inclusion of extra interface terms. While Foreman has also addressed these issues in great depth,[12,21] his approach leads to a more complex Hamiltonian for the valence band with a large number of parameters that must be determined from atomic pseudopotential calculations. Although more precise, especially in superlattice materials with a large band offset, it does not provide a simple prescription for the operator ordering in the standard Kane-like form.

In this work, the method of Takhtamirov and Volkov[8] is used to derive 6×6 and 8×8 Kane-like Hamiltonians, which include all important $\ell=1$ and $\ell=2$ contributions. While it is fairly straight forward to write down the Hamiltonian based on a suitable transformation method that separates local and remote states,[10,12] it is more difficult to relate the results so obtained to the familiar bulk parameters. By so doing, the correct operator ordering scheme can be derived for the off-diagonal bulk terms. The ordering scheme obtained in this way for the valence band is shown to differ from the widely adopted Burt scheme. For the linear-k P terms that couple conduction and valence bands, no reliable operator ordering scheme has yet been derived. Burt used symmetry arguments to justify the omission of several terms proportional to $\delta\bar{V}/\Delta E$, where ΔE is a typical energy separation between local and remote bands. One of these terms is in fact finite at the interfaces and, when included, the operator ordering of the linear-k P terms can be deduced. By assuming that the derivative of the profile function, $G(z)$, is essentially symmetric about the plane of atoms that constitutes an interface, where $\delta V(\mathbf{r})=\delta U(\mathbf{r})G(z)$ and $\delta U(\mathbf{r})$ is the difference in the microscopic potentials of the two bulk materials, the present derivation also produces a δ-functionlike interface matrix with only off-diagonal elements and a derivative of a delta-functionlike interface matrix with only diagonal elements. All but two of the elements in these matrices are of order $\ell=2$, the exceptions being the zone center $\ell=1$ interface-band mixing terms previously considered by Foreman,[11] similar to $\Omega_{nn'}\delta(z-z_i)$ described above. The δ-functionlike interface matrix also contains linear k terms that mix Γ_{15x} and Γ_{15y} with Γ_{15z} and Γ_1. When the derivative of the profile function is not symmetric, more terms must be included in the interface matrices. It is argued that the two cases of symmetric and nonsymmetric profile functions at a metallurgically abrupt interface correspond to common atom superlattices (e.g., $GaAs/Al_xGa_{1-x}As$) and no common atom superlattices (e.g., InAs/GaSb), respectively. Relativistic corrections introduce a plethora of additional interface related parameters that also depend on the microscopic interface structure. However these terms are only likely to be important in superlattice material combinations in which the difference in the spin-orbit splitting energies is comparable with the valence-band offset. For this case, the most important interface terms are identified.

The next section contains a brief review of the derivation of the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian in Fourier representation and its subsequent transformation back to real space, following closely the treatment of Takhtamirov and Volkov.[10] This yields both δ-functionlike and derivative of a δ-functionlike interface terms, which depend on the microscopic interface structure. In Sec. III the sensitivity of these terms to interface abruptness and symmetry is discussed. In Sec. IV, the transformation scheme of Pikus and Bir is used to lowest order to derive an 8×8 Hamiltonian in which all terms up to $\delta\bar{V}\cdot(\bar{k}a)$ are included. This Hamiltonian demonstrates the correct operator ordering procedure for the linear-k P term coupling conduction and valence bands and includes only the simple $\Omega_{nn'}\delta(z-z_i)$ interface-band mixing term. The Hamiltonian is not sensitive to mass differences between the different superlattice materials and does not include any derivative of a δ-functionlike interface terms. These, and additional δ-functionlike terms are added in Sec. V, where all contributions greater than or equal to $\delta\bar{V}\cdot(\bar{k}a)^2$ are included. Several differences between the 6×6 and 8×8 cases are pointed out, including different operator ordering schemes. In Sec. VI, the results of the preceding sections are used to derive the full 6×6 and 8×8 Hamiltonian *matrices* for Γ_{15} valence and Γ_1 conduction states. In Sec. VII, the operator ordering in the present treatment is compared with Burt's result for a number of common superlattice materials. The values of the interface potentials which depend on the bulk material parameters are also estimated. The relativistic corrections are discussed in Sec. VIII and in Sec. IX, conclusions are presented.

II. $k\cdot p$ HAMILTONIAN IN THE REPRESENTATION OF A REFERENCE CRYSTAL

The potential of a semiconductor microstructure or superlattice, V_{SL}, can be expressed as the sum of the potential of a reference crystal, V, and a perturbing potential δV so that $V_{SL}=V+\delta V$. In the case of a superlattice made from two-dimensional layers of materials A and B, the reference po-

tential, V, could be the average of the crystal potentials, U_A and U_B, for the two materials, which then minimizes the size of δV. However, for simplicity of notation the reference crystal will be taken to be material A, as in the case of Ref. 10. The results will be valid for any choice of reference crystal.

The superlattice Schrödinger equation for a state of interest, Ψ_1, is

$$-\frac{\hbar^2}{2m_0}\frac{d^2\Psi_1}{dz^2}+V_{SL}\Psi_1=E\Psi_1, \tag{1}$$

where $\Psi_1=\Sigma_n\tilde{F}_n u_n$ in which u_n are the complete set of Bloch functions from a specific symmetry point of the *reference* crystal. The envelope functions, $\tilde{F}_n$, vary on a length scale, L, typical of the superlattice layer widths. This is usually much larger than the length scale, a, characteristic of the Bloch functions, which is also the dimension of a unit cell in the reference crystal. The envelope functions may be expanded in terms of their Fourier components, where the range of wave vectors is limited to the first Brillouin zone,

$$\tilde{F}_n=\int_{\substack{1\mathrm{st}\\ BZ}} d^3k' F_n(\mathbf{k}')e^{i\mathbf{k}'\cdot\mathbf{r}}. \tag{2}$$

Following the treatment described in Ref. 8, the envelope function Hamiltonian in reciprocal space is

$$\begin{aligned}EF_n(\mathbf{k})=&\left(\frac{\hbar^2k^2}{2m_0}+E_n\right)F_n(\mathbf{k})+\sum_{n'}\frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p}_{nn'}F_{n'}(\mathbf{k})\\&+\sum_{n'}\sum_{z_i}\int\left[G(k_z-k_z')\delta U_{nn'}+\frac{\pi_i e^{-i(k_z-k_z')z_i}}{2\pi}\right.\\&\left.\times\{D_{0,nn'}+(k_z-k_z')D_{1,nn'}+\cdots\}\right]\\&\times\delta(\mathbf{k}_\parallel-\mathbf{k}_\parallel')F_{n'}(\mathbf{k}')d^3k'\end{aligned} \tag{3}$$

in which

$$\begin{aligned}D_{l,nn'}=\langle n|D_l|n'\rangle=&\sum_{j\neq 0}B_j^{nn'}\frac{1}{iK_{zj}}\int_{-d}^{d}G'(z)e^{-iK_{zj}z}\\&\times\left(-\frac{1}{K_{zj}}-iz\right)^l dz,\end{aligned} \tag{4}$$

where $\pi_i=+1$ for an inverted interface (B on A) and $\pi_i=-1$ for a normal interface (A on B). $\delta U_{nn'}=\langle u_n|\delta U|u_{n'}\rangle$ and $B_j^{n,n'}=\langle u_n|e^{iK_{zj}z}\delta U|u_{n'}\rangle$ in which $\delta V(\mathbf{r})=\delta U(\mathbf{r})G(z)$ for a multilayer heterostructure grown in the z direction and $\boldsymbol{K}_j$ is a reciprocal-lattice vector. E_n is the band edge in the reference crystal of the state with Bloch symmetry $|n\rangle$ and the interfaces are located at (x,y,z_i). For an interface located at $z_i=0$, $\pm d$ is the region over which the step like function $G(z)$ is changing. $G(z)$ defines the abruptness of the interface. Since the reference crystal is material A, then $\delta U=U_B-U_A$ and $G(z)=0$ in material A and $G(z)=1$ in material B. The advantage of Eq. (3) is that the expansion in the square bracket contains terms related to the confining potential whose order of magnitude reduces by a factor $\bar{k}a$ for each successive term.

In Appendix A, Eq. (3) is transformed back to real space to yield the envelope function equation,

$$\begin{aligned}E\tilde{F}_n(r)=&\left(-\frac{\hbar^2}{2m_0}\nabla^2+E_n^{(1)}\right)\tilde{F}_n(r)-\sum_{n'}\frac{i\hbar}{m_0}\mathbf{p}_{nn'}\cdot\boldsymbol{\nabla}\tilde{F}_{n'}(r)\\&+\sum_{n'\neq n}\delta U_{nn'}\tilde{G}(z)\tilde{F}_{n'}(r)+\sum_{z_i}\sum_{n'}\pi_i\{D_{0,nn'}\tilde{\delta}(z-z_i)\\&-iD_{1,nn'}\tilde{\delta}'(z-z_i)\}\tilde{F}_{n'}(r),\end{aligned} \tag{5}$$

where $E_n^{(1)}(z)=E_n+\delta U_{nn}\tilde{G}(z)$ is the local band edge in the heterostructure of the state $|n\rangle$, correct to first order in δU. The tilde symbol ($\sim$) above any function indicates that this function is made up of Fourier components limited to the first Brillouin zone. Thus $\tilde{\delta}(z)$ is a delta function of width $\sim a$. Note that $E_n^{(1)}(z)$ changes over a distance of $\sim a$ when passing through an abrupt interface due to the behavior of $\tilde{G}(z)$.

III. INTERFACE STRUCTURE AND THE BEHAVIOR OF THE D_0 AND D_1 INTERFACE POTENTIALS

In the remainder of this paper the interface structure will be restricted to situations where the microscopic potential changes from U_A to U_B and vice versa in a fairly abrupt fashion, typically over a distance $\sim a$. This will usually be the case when the interface is grown metallurgically abrupt, with a low level of atomic interdiffusion. To begin with, let us also assume that $G'(z)$ in Eq. (4) is a symmetric function about $z=0$, denoted $G'(z)|_s$. The consequences of this assumption are discussed at the end of the section. If we define $I_G^s(K_{zj})=\int_{-d}^{d}G'(z)|_s\cos(K_{zj}z)dz$ and $\bar{I}_G^s(K_{zj})=\int_{-d}^{d}zG'(z)|_s\sin(K_{zj}z)dz$, it is easy to see that I_G^s is an even function of K_{zj}, and $\bar{I}_G^s$ is an odd function. Three real functions are also defined: $\Phi_0^s=\Sigma_{j\neq 0}(e^{iK_{zj}z}/iK_{zj})I_G^s(K_{zj})$, $\Phi_1^s=\Sigma_{j\neq 0}(e^{iK_{zj}z}/K_{zj}^2)I_G^s(K_{zj})$, and $\bar{\Phi}_1^s=\Sigma_{j\neq 0}(e^{iK_{zj}z}/K_{zj})\bar{I}_G^s(K_{zj})$. Φ_0^s is an odd function of z, and Φ_1^s and $\bar{\Phi}_1^s$ are even functions. From Eq. (4) it follows that $D_l=D_l^s=i^l\delta U(\Phi_l^s+\bar{\Phi}_l^s)$, where $\bar{\Phi}_0^s=0$. In Figs. 1 and 2, Φ_0^s and $\Phi_1^s+\bar{\Phi}_1^s$ are plotted as solid lines for a mathematically abrupt interface in which $G'(z)|_s$ is a δ function and as dashed lines for a more realistic interface in which $G'(z)|_s$ is a Gaussian with a full width at half maximum of 0.8 Å. The unit cell of the reference crystal is taken to be 3 Å. It can be seen that the broadening of the interface region has a slight weakening effect, more so on the first-order potential, D_0^s, than on the second-order potential, D_1^s. From the symmetry properties of D_0^s and D_1^s, it follows that if $|n\rangle$ and $|n'\rangle$ are limited to the Γ_{15} valence and Γ_1 conduction states in a common atom superlattice (where a plane of the common atoms defines an interface at $z=0$), $D_{0,nn'}^s$ has only off-diagonal contributions ($D_{0,\sigma Z}^s, D_{0,\mathrm{XY}}^s$) while the contributions to $D_{1,nn'}^s$ are all diagonal ($D_{1,\sigma\sigma}^s$, $D_{1,\mathrm{XX}}^s=D_{1,\mathrm{YY}}^s$ and $D_{1,ZZ}^s$).

The present treatment shows that a reasonable expression for the first-order interface-band mixing potential is $D_{0,nn'}^s$

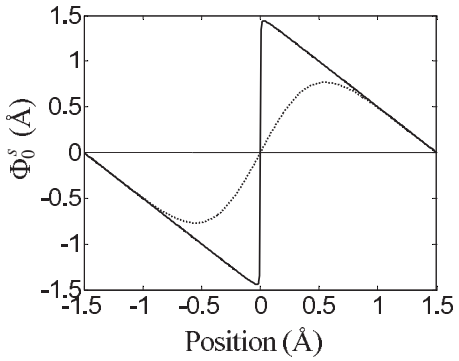

FIG. 1. Interface function Φ_0^s for a mathematically abrupt interface in which $G'(z)$ is a δ function (solid line) and for an interface in which $G'(z)$ is a Gaussian with a full width at half maximum of 0.8 Å (dashed line).

$=\langle n|\delta U\cdot\Phi_0^s(z)|n'\rangle$, where for a mathematically abrupt interface at $z=0$, $\Phi_0^s(z)=G_F(z)a/2-z$ and $G_F(z)$ is a step function that takes the value -1 on the left side of the interface and $+1$ on the right. The integral in the matrix element is evaluated over a unit cell: $-a/2<z<a/2$. This expression is slightly different from the expression: $\langle n|\delta U\cdot G_F(z)|n'\rangle a/2$, used by Foreman for a planar mathematically abrupt interface.[11,22] It puts greater weight on contributions to the integral closer to the interface. Both Foreman[11] and Takhtamirov and Volkov[10] also considered the effect of taking into account a more realistic three-dimensional form for the interface potential instead of simply averaging over the x-y plane. Takhtamirov and Volkov[10] showed that this simply renormalizes the values of some vanishingly small parameters and introduces nothing qualitatively new into the treatment of the interface. They concluded that the simple one-dimensional model used here should be sufficient. According to Foreman's most recent treatment,[12] this model should give reasonable results, provided the interfaces are not graded significantly.

Since a typical value for $D_{0,nn'}^s$ is 0.3–3 eV Å,[11,23] typical values for $D_{1,nn}^s$ are expected to be comparable, i.e., 0.3–3 eV Å^2. This follows from the fact that the peak amplitude in angstrom units for $\Phi_1^s+\bar{\Phi}_1^s$ in Fig. 2 is comparable

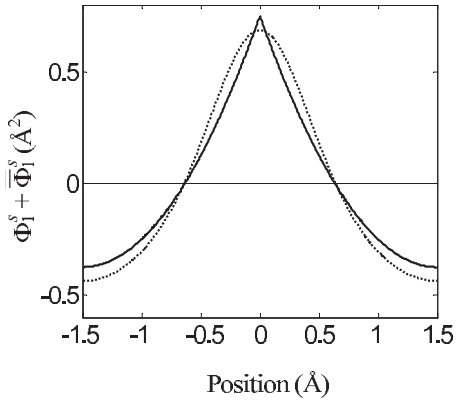

FIG. 2. Interface function $\Phi_1^s+\overline{\Phi_1^s}$ for a mathematically abrupt interface in which $G'(z)$ is a δ function (solid line) and for an interface in which $G'(z)$ is a Gaussian with a full width at half maximum of 0.8 Å (dashed line).

with that for Φ_0^s in Fig. 1. The D_1^s contribution to the ground-state energy can be estimated as follows. For a ground $|X\rangle$ hole state with envelope function $F_{X(1)}$, in a quantum well of width L, the D_1^s energy contribution is of magnitude $D_{1,XX}^s\Sigma_{z_i}\pi_i\int\tilde{\delta}(z-z_i)\,\partial/\partial z(F_{X(1)}F_{X(1)}^*)dz\sim D_{1,XX}^s\pi/L^2$. For $L=100$ Å and $D_{1,XX}^s=1$ eV Å^2 this takes a value of about 0.25 meV, which is very small. In contrast, $D_{0,XY}^s=1$ eV Å would contribute an energy matrix element between the first confined $|X\rangle$ state and the second confined $|Y\rangle$ state of roughly $D_{0,XY}^s/L$ which takes a value of $\sim$10 meV. From these values it seems likely that in many cases the $D_{1,nn}^s$ contributions can be ignored without a significant loss of accuracy. This proposal is also supported by the fact that a one monolayer increase in the thickness of material B in a superlattice with a fixed period corresponds to the addition of diagonal terms to Eq. (5) of the form $\Sigma_{z_i}\Sigma_{n'}T_{0,n'n'}\tilde{\delta}(z-z_i)\tilde{F}_{n'}(r)$, where $T_{0,n'n'}=\langle n'|\delta U|n'\rangle a/2$. This T_0 contribution should be comparable in size to the D_0^s contribution and couples to exactly the same states as the much smaller D_1^s contribution. Thus the effect of the D_1^s contribution is on the level of changes in layer thickness of much less than a monolayer, which is much below the typical experimental uncertainty in specifying the layer thickness.

If the restriction of the interface to one in which $G'(z)$ is a symmetrical function is relaxed, then a more general interface can be represented by the sum of symmetrical and antisymmetrical functions: $G'(z)=G'(z)|_s+G'(z)|_a$. A nonzero $G'(z)|_a$ may allow new mixing channels. In a common atom superlattice such as GaAs/Al_xGa_{1-x}As in which the metallurgically abrupt interfaces are located on planes of the common atom (As planes), $G'(z)|_a$ should be much smaller than $G'(z)|_s$ because $G(z)$ should approximate to an odd function when the reference crystal is taken to be the virtual-crystal average of the well and barrier materials. If a different reference crystal is used, there will be a constant offset to $G(z)$ which will not contribute to its derivative. Thus the treatment presented above should apply reasonably well. On the other hand, for superlattices made from materials with no common atom, such as InAs/GaSb, the contribution from $G'(z)|_a$ can be significant. This situation is discussed in more detail in Appendix B, where it is shown that diagonal D_0 terms ($D_{0,\sigma\sigma}^a$, $D_{0,XX}^a=D_{0,YY}^a$ and $D_{0,ZZ}^a$) and off-diagonal D_1 terms ($D_{1,\sigma Z}^a$ and $D_{1,XY}^a$) are then included in the δ-functionlike and derivative of a δ-functionlike interface matrices, respectively.

IV. SEPARATION INTO LOCAL AND REMOTE STATES

The next step in the development of a Kane-like Hamiltonian for semiconductor superlattice structures is to chose the set of local states, $m,m',m'',\ldots$, which are of interest and to perform a suitable transformation of Eq. (5) that removes any interaction between the local states and all the other remote states, $s,s',s'',\ldots$ The transformation used by Burt leads to energy-dependent material parameters which also

depend on the choice of the reference crystal. As pointed out by Takhtamirov and Volkov,[10] the resulting Hamiltonian is not precise enough to take into account any differences in the bulk material parameters. They point out that a preferable scheme is that described by Pikus and Bir in Eq. (15.46) of Ref. 24. This yields energy-independent parameters and allows them to be determined to any desired order in the small parameter, $\delta\bar{V}/\Delta E$. The first four terms in the transformed Hamiltonian, $\bar{H}$, are given as follows:

$$\bar{H}_{mm'} = H_{mm'} - \frac{1}{2}\sum_s H'_{ms}H'_{sm'}\left(\frac{1}{E_s - E_m} + \frac{1}{E_s - E_{m'}}\right) - \frac{1}{2}\sum_{m''s}\left[\frac{H'_{ms}H'_{sm''}H'_{m''m'}}{(E_s - E_{m''})(E_s - E_{m'})} + \frac{H'_{mm''}H'_{m''s}H'_{sm'}}{(E_s - E_{m''})(E_s - E_m)}\right]$$
$$+ \frac{1}{2}\sum_{ss'} H'_{ms}H'_{ss'}H'_{s'm'}\left[\frac{1}{(E_s - E_m)(E_{s'} - E_m)} + \frac{1}{(E_s - E_{m'})(E_{s'} - E_{m'})}\right]. \tag{6}$$

In this equation, $H=H_0+H'$, $H'=H_1+H_2$, $H_1=\hbar^2k^2/2m_0$, and $H_2=\delta\chi+(\hbar/m_0)\mathbf{k}\cdot\mathbf{p}$, where $\delta\chi_{nn'}=\delta U_{nn'}\tilde{G}(z)+\pi_i D_{0,nn'}(z_i)\tilde{\delta}(z-z_i)-i\pi_i D_{1,nn'}(z_i)\tilde{\delta}'(z-z_i)$.

It will be assumed to start with that there are two dominant states with indices 1 and 2 and that the rest of the states are remote (the extension to a greater number of dominant states is obvious). This will avoid the excessive use of summations and subscripts. Using only the first two terms of Eq. (6) a Kane-like Hamiltonian (ignoring spin) can be written down, as follows, for the dominant envelope function $\tilde{F}_1$. The result for $\tilde{F}_2$ looks the same but with indices 1 and 2 interchanged,

$$E\tilde{F}_1 = \frac{\hbar^2}{2}\sum_{\substack{\mu,\nu=\\ x,y,z}} k_\mu \frac{1}{m_{1,\mu\nu}} k_\nu \tilde{F}_1 + E_1^{(lc)}\tilde{F}_1 + i\sum_\mu P_\mu^{12}k_\mu\tilde{F}_2 + \sum_{\mu,\nu} k_\mu C_{\mu\nu}^{12}k_\nu\tilde{F}_2 + \frac{\hbar}{m_0}\sum_\mu\left[k_\mu\sum_s \theta_{1,s}\tilde{G}(z)p_{1s}^\mu\delta U_{s1} + \sum_s \theta_{1,s}\tilde{G}(z)\delta U_{1s}p_{s1}^\mu k_\mu\right]\tilde{F}_1$$
$$+ \frac{\hbar}{m_0}\sum_{\mu,z_i}\pi_i\left[k_\mu\sum_s \theta_{1,s}p_{1s}^\mu D_{0,s1}\tilde{\delta}(z-z_i) + \sum_s \theta_{1,s}D_{0,1s}p_{s1}^\mu\tilde{\delta}(z-z_i)k_\mu\right]\tilde{F}_1 - i\sum_{z_i}\pi_i D_{1,11}\tilde{\delta}'(z-z_i)\tilde{F}_1(r)$$
$$+ \frac{\hbar}{m_0}\sum_\mu\left[k_\mu\sum_s \theta_{12,s}\tilde{G}(z)p_{1s}^\mu\delta U_{s2} + \sum_s \theta_{12,s}\tilde{G}(z)\delta U_{1s}p_{s2}^\mu k_\mu\right]\tilde{F}_2 + \frac{\hbar}{m_0}\sum_{\mu,z_i}\pi_i\left[k_\mu\sum_s \theta_{12,s}p_{1s}^\mu D_{0,s2}\tilde{\delta}(z-z_i)\right.$$
$$\left. + \sum_s \theta_{12,s}D_{0,1s}p_{s2}^\mu\tilde{\delta}(z-z_i)k_\mu\right]\tilde{F}_2 + \sum_{z_i} D_{0,12}\pi_i\tilde{\delta}(z-z_i)\tilde{F}_2(r), \tag{7}$$

where $\theta_{1,s}=1/(E_1-E_s)$ and $\theta_{12,s}=1/([E_1+E_2]/2-E_s)$ in which E_1, E_2, and E_s are the energy values for the reference crystal. It is assumed that $\delta U_{1m}=0$ for $m\neq 1$, which is true if $|m\rangle$ is restricted to the Γ_{15} valence and Γ_1 conduction states. The momentum matrix element of the reference crystal is $p_{nn'}^\mu=\langle u_n|p_\mu|u_{n'}\rangle$ in which μ represents x, y, or z. The mass tensor in Eq. (7) is given by $m_0/m_{1,\mu\nu}=\delta_{\mu\nu}+(2/m_0)\Sigma_s\theta_{1,s}p_{1s}^\mu p_{s1}^\nu$ in which $\delta_{\mu\nu}$ is the Kronecker delta function. The energy $E_1^{(lc)}$ is the local band-edge energy of the $m=1$ state correct to second order, such that $E_1^{(lc)}=E_1+\Delta U_{11}\Gamma(z)$, where $\Gamma(z)$ is a step like function equal to $G(z)$ at distances greater than $\sim a$ from a metallurgically abrupt interface: $\Delta U_{11}\Gamma(z)=\tilde{G}(z)\delta U_{11}+\Sigma_s\tilde{G}^2(z)\theta_{1,s}\delta U_{1s}\delta U_{s1}$. The parameters $P_\mu^{12}=\hbar p_{12}^\mu/im_0$ and $C_{\mu\nu}^{12}=(\hbar^2/m_0^2)\Sigma_s\theta_{12,s}p_{1s}^\mu p_{s2}^\nu$ are the k-linear and k-quadratic off-diagonal $\mathbf{k}.\mathbf{p}$ terms, respectively.

In Eq. (7) all terms of magnitude $\delta\bar{V}\cdot(\bar{k}a)^2$ or larger have been kept. The way to estimate the size of each term has been discussed extensively in Refs. 9 and 12, so will not be repeated in any detail here. In Ref. 12, it is shown that $(\delta\bar{V}/\Delta E)\sim(\bar{k}\lambda)^2\sim(\bar{k}a)^2$, based on the fact that $\lambda\approx\hbar(2m^*\Delta E)^{-1/2}$. The parameter, m^*, refers to the effective mass at the edge of the nearest remote band due to its interaction with the local bands. λ has a value of ~ 6 Å in GaAs if ΔE is set equal to the band gap, so $\lambda\approx a$. A typical value for $(\bar{k}a)^{-1}\approx L/2\pi\lambda$ in different materials is thus in the range of 3 or larger. Equation (7) is generally true but the δ-functionlike and derivative of a δ-functionlike interface terms have been restricted to the simplest case, discussed in the previous section, of off-diagonal and diagonal terms, respectively, appropriate to common atom superlattices with a negligible $G'(z)|_a$. The more general case is treated at the end of Sec. V. Terms with numerators containing $\delta U_{1s}D_{0,s1}$, $D_{0,1s}\delta U_{s1}$, $\delta U_{1s}D_{0,s2}$, $D_{0,1s}\delta U_{s2}$, $D_{0,1s}D_{0,s1}$, or $D_{0,1s}D_{0,s2}$ are omitted since they are of order $\delta\bar{V}\cdot(\bar{k}a)^3$. Terms containing $\delta U_{1s}\delta U_{s2}$ are zero on symmetry grounds if $|1\rangle$ and $|2\rangle$ are restricted to the Γ_{15} valence and Γ_1 conduction states.

Equation (7) can be simplified as follows. The first square bracket is zero since the operators p_μ and δU have opposite parity. Assuming the Bloch functions are real, the

second square bracket reduces to $(\hbar/m_0)\tilde{F}_1\Sigma_{z_i}\pi_i k_z\tilde{\delta}(z-z_i)\Sigma_s\theta_{1,s}p^z_{1s}D_{0,s1}$ which is proportional to $-i\tilde{F}_1(z)\tilde{\delta}'(z-z_i)$, so it makes an interface contribution. The fourth bracket can also contribute interface terms proportional to $-i\tilde{F}_2(z)\tilde{\delta}'(z-z_i)$ or $\tilde{\delta}(z-z_i)k_\mu\tilde{F}_2(z)$. The sum of all interface terms can be written $\Sigma_{z_i}\pi_i\tilde{\delta}(z-z_i)\Omega_{12}\tilde{F}_2(r)+\pi_i\tilde{\delta}'(z-z_i)\{\Upsilon_{11}\tilde{F}_1(r)+\Upsilon_{12}\tilde{F}_2(r)\}$ in which

$$\Omega_{12}=D_{0,12}+\sum_{\mu=x,y,z}\{Q^\mu_{L,12}+Q^\mu_{R,12}\}k_\mu,$$

$$\Upsilon_{11}=-i\{D_{1,11}+Q^z_{L,11}\},$$

$$\Upsilon_{12}=-i\{D_{1,12}+Q^z_{L,12}\}. \tag{8}$$

In Eq. (8) $Q^\mu_{L,12}=(\hbar/m_0)\Sigma_s\theta_{12,s}p^\mu_{1s}D_{0,s2}$, $Q^\mu_{R,12}=(\hbar/m_0)\Sigma_s\theta_{12,s}D_{0,1s}p^\mu_{s2}$, and $k_z=-i\partial/\partial z$. If we define the magnitude of the interface terms in Eq. (8) as $\delta\bar{V}(\bar{k}a)^\ell$, the two terms in Ω_{12} are formally of type $\ell=1$ and 2, respectively, while Υ_{11} and Υ_{12} all correspond to $\ell=2$. There is no Ω_{11} term since $D_{0,11}=Q^\mu_{L,11}+Q^\mu_{R,11}=0$.

The third square bracket in Eq. (7) may be simplified by noting that we may expand the Bloch functions of the reference crystal in terms of the Bloch functions of the local crystal to obtain the relationship between the local and reference momentum matrix elements,

$$\langle u^{(lc)}_1|p_\mu|u^{(lc)}_2\rangle-\langle u_1|p_\mu|u_2\rangle=\frac{im_0(P^{12(lc)}_\mu-P^{12}_\mu)}{\hbar}=\sum_{n'\neq 2}\frac{\langle u_1|p_\mu|u_{n'}\rangle\langle u_{n'}|\delta U|u_2\rangle}{E_2-E_{n'}}+\sum_{n'\neq 1}\frac{\langle u_1|\delta U|u_{n'}\rangle\langle u_{n'}|p_\mu|u_2\rangle}{E_1-E_{n'}} \tag{9}$$

in which $\delta U=U^{(lc)}-U$, where the parameters with a superscript, (lc), are those of the local crystal while the parameters without a superscript belong to the reference crystal, and where higher order terms in $\delta\bar{V}/\Delta E$ have been neglected. At this level of accuracy both denominators may be replaced by $(E_1+E_2)/2-E_{n'}$. If the local states are restricted to the Γ_{15} valence and Γ_1 conduction bands, the summations can be made just over all of the remote states, s, since any contribution when n' is a local state is symmetry forbidden.

Substituting Eqs. (8) and (9) into Eq. (7) we have

$$E\tilde{F}_1=\frac{\hbar^2}{2}\sum_{\substack{\mu,\nu=\\ x,y,z}}k_\mu\frac{1}{m_{1,\mu\nu}}k_\nu\tilde{F}_1+E^{(lc)}_1\tilde{F}_1+i\sum_\mu P^{12(lc)}_\mu k_\mu\tilde{F}_2+\sum_{\mu,\nu}k_\mu C^{12}_{\mu\nu}k_\nu\tilde{F}_2+\sum_{z_i}\pi_i\tilde{\delta}'(z-z_i)\Upsilon_{11}\tilde{F}_1(r)+\sum_{z_i}\pi_i\{\tilde{\delta}(z-z_i)\Omega_{12}+\tilde{\delta}'(z-z_i)\Upsilon_{12}\}\tilde{F}_2(r)$$

$$+\tilde{F}_2\frac{\hbar}{m_0}\sum_\mu\left[k_\mu\sum_s\theta_{12,s}\tilde{G}(z)p^\mu_{1s}\delta U_{s2}\right]. \tag{10}$$

Note that in Eq. (10) the first-order $\mathbf{k}\cdot\mathbf{p}$ terms containing P^{12}_μ have been replaced by their local counterparts containing $P^{12(lc)}_\mu$. The last term in Eq. (10) establishes the correct operator ordering of these terms, as may be seen by integrating Eq. (10) across an interface. Comparing the result with Eq. (9) shows that the last term in Eq. (10) can be omitted if $P^{12(lc)}_\mu k_\mu$ is replaced with $(1-f^\mu_{12})k_\mu P^{12(lc)}_\mu+f^\mu_{12}P^{12(lc)}_\mu k_\mu$, where

$$f^\mu_{12}=\frac{-i\hbar/m_0}{(P^{12+}_\mu-P^{12-}_\mu)}\sum_s\frac{\langle u_1|U^+-U^-|u_s\rangle\langle u_s|p_\mu|u_2\rangle}{(E_1+E_2)/2-E_s} \tag{11}$$

and $f^\mu_{21}=1-f^\mu_{12}$. This operator ordering only matters for $\mu=z$, but it has also been retained for $\mu=x,y$, in order to keep the notation consistent. In Eq. (11) symbols with a plus refer to the material on the right-hand side of the interface and those with a minus, to the material on the left-hand side. Note that on going from a normal to an inverted interface, both (U^+-U^-) and $(P^{12+}_\mu-P^{12-}_\mu)$ change sign, so the definition of f^μ_{12} is not sensitive to the interface type.

It is not straightforward to estimate the value of f^μ_{12}. For $|1\rangle=|Z\rangle$ (bonding p state) and $|2\rangle=|\sigma\rangle$ (antibonding s state), the states, s, that can contribute to the sum in Eq. (11) are antibonding p states (Γ^-_{15}), and bonding and antibonding f states ($\Gamma^\pm_{25}$). These, and bonding and antibonding d states ($\Gamma^\pm_{12}$), contribute to the denominator $(P^{12+}_\mu-P^{12-}_\mu)$. Thus $f^z_{Z\sigma}$ can be expressed as

$$f^z_{Z\sigma}=\Sigma_{s=\Gamma^-_{15},\Gamma^\pm_{25}}\theta_{Z,s}\delta U_{Zs}p^z_{s\sigma}/\{\Sigma_{s=\Gamma^\pm_{12}}\theta_{\sigma,s}p^z_{Zs}\delta U_{s\sigma}+\Sigma_{s=\Gamma^-_{15},\Gamma^\pm_{25}}\theta_{Z,s}\delta U_{Zs}p^z_{s\sigma}\}.$$

The antibonding p-state contribution would be zero in the presence of inversion symmetry and thus has a relatively small matrix element, $p^z_{Z'\sigma}$. It is typically about three times smaller than the matrix element, $p^z_{Z\sigma}$, with a bonding p state,[25,26] so we can write $p^z_{Z'\sigma}\sim(\bar{k}a)p^z_{Z\sigma}$ (which is a useful expression for later on). The combination of the weak antibonding p-state contribution, and the small f-state contribution, could yield a term comparable with the d-state term, so $f^z_{Z\sigma}$ will be nonzero. It is not easy to make a simple theoretical estimate of $f^z_{Z\sigma}$ but it can be treated as a fitting parameter in the same way as the Luttinger parameters. However, the Luttinger parameters are fitted to bulk energy dispersion data for each individual material while $f^z_{Z\sigma}$ must be fitted to dispersion data for the superlattice.

If we only include terms of magnitude $\delta\bar{V}\cdot(\bar{k}a)$ or larger, a first version of the Hamiltonian for superlattice structures finally takes the form

$$EF_1 = \frac{\hbar^2}{2}\sum_{\substack{\mu,\nu= \\ x,y,z}} k_\mu \frac{1}{m_{1,\mu\nu}} k_\nu F_1 + E_1^{(lc)} F_1 + i\sum_\mu [(1-f_{12}^\mu)k_\mu P_\mu^{12(lc)} + f_{12}^\mu P_\mu^{12(lc)} k_\mu] F_2 + \sum_{\mu,\nu} k_\mu C_{\mu\nu}^{12} k_\nu F_2 + D_{0,12} F_2 \sum_{z_i} \pi_i \delta(z-z_i). \quad (12)$$

In Eq. (12) the band-edge energy $E_1^{(lc)}(z)$ and the $P_\mu^{12(lc)}$ parameter are the local bulk values. Reference crystal values appear for the $m_{1,\mu\nu}$ and $C_{\mu\nu}^{12}$ parameters. Since the accuracy of Eq. (12) is limited to $\delta\bar{V}\cdot(\bar{k}a)$, only the $D_{0,12}$ interface term has been kept. In Eq. (12) the tilde symbols have also been dropped in order to allow all Fourier components, and the band-edge potential, $E_1^{(lc)}(z)$, is taken to have a square piecewise variation instead of varying as $\Gamma(z)$. The justification for these simplifications is discussed by Takhtamirov and Volkov[10] who argue that the error introduced by allowing all Fourier components should be $\sim\delta\bar{V}\cdot(\bar{k}a)^3$, which is small enough to be ignored. Burt also provided a justification by comparing the exact solution with the square-well envelope function solution, for a one-dimensional Mathieu lattice.[7,27] Equation (12) appears similar to a standard Kane Hamiltonian, the main differences being the ordering of the k-linear operator containing the material parameter $P_\mu^{12(lc)}$, the absence of a piecewise variation in the k-quadratic material parameters, and the appearance of a delta functionlike interface term.

V. ELIMINATION OF THE DEPENDENCE ON THE REFERENCE CRYSTAL

A second more precise version of the Hamiltonian for superlattice structures will now be discussed which has an accuracy of $\delta\bar{V}\cdot(\bar{k}a)^2$ so that smaller interface terms omitted from Eq. (12) can be included, and so that differences in the $m_{1,\mu\nu}$ and $C_{\mu\nu}^{12}$ parameters on each side of an interface can properly be taken into account. Note that in Eq. (12) these parameters take the reference crystal values, $m_{1,\mu\nu}^A$ and $C_{\mu\nu}^{12,A}$, corresponding to material A. The transformation in Eq. (6) must now include the third and fourth terms that have not been considered so far. Evaluating these terms but neglecting contributions of magnitude $\delta\bar{V}\cdot(\bar{k}a)^\ell$ with $\ell\geq 3$, results in the addition of two more components of order $\delta\bar{V}\cdot(\bar{k}a)^2$ to the right-hand side of Eq. (12). The first of these modifies the diagonal kinetic-energy terms such as, $\bar{H}_{11}$, as follows:

$$\bar{H}_{11} = \frac{\hbar^2}{2}\left\{\sum_{\substack{\nu= \\ x,y,z}} k_\nu \frac{1}{m_{1,\nu\nu}^A} k_\nu - \frac{\{\mu_{\alpha,\nu\nu}^{11} + \bar{\mu}_{\alpha,\nu\nu}^{11}\}}{2}[\tilde{G}(z)k_\nu^2 + k_\nu^2\tilde{G}(z)] + \{\mu_{\beta,\nu\nu}^{11} + \bar{\mu}_{\beta,\nu\nu}^{11}\}k_\nu\tilde{G}(z)k_\nu\right\}, \quad (13)$$

where

$$\mu_{\alpha,\nu\nu}^{11} = \frac{2}{m_0^2}\sum_{m''s}\theta_{s,1}\theta_{s,m''}\delta U_{1m''}p_{m''s}^\nu p_{s1}^\nu - \frac{4}{m_0^2}\sum_{ss'}\theta_{s,1}\theta_{s',1}\delta U_{1s}p_{ss'}^\nu p_{s'1}^\nu,$$

$$\mu_{\beta,\nu\nu}^{11} = \frac{2}{m_0^2}\sum_{ss'}\theta_{s,1}\theta_{s',1}p_{1s}^\nu\delta U_{ss'}p_{s'1}^\nu - \frac{4}{m_0^2}\sum_{m''s}\theta_{s,1}\theta_{s,m''}p_{1s}^\nu\delta U_{sm''}p_{m''1}^\nu,$$

$$\bar{\mu}_{\alpha,\nu\nu}^{11} = \frac{2}{m_0^2}\sum_{m''s}\theta_{s,1}\theta_{s,m''}\delta U_{1s}p_{sm''}^\nu p_{m''1}^\nu,$$

$$\bar{\mu}_{\beta,\nu\nu}^{11} = \frac{2}{m_0^2}\sum_{m''s}\theta_{s,1}\theta_{s,m''}p_{1s}^\nu\delta U_{sm''}p_{m''1}^\nu. \quad (14)$$

By substituting Eq. (9) into the formula for the effective mass, $m_0/m_{1,\mu\nu} = \delta_{\mu\nu} + (2/m_0)\Sigma_s p_{1s}^\mu p_{s1}^\nu/(E_1 - E_s)$, it can be shown that $1/m_{1,\nu\nu}^B = 1/m_{1,\nu\nu}^A + (\mu_{\beta,\nu\nu}^{11} - \mu_{\alpha,\nu\nu}^{11})$.

For the case of a 6×6 Hamiltonian based on Γ_{15} valence states, the $\bar{\mu}_{\alpha,\nu\nu}^{11}$ and $\bar{\mu}_{\beta,\nu\nu}^{11}$ terms are zero. For the 8×8 case which also includes the Γ_1 conduction states, $\bar{\mu}_{\alpha,\nu\nu}^{11}$ and $\bar{\mu}_{\beta,\nu\nu}^{11}$ either contain terms with momentum matrix elements which are zero when inversion symmetry applies, and so as discussed earlier, are reduced in the present case roughly by a factor of $(\bar{k}a)$, or they contain terms which are very small because they have large denominators (involving d- or higher energy states). For this reason, both $\bar{\mu}_{\alpha,\nu\nu}^{11}$ and $\bar{\mu}_{\beta,\nu\nu}^{11}$ should be of order $\delta\bar{V}\cdot(\bar{k}a)^3$ and can be ignored. Takhtamirov and Volkov[9] have shown that Eq. (13) can then be rearranged to give

$$\bar{H}_{11} = \frac{\hbar^2}{2}\sum_{\substack{\nu= \\ x,y,z}} k_\nu \frac{1}{m_{1,\nu\nu}^{(lc)}} k_\nu + \hbar^2 \sum_{z_i} \frac{\mu_{\alpha,zz}^{11}}{4}\pi_i\tilde{\delta}'(z-z_i), \quad (15)$$

where $m_{1,\nu\nu}^{(lc)}$ is the local mass value.

Estimates can be made for $\mu_{\alpha,zz}^{11}$ with $|1\rangle = |\sigma\rangle$, $|X\rangle$, $|Y\rangle$, or $|Z\rangle$, by ignoring all terms with momentum matrix elements that are zero when inversion symmetry applies. Also any term with a very large denominator (involving d- or higher energy states) can reasonably be ignored in favor of other terms with a much smaller denominator. Since $\mu_{\alpha,zz}^{11}$ is of order $\delta\bar{V}\cdot(\bar{k}a)^2$ any such the terms can be considered to be below the required accuracy limit. For example, for the 6×6 case $\mu_{\alpha,zz}^{ZZ}$ is given by

$$\mu_{\alpha,zz}^{ZZ} = \frac{2}{m_0^2}\theta_{C,V}^2\delta U_{ZZ}p_{Z\sigma}^z p_{\sigma Z}^z = -\frac{2}{\hbar^2}\frac{F'}{E_G}\delta E_V, \quad (16)$$

where F' is the Kane parameter of the reference crystal (which includes contributions from both bonding and *anti-bonding s* states), E_C and E_V are the conduction and valence-band edges of the reference crystal ($E_G = E_C - E_V$), and δE_V is the valence-band offset. The expressions for $\mu_{\alpha,zz}^{XX}$, $\mu_{\alpha,zz}^{YY}$, and

$\mu^{\sigma\sigma}_{\alpha,zz}$ can be deduced in terms of the Kane parameters in a similar way and these are listed in Sec. VI.

The second component that must be added to Eq. (12), due to the higher order terms in Eq. (6), concerns a correction to the off-diagonal energy term, $\Sigma_{\mu,\nu=x,y,z}k_\mu C^{12}_{\mu\nu}k_\nu$. Since $C^{12}_{\mu\nu}$ in Eq. (12) is equal to $C^{12,A}_{\mu\nu}$, which is a parameter of the reference crystal, A, and is constant throughout, this term can be rewritten: $N^A_{12}k_\mu k_\nu=\Sigma_{\mu',\nu'=x,y,z}C^{12,A}_{\mu'\nu'}k_{\mu'}k_{\nu'}$. With the correction, the off-diagonal energy term becomes

$$\bar{H}_{12}=N^A_{12}k_\mu k_\nu+r_{\mu\nu}k_\mu(\Delta N_{12}+\Delta\bar{n}_{12})\cdot\tilde{G}(z)k_\nu + r_{\nu\mu}k_\nu(\Delta N_{12}+\Delta\bar{n}_{12})\cdot\tilde{G}(z)k_\mu,$$

where the local value, $N^{(lc)}_{12}$ is given by $N^{(lc)}_{12}=N^A_{12}+\Delta N_{12}\cdot\tilde{G}(z)$ and $r_{\nu\mu}=1-r_{\mu\nu}$. The term $\Delta\bar{n}_{12}(z)=\Delta\bar{n}_{12}\cdot\tilde{G}(z)$ that appears in the Hamiltonian is not related to the bulk Kane parameter, N_{12}, but is an extra term produced by the expansion in Eq. (6). For clarity let us consider a specific case where the local states have Γ_{15} symmetry and are $|1\rangle=|Z\rangle$ and $|2\rangle=|X\rangle$. In this case $C^{ZX}_{xz}=H_1$, $C^{ZX}_{zx}=D=F'-G$, and all other $C^{ZX}_{\mu\nu}$ are zero. F', H_1, and G are the Kane parameters based on states of Γ_1, Γ_{15}, and Γ_{12} symmetries, respectively. Performing an analysis similar to that for the diagonal terms in Eq. (13) and assuming the Bloch functions are real, the corrections for the off-diagonal energy term in Eq. (12) are

$$\begin{aligned}r_{xz}\Delta N_{ZX}=&-\frac{\hbar^2}{2m_0^2}\sum_{m''s}^{B/2}\theta_{s,m''}\theta_{s,X}\delta U_{Zm''}p^x_{m''s}p^z_{sX}\\&-\frac{\hbar^2}{2m_0^2}\sum_{m''s}^{H/2}\theta_{s,m''}\theta_{s,X}\delta U_{Zm''}\{p^z_{m''s}\}\{p^x_{sX}\}\\&+\frac{\hbar^2}{m_0^2}\sum_{ss'}^{J}\theta_{s,X}\theta_{s',X}\delta U_{Zs}p^z_{ss'}\{p^x_{s'X}\}\\&+\frac{\hbar^2}{m_0^2}\sum_{ss'}^{R}\theta_{s,X}\theta_{s',X}\delta U_{Zs}p^x_{ss'}p^z_{s'X}\\&+\frac{\hbar^2}{m_0^2}\sum_{ss'}^{A}\theta_{s,X}\theta_{s',X}p^x_{Zs}\delta U_{ss'}p^z_{s'X},\end{aligned}$$

$$r_{xz}\Delta\bar{n}_{ZX}=-\frac{\hbar^2}{2m_0^2}\sum_{m''s}^{M/2}\theta_{s,m''}\theta_{s,X}\delta U_{Zs}\{p^z_{sm''}\}(p^x_{m''X})$$

and

$$\begin{aligned}r_{zx}\Delta N_{ZX}=&-\frac{\hbar^2}{m_0^2}\sum_{m''s}^{L}\theta_{s,m''}\theta_{s,X}\{p^z_{Zs}\}\delta U_{sm''}(p^x_{m''X})\\&-\frac{\hbar^2}{m_0^2}\sum_{m''s}^{K}\theta_{s,m''}\theta_{s,X}(p^z_{Zm''})\delta U_{m''s}\{p^x_{sX}\}\\&-\frac{\hbar^2}{2m_0^2}\sum_{m''s}^{H/2}\theta_{s,m''}\theta_{s,X}\{p^z_{Zs}\}\{p^x_{sm''}\}\delta U_{m''X}\\&-\frac{\hbar^2}{2m_0^2}\sum_{m''s}^{B/2}\theta_{s,m''}\theta_{s,X}p^x_{Zs}p^z_{sm''}\delta U_{m''X}\\&+\frac{\hbar^2}{m_0^2}\sum_{ss'}^{T}\theta_{s,X}\theta_{s',X}\{p^z_{Zs}\}\delta U_{ss'}\{p^x_{s'X}\}\\&+\frac{\hbar^2}{m_0^2}\sum_{ss'}^{I}\theta_{s,X}\theta_{s',X}\{p^z_{Zs}\}p^x_{ss'}\delta U_{s'X}\\&+\frac{\hbar^2}{m_0^2}\sum_{ss'}^{C}\theta_{s,X}\theta_{s',X}p^x_{Zs}p^z_{ss'}\delta U_{s'X}\\=&(1-r_{xz})\Delta N_{ZX},\end{aligned}$$

$$\begin{aligned}r_{zx}\Delta\bar{n}_{ZX}=&\frac{\hbar^2}{2m_0^2}\sum_{m''s}^{-L/2}\theta_{s,m''}\theta_{s,X}\{p^z_{Zs}\}\delta U_{sm''}(p^x_{m''X})\\&+\frac{\hbar^2}{2m_0^2}\sum_{m''s}^{-K/2}\theta_{s,m''}\theta_{s,X}(p^z_{Zm''})\delta U_{m''s}\{p^x_{sX}\}\\&-\frac{\hbar^2}{2m_0^2}\sum_{m''s}^{N/2}\theta_{s,m''}\theta_{s,X}(p^z_{Zm''})\{p^x_{m''s}\}\delta U_{sX},\end{aligned}\quad(17)$$

where $\Delta N_{ZX}=[N^B_{ZX}-N^A_{ZX}]$, and where each term has been labeled with a superscript above its summation sign for ease of identification later on. In Eq. (17), terms containing momentum matrix elements $p^z_{m''X}=p^x_{m''Z}=0$ have been dropped. Round brackets are used to identify momentum matrix elements which are zero for the 6×6 case. Curly brackets are used to identify elements which are rather small for remote s and p states in the 8×8 case, because they vanish in the presence of inversion symmetry, and so are suppressed in the present case by a factor of $\sim(\bar{k}a)$. These matrix elements can be larger for remote d states but then the term to which they belong will be very small because it contains the square of the energy gap E_d-E_X in the denominator, where E_d is a d-state energy. Matrix elements suppressed by inversion symmetry include elements of the form $p^z_{\sigma'Z}$ and $p^z_{\sigma Z'}$ in which σ (σ') is the antibonding (bonding) s state and Z (Z') is the bonding (antibonding) p state. The appearance of the $\Delta\bar{n}$ term in Eq. (17), similar to the $\bar{\mu}^{11}_{\alpha,\nu\nu}$ and $\bar{\mu}^{11}_{\beta,\nu\nu}$ terms above, introduces a dependence on the choice of reference crystal into the Hamiltonian. However, this dependence is much weaker than for the lower order Hamiltonian of Eq. (12) because, similar to the $\bar{\mu}^{11}_{\alpha,\nu\nu}$ and $\bar{\mu}^{11}_{\beta,\nu\nu}$ terms, $\Delta\bar{n}$ is either zero (in the 6×6 case) or else it is of order $\delta\bar{V}\cdot(\bar{k}a)^3$ which is small enough to be ignored (in the 8×8 case).

The separation of the terms in Eq. (17) between ΔN_{ZX} and $\Delta\bar{n}_{ZX}$ is based on an expression for ΔN_{ZX}, obtained by substituting Eq. (9) into the expression for the coefficient of the off-diagonal energy term in the reference crystal: $C^{ZX}_{\mu\nu}=(\hbar^2/m_0^2)\Sigma_s p^\mu_{Zs}p^\nu_{sX}/(E_v-E_s)$, where $C^{ZX}_{zx}=D$, $C^{ZX}_{xz}=H_1$, and $\Delta N_{ZX}=\Delta D+\Delta H_1$. On performing this substitution, the following result is obtained:

$$\Delta H_1 = \frac{\hbar^2}{m_0^2}\sum_{s'}^{A}\sum_{s}\theta_{\mathrm{X},s}\theta_{\mathrm{X},s'}p^x_{\mathrm{Z}s'}\delta U_{s's}p^z_{s\mathrm{X}} - \frac{\hbar^2}{m_0^2}\sum_{s}^{B}\theta^2_{\mathrm{X},s}p^x_{\mathrm{Z}s}p^z_{s\mathrm{X}}\delta U_{\mathrm{ZZ}} + \frac{\hbar^2}{m_0^2}\sum_{s}\sum_{s'}^{C}\theta_{\mathrm{X},s}\theta_{\mathrm{X},s'}p^x_{\mathrm{Z}s}p^z_{ss'}\delta U_{s'\mathrm{X}} + \frac{\hbar^2}{m_0^2}\sum_{s}\sum_{s'}^{R}\theta_{\mathrm{X},s}\theta_{\mathrm{X},s'}\delta U_{\mathrm{Z}s'}p^x_{s's}p^z_{s\mathrm{X}}$$

and

$$\Delta D = \frac{\hbar^2}{m_0^2}\sum_{s'}\sum_{s}^{T}\theta_{\mathrm{X},s}\theta_{\mathrm{X},s'}p^z_{\mathrm{Z}s'}\delta U_{s's}p^x_{s\mathrm{X}} - \frac{\hbar^2}{m_0^2}\sum_{s}^{H}\theta^2_{\mathrm{X},s}p^z_{\mathrm{Z}s}p^x_{s\mathrm{X}}\delta U_{\mathrm{ZZ}} + \frac{\hbar^2}{m_0^2}\sum_{s}\sum_{s'}^{I}\theta_{\mathrm{X},s}\theta_{\mathrm{X},s'}p^z_{\mathrm{Z}s}p^x_{ss'}\delta U_{s'\mathrm{X}} + \frac{\hbar^2}{m_0^2}\sum_{s}\sum_{s'}^{J}\theta_{\mathrm{X},s}\theta_{\mathrm{X},s'}\delta U_{\mathrm{Z}s'}p^z_{s's}p^x_{s\mathrm{X}} + \frac{\hbar^2}{m_0^2}\sum_{s}\sum_{m''}^{K}\theta_{s,m''}\theta_{\mathrm{X},s}p^z_{\mathrm{Z}m''}\delta U_{m''s}p^x_{s\mathrm{X}} + \frac{\hbar^2}{m_0^2}\sum_{s}\sum_{m''}^{L}\theta_{s,m''}\theta_{\mathrm{X},s}p^z_{\mathrm{Z}s}\delta U_{sm''}p^x_{m''\mathrm{X}}. \quad (18)$$

In Eq. (18), terms containing momentum matrix elements $p^z_{m''\mathrm{X}}=p^x_{\mathrm{Z}m''}=0$ have been dropped. The widely accepted form of the $\bar{H}_{\mathrm{ZX}}$ term based on the Burt formulation[13,14,16–18] is

$$\bar{H}^{Burt}_{\mathrm{ZX}} = k_z D^{(lc)}k_x + k_x H_1^{(lc)}k_z = N^A_{\mathrm{ZX}}k_zk_x + k_z\Delta D\cdot\tilde{G}(z)k_x + k_x\Delta H_1\cdot\tilde{G}(z)k_z.$$

If we ignore $\Delta\bar{n}_{\mathrm{ZX}}$ for the reasons given above, the present treatment gives $\bar{H}_{\mathrm{ZX}}=N^A_{\mathrm{ZX}}k_zk_x+k_zr_{zx}\Delta N_{\mathrm{ZX}}\cdot\tilde{G}(z)k_x+k_xr_{xz}\Delta N_{\mathrm{ZX}}\cdot\tilde{G}(z)k_z$. Comparing Eqs. (17) and (18) shows that $r_{zx}\Delta N_{\mathrm{ZX}}\neq\Delta D$ [for ease of comparison each term in Eqs. (17) and (18) is labeled with an alphabetic superscript above its summation sign]. For example, the second term in ΔH_1 is made up from the sum of the first term in $r_{xz}\Delta N_{\mathrm{ZX}}$ and the fourth term in $r_{zx}\Delta N_{\mathrm{ZX}}$. Therefore the Burt formulation is not correct and the formulation presented here must be adopted instead.

In the 6×6 case, a reasonable approximation can be found for $r_{xz}\Delta N_{\mathrm{ZX}}$, in terms of the Kane or Luttinger parameters, as follows. This expression is written as $r_{xz}\Delta N_{\mathrm{ZX}}=-B/2-H/2+A+J+R$, where each of the five terms $B/2$, etc., represents a (labeled) term in the first part of Eq. (17). In evaluating these terms, only s, p, and d states are considered since the f states will make a negligible contribution. Also, contributions are ignored which have matrix elements suppressed by a factor $\sim(\bar{k}a)$, due to their vanishing in the presence of inversion symmetry. Each term can be expanded in terms of the Kane parameters and appropriate band gaps and band offsets, as follows: $B=\frac{\hbar^2}{m_0^2}\Sigma_{s=\Gamma_{15}^-}\theta^2_{s,\mathrm{X}}\delta U_{\mathrm{ZZ}}p^x_{\mathrm{Z}s}p^z_{s\mathrm{X}}=-H_1\frac{\delta E_{\mathrm{X}}}{E_{\mathrm{X}'}-E_{\mathrm{X}}}$, where X and X′ are the bonding (Γ_{15}^+) and antibonding (Γ_{15}^-) p states, respectively, and $\delta E_{\mathrm{X}}=\delta E_V=E_V^B-E_V^A$ is the valence-band offset.

$H=\frac{\hbar^2}{m_0^2}\Sigma_{s=\Gamma_1^\pm,\Gamma_{12}^\pm}\theta^2_{s,\mathrm{X}}\delta U_{\mathrm{ZZ}}p^z_{\mathrm{Z}s}p^x_{s\mathrm{X}}=-F'\frac{\delta E_V}{E_G}+G\frac{\delta E_V}{E_{D'}-E_{\mathrm{X}}}$, where $\Gamma_1^\pm$ are the bonding and antibonding s states and $\Gamma_{12}^\pm$ are the bonding and antibonding d states. In deriving this formula it was assumed that contributions containing the matrix element $p^z_{\sigma'\mathrm{Z}}\sim p^z_{\sigma\mathrm{Z}}(\bar{k}a)$ can be ignored, as discussed above. $E_{D'}$ is the energy of the antibonding d states (Γ_{12}^-).

$A=\frac{\hbar^2}{m_0^2}\Sigma_{s=\Gamma_{15}^-,s'=\Gamma_{15}^-}\theta_{s,\mathrm{X}}\theta_{s',\mathrm{X}}p^x_{\mathrm{Z}s}\delta U_{ss'}p^z_{s'\mathrm{X}}=-H_1\frac{\delta E_{\mathrm{X}'}}{|E_{\mathrm{X}'}-E_{\mathrm{X}}|}$, where $\delta E_{\mathrm{X}'}\approx\alpha_{\mathrm{X}}\delta E_V$ is the band offset of the antibonding p states. Since the bonding and antibonding p states should have nearly the same probability densities, it is to be expected that α_{X} is fairly close to unity.

The other two terms in $r_{xz}\Delta N_{\mathrm{ZX}}$ are negligible. $J=(\hbar^2/m_0^2)\Sigma_{s=\Gamma_{15}^-,\ s'=\Gamma_1^\pm,\Gamma_{12}^\pm}\theta_{s,\mathrm{X}}\theta_{s',\mathrm{X}}\delta U_{\mathrm{Z}s}p^z_{ss'}p^x_{s'\mathrm{X}}$ is negligible since each term in the sum, *including terms with d* states, contains a momentum matrix element which is zero when the crystal exhibits inversion symmetry. $R=(\hbar^2/m_0^2)\Sigma_{ss'}\theta_{s,\mathrm{X}}\theta_{s',\mathrm{X}}\delta U_{\mathrm{Z}s}p^x_{ss'}p^z_{s'\mathrm{X}}$ is negligible since it has a very large denominator involving the product of antibonding p states and bonding or antibonding f states.

Combining all terms, we have $r_{xz}\Delta N_{\mathrm{ZX}}=\{F'/E_G-G/(E_{D'}-E_V)-\{2\alpha_{\mathrm{X}}-1\}H_1/(E_{\mathrm{X}'}-E_{\mathrm{X}})\}(\delta E_V/2)$. The Kane parameters F', H_1, and G may be evaluated from the Luttinger parameters as described in Sec. VI. Typical values for GaAs in units of $3\hbar^2/m_0$ are −2.4, −0.61, and −0.14 respectively. The energy gap between p states has a value of approximately $E_{\mathrm{X}'}-E_{\mathrm{X}}\sim5$ eV. If we also assume that $E_{D'}-E_V>10$ eV, it is found that the term proportional to G contributes less than 1% to the value of $r_{xz}\Delta N_{\mathrm{ZX}}$ and so can be neglected. Its contribution is also negligible in other common superlattice systems, such as those considered below in Table II. This term will therefore be ignored. Thus we can write

$$r_{xz}\Delta N_{\mathrm{ZX}} = \left\{\frac{1}{E_G}F' - \frac{\{2\alpha_{\mathrm{X}}-1\}}{E_{\mathrm{X}'}-E_{\mathrm{X}}}H_1\right\}\frac{\delta E_V}{2}. \quad (19)$$

A similar treatment can be performed for $r_{zx}\Delta N_{\mathrm{ZX}}=(1-r_{xz})\Delta N_{\mathrm{ZX}}$ by ignoring terms with matrix elements that are suppressed by inversion symmetry and also terms with denominators in which at least one of the remote states is an f state. Also terms are ignored where the two remote states are d states or a combination of d and bonding s states since the latter are as remote as d states and even d states were shown above to make a negligible contribution. The one exception is the term labeled T in the second part of Eq. (17), which contributes a term with a denominator containing both antibonding s and d states. It also contributes a much larger term whose denominator contains two antibonding s states. This is

shown explicitly in Eq. (20) in which δE_C is the conduction-band offset,

$$T = \frac{\hbar^2}{m_0^2} \sum_{s,s'=\Gamma_1^{\pm},\Gamma_{12}^{\pm}} \theta_{s,\mathrm{X}} \theta_{s',\mathrm{X}} p_{\mathrm{Z}s}^z \delta U_{ss'} p_{s'\mathrm{X}}^x$$

$$\approx \frac{\hbar^2}{m_0^2} \theta_{\sigma,\mathrm{X}}^2 p_{\mathrm{X}\sigma}^x p_{\sigma\mathrm{X}}^x \delta U_{\sigma\sigma} - 2\frac{\hbar^2}{m_0^2} \theta_{\sigma,\mathrm{X}} \theta_{D',\mathrm{X}} p_{\mathrm{X}\sigma}^x p_{\mathrm{X}D'}^x \delta U_{\sigma D'}$$

$$\approx -\frac{F'}{E_G} \delta E_C + 2P_z \frac{(1-f_{\mathrm{Z}\sigma}^z)}{E_G} \delta P_z^{(lc)} \left[1 - \frac{E_G}{E_{D'} - E_\sigma} \right]. \quad (20)$$

In Eq. (20), the term in the middle line proportional to $\delta U_{\sigma D'}$ has been expressed in the last line in terms of $\delta P_z^{(lc)}$, using the expressions in Eqs. (9) and (11). Setting the square bracket in the last line equal to one since $E_G \ll E_{D'} - E_\sigma$, the result for $(1-r_{xz})\Delta N_{\mathrm{ZX}}$, analogous to Eq. (19), is

$$(1-r_{xz})\Delta N_{\mathrm{ZX}} = \frac{H_1}{2} \frac{\delta E_V}{E_{\mathrm{X}'} - E_{\mathrm{X}}} + \frac{F'}{2E_G} (\delta E_V - 2\delta E_C) + 2\frac{(1-f_{\mathrm{Z}\sigma}^z)P_z}{E_G} \delta P_z^{(lc)}. \quad (21)$$

Combining Eqs. (19) and (21) yields

$$\Delta N_{\mathrm{ZX}} = r_{xz}\Delta N_{\mathrm{ZX}} + (1-r_{xz})\Delta N_{\mathrm{ZX}} \approx -F' \frac{\Delta E_G}{E_G} + 2\frac{(1-f_{\mathrm{Z}\sigma}^z)P_z}{E_G} \delta P_z^{(lc)} + \{1-\alpha_{\mathrm{X}}\} \frac{H_1}{E_{\mathrm{X}'} - E_{\mathrm{X}}} \delta E_V. \quad (22)$$

Equation (22) shows that on crossing an interface, the main change in $N = F' - G + H_1$, is the term proportional to ΔE_G, which is due to the denominator of F' that depends mainly on the antibonding s states. Changes in the squared momentum matrix element of the numerator make a much smaller contribution, proportional to $\delta P_z^{(lc)}$. The change in H_1 is given by the third term in Eq. (22) and is very small, vanishing for $\alpha_{\mathrm{X}} = 1$. This term is due to the change in the band gap between the bonding and antibonding p states, which is fairly similar in both materials. Any change in H_1 due to the squared momentum matrix element in its numerator is negligible because the change in the numerator involves f, or higher states, according to Eq. (9). The contribution from the G term is negligible because it has a very large denominator. Its variation is expected to be of order $\Delta G/G \sim \delta\bar{V}/\Delta E$ which yields $\Delta G \sim G(\bar{k}a)^2 < \delta\bar{V}\cdot a^2$ since $G\bar{k}^2 < F\bar{k}^2 \sim \delta\bar{V}$. Since $\delta\bar{V}\cdot a^2$ corresponds to an energy contribution $\delta\bar{V}\cdot(\bar{k}a)^2$, which is the accuracy limit in this section, we can write $\Delta G \sim 0$. Equation (22) means that in the 8×8 case considered below, where the contribution from the antibonding s band is excluded, $\Delta N_{\mathrm{ZX}} \approx \Delta H_1 \approx \{1-\alpha_{\mathrm{X}}\}(H_1/E_{\mathrm{X}'} - E_{\mathrm{X}})\delta E_V$, which vanishes for $\alpha_{\mathrm{X}} = 1$.

Substituting Eq. (22) into Eq. (21), we end up with the final result for the operator ordering parameter, r_{xz}:

$$r_{xz}(6\times 6) = \frac{\frac{1}{2}\left[(2\alpha_{\mathrm{X}} - 1)\frac{E_G}{E_{\mathrm{X}'} - E_{\mathrm{X}}} \frac{H_1}{F'} - 1 \right] \frac{\delta E_V}{\Delta E_G}}{1 - 2(1 - f_{\mathrm{Z}\sigma}^z)\frac{P_z}{F'} \frac{\delta P_z^{(lc)}}{\Delta E_G} - \{1-\alpha_{\mathrm{X}}\}\frac{H_1}{F} \frac{E_G}{E_{\mathrm{X}'} - E_{\mathrm{X}}} \frac{\delta E_V}{\Delta E_G}}. \quad (23)$$

Note that H, F', and the band-gap energies E_G and $E_{\mathrm{X}'} - E_{\mathrm{X}}$ in Eq. (23) refer to the reference crystal, and that $\delta E_V/\Delta E_G$ is simply the valence-band offset ratio at each interface. As shown below in Sec. VII, the first term in the denominator of Eq. (23), and the second term in the brackets of the numerator, will dominate in narrow gap systems and r_{xz} then takes a value close to minus half the valence-band offset ratio.

In arriving at the expression for r_{xz}, where $(1-r_{xz})k_z N_{\mathrm{ZX}} k_x$ makes an interface contribution of order $\delta\bar{V}\cdot(\bar{k}a)^2$, a number of small terms have been neglected due to small momentum matrix elements which would be zero in the presence of inversion symmetry or due to large energy denominators. This can be justified by supposing that they will each make a contribution at least $\sim(\bar{k}a)$ times smaller than other larger terms, of order $\delta\bar{V}\cdot(\bar{k}a)^2$, and so can reasonably be neglected. The same argument was already applied above to the diagonal $\mu_{\alpha,zz}^{11}$ terms. It should also be noted that if r_{xz} is determined by substituting $\Delta N_{\mathrm{ZX}} = -3\hbar^2\Delta\gamma_3/m_0$ into Eq. (19), the results are less reliable, being much more dependent on the choice of reference crystal than those obtained by substituting Eq. (22). This is because ΔN_{ZX} has a nonlinear variation with composition, as evident from Eq. (22).

For the 8×8 case, there is no contribution from the antibonding s states, so the F' and P_z terms can be dropped in Eqs. (19), (21), and (22). No other significant terms are introduced. This gives $r_{xz}\Delta N_{\mathrm{ZX}} = -\{2\alpha_{\mathrm{X}} - 1\}\overline{\Delta N}$ and $(1-r_{xz})\Delta N_{\mathrm{ZX}} = \overline{\Delta N}$ with $\overline{\Delta N} = \{H_1/(E_{\mathrm{X}'} - E_{\mathrm{X}})\}\delta E_V/2$. Hence $\Delta N_{\mathrm{ZX}} = -2\{\alpha_{\mathrm{X}} - 1\}\overline{\Delta N}$ and r_{xz} is given by the following simple relationship:

$$r_{xz}(8\times 8) = \frac{\alpha_{\mathrm{X}} - 0.5}{\alpha_{\mathrm{X}} - 1}. \quad (24)$$

Note that for $\alpha_{\mathrm{X}} \to 1$, $\Delta N_{\mathrm{ZX}} \to 0$. However, the product $r_{xz}\Delta N_{\mathrm{ZX}}$ remains finite.

Based on the preceding results, a second version of the Hamiltonian for superlattice structures can be constructed which now includes all terms up to order $\ell = 2$ in $\delta\bar{V}\cdot(\bar{k}a)^\ell$. It takes the form

$$EF_{\mathrm{Z}} = \left\{ \begin{array}{l} \dfrac{\hbar^2}{2}\left\{ k_x \dfrac{1}{m^{(lc)}_{\mathrm{Z},xx}} k_x + k_y \dfrac{1}{m^{(lc)}_{\mathrm{Z},yy}} k_y + k_z \dfrac{1}{m^{(lc)}_{\mathrm{Z},zz}} k_z \right\} + \sum_{z_i} \left\{ \dfrac{\hbar^2}{4} \mu^{\mathrm{Z}}_{\alpha,zz} + \Upsilon_{\mathrm{ZZ}} \right\} \pi_i \delta'(z - z_i) \\ + \alpha_{0,zz} k_z^4 + \alpha_{1,zz}\{k_x^4 + k_y^4\} + \beta_{0,zz} k_x^2 k_y^2 + \beta_{1,zz}\{k_x^2 k_z^2 + k_y^2 k_z^2\} \end{array} \right\} F_{\mathrm{Z}} + E^{(lc)}_{\mathrm{Z}} F_{\mathrm{Z}} - i\{f P^{(lc)}_z k_z + (1-f) k_z P^{(lc)}_z\} F_\sigma$$
$$+ \{r k_x N^{(lc)} k_z + (1-r) k_z N^{(lc)} k_x\} F_{\mathrm{X}} + \{r k_y N^{(lc)} k_z + (1-r) k_z N^{(lc)} k_y\} F_{\mathrm{Y}} + \sum_{z_i} \pi_i \delta(z - z_i)\{\Omega_{\mathrm{Z}\sigma} F_\sigma + \Omega_{\mathrm{ZX}} F_{\mathrm{X}} + \Omega_{\mathrm{ZY}} F_{\mathrm{Y}}\}$$
$$+ \sum_{z_i} \delta(z - z_i)\{\Omega^a_{\mathrm{Z}\sigma} F_\sigma + \Omega^a_{\mathrm{ZX}} F_{\mathrm{X}} + \Omega^a_{\mathrm{ZY}} F_{\mathrm{Y}} + \Omega^a_{\mathrm{ZZ}} F_{\mathrm{Z}}\} + \sum_{z_i} \delta'(z - z_i) \Upsilon^a_{\mathrm{Z}\sigma} F_\sigma, \tag{25}$$

where the inclusion of the $\alpha_{0,11}$, $\alpha_{1,11}$, $\beta_{0,11}$, and $\beta_{1,11}$ nonparabolicity terms was first pointed out by Takhtamirov and Volkov.[9,10] These (and additional off-diagonal contributions not explicitly included) come, for example, from the next term in the expansion of Eq. (6) and are evaluated for the reference crystal. For low lying confined states these terms can probably be ignored, especially in an 8×8 treatment, where the remote states of the reference crystal that contribute to the nonparabolicity coefficients are more distant in energy than in the 6×6 case.

The terms on the last line of Eq. (25) with superscript "a" are due to the antisymmetric part of $G'(z)$ and apply in the case of a no common atom superlattice, as discussed in Sec. III. Note that they do not contain a factor π_i since $G'(z)|_a$ has the same sign at each interface (see Appendix B). Note also that the notation has been simplified by invoking cubic crystal symmetry and Hermiticity of the Hamiltonian: $r = r_{xz} = r_{yz}$, $f = f^z_{\mathrm{Z}\sigma}$, $P^{(lc)}_z = P^{\sigma\mathrm{Z}(lc)}_z$, and $N^{(lc)} = N^{(lc)}_{\mathrm{ZX}} = N^{(lc)}_{\mathrm{ZY}}$. r is given by Eqs. (23) and (24) for the 6×6 and 8×8 cases, respectively.

In the next section the full 6×6 and 8×8 Hamiltonian *matrices* are presented, based on the forgoing treatment.

VI. HAMILTONIAN FOR Γ_1 CONDUCTION AND Γ_{15} VALENCE STATES

Following from the preceding results, it is possible to construct a complete 6×6 Hamiltonian matrix for the zone-center Γ_{15} valence states. Similarly a complete 8×8 Hamiltonian matrix can be constructed which also includes the Γ_1 conduction states. These Hamiltonians matrices are presented below. The nonparabolicity terms are not included for the reasons discussed in Sec. V but could easily be incorporated at the expense of adding several more fitting parameters. Additional contributions due to relativistic corrections are considered in Sec. VIII. The Hamiltonian matrix is made up of two diagonal blocks, $\bar{\bar{M}}$, one for each spin direction, where $\bar{\bar{M}} = \bar{\bar{M}}_1 + \bar{\bar{M}}_{IF_1} + \bar{\bar{M}}_{IF_2} + \bar{\bar{M}}'_{IF_1} + \bar{\bar{M}}'_{IF_2}$. The matrices $\bar{\bar{M}}_{IF_2}$ and $\bar{\bar{M}}'_{IF_2}$ may be omitted for common atom superlattices, which have a negligible $G'(z)|_a$ (see Appendix B). Moreover, as discussed below, the matrices $\bar{\bar{M}}'_{IF_1}$ and $\bar{\bar{M}}'_{IF_2}$ are usually small enough to be below the level of uncertainty in any comparison with experimental data and can be omitted in most cases. The main exception is $\bar{\bar{M}}'_{IF_1}$ in the 6×6 case. Table I shows the definitions of the terms that appear in the matrix $\bar{\bar{M}}$, which is written explicitly below. The 8×8 Hamiltonian matrix has the following states as the local basis: S↑, X↑, Y↑, Z↑, S↓, X↓, Y↓, and Z↓ while in the 6×6 Hamiltonian matrix the S↑ and S↓ states are excluded. Only the spin-up matrices are given below.

The 8×8 Hamiltonian is as follows, where the superscript (lc) refers to local piecewise values,

$$\bar{\bar{M}}_1 = \begin{bmatrix} \left\{ \begin{array}{l} A'^{(lc)}(k_x^2 + k_y^2) \\ + k_z A'^{(lc)} k_z + E^{(lc)}_C \end{array} \right\} & i P^{(lc)} k_x & i P^{(lc)} k_y & i \left\{ \begin{array}{l} (1-f) P^{(lc)} k_z \\ + f k_z P^{(lc)} \end{array} \right\} \\ - i P^{(lc)} k_x & \left\{ \begin{array}{l} L'^{(lc)} k_x^2 + M^{(lc)} k_y^2 \\ + k_z M^{(lc)} k_z + E^{(lc)}_V \end{array} \right\} & N^{(lc)} k_x k_y & (1-r) k_x N^{(lc)} k_z + r k_z N^{(lc)} k_x \\ - i P^{(lc)} k_y & N^{(lc)} k_x k_y & \left\{ \begin{array}{l} M^{(lc)} k_x^2 + L'^{(lc)} k_y^2 \\ + k_z M^{(lc)} k_z + E^{(lc)}_V \end{array} \right\} & (1-r) k_y N^{(lc)} k_z + r k_z N^{(lc)} k_y \\ - i \left\{ \begin{array}{l} f P^{(lc)} k_z \\ + (1-f) k_z P^{(lc)} \end{array} \right\} & r k_x N^{(lc)} k_z + (1-r) k_z N^{(lc)} k_x & r k_y N^{(lc)} k_z + (1-r) k_z N^{(lc)} k_y & \left\{ \begin{array}{l} M^{(lc)}(k_x^2 + k_y^2) \\ + k_z L'^{(lc)} k_z + E^{(lc)}_V \end{array} \right\} \end{bmatrix}, \tag{26}$$

$$\bar{\bar{M}}_{IF_1} = \sum_i \pi_i \delta(z - z_i) \times \begin{bmatrix} 0 & i\kappa_1 k_y & i\kappa_1 k_x & \beta \\ -i\kappa_1 k_y & 0 & \alpha & i(\kappa_0 + \kappa_2)k_x \\ -i\kappa_1 k_x & \alpha & 0 & i(\kappa_0 + \kappa_2)k_y \\ \beta & -i(\kappa_0 + \kappa_2)k_x & -i(\kappa_0 + \kappa_2)k_y & 0 \end{bmatrix}, \tag{27}$$

$$\bar{\bar{M}}_{IF_2} = \sum_i \delta(z - z_i) \begin{bmatrix} D^a_{0,\sigma\sigma} & i\chi_1 k_x & i\chi_1 k_y & i\chi_1 k_z \\ -i\chi_1 k_x & D^a_{0,\mathrm{XX}} & 0 & i\chi_0 k_y \\ -i\chi_1 k_y & 0 & D^a_{0,\mathrm{XX}} & i\chi_0 k_x \\ -i\chi_1 k_z & -i\chi_0 k_y & -i\chi_0 k_x & D^a_{0,\mathrm{ZZ}} \end{bmatrix}, \tag{28}$$

$$\bar{\bar{M}}'_{IF_1} = \sum_i \pi_i \delta'(z - z_i) \begin{bmatrix} d_{1,\sigma\sigma} & 0 & 0 & 0 \\ 0 & \eta_{\mathrm{X}} - \kappa_0 + d_{1,\mathrm{XX}} & 0 & 0 \\ 0 & 0 & \eta_{\mathrm{X}} - \kappa_0 + d_{1,\mathrm{XX}} & 0 \\ 0 & 0 & 0 & \kappa_2 + d_{1,\mathrm{ZZ}} \end{bmatrix}, \tag{29}$$

and

$$\bar{\bar{M}}'_{IF_2} = \sum_i \delta'(z - z_i) \begin{bmatrix} 0 & 0 & 0 & \bar{\beta} \\ 0 & 0 & \bar{\alpha} + \chi_2 & 0 \\ 0 & \bar{\alpha} + \chi_2 & 0 & 0 \\ \bar{\beta} - \chi_1 & 0 & 0 & 0 \end{bmatrix}. \tag{30}$$

A term of the form Bk_yk_z can be added to $iP^{(lc)}k_x$, with similar combinations for the other $P^{(lc)}$ terms. It contributes to a small spin splitting in the conduction band.[26] However, it is often ignored since it vanishes in the presence of inversion symmetry and is not included here explicitly. P is given by $P=(\hbar/im_0)p^x_{\sigma\mathrm{X}}$.

Equations (27) and (28) contain matrix elements due to $Q^{\mu}_{L,12}+Q^{\mu}_{R,12}$ and Eqs. (29) and (30) contain matrix elements due to $Q^{z}_{L,12}$, as defined in Eq. (8). Contributions to these elements from Γ_1 bonding s states are ignored (since they are

TABLE I. Definition of parameters appearing in the 8×8 and 6×6 Hamiltonians. E_G is the band gap, in the *absence* of the spin-orbit interaction, between antibonding s states which form the conduction-band edge, E_C, and bonding p states which form the valence-band edge, E_V. $\delta E_V=E^B_V-E^A_V$ is the valence-band offset and $E_{\mathrm{X}'}-E_{\mathrm{X}}$ is the band gap between the antibonding ($\Gamma_{15\mathrm{c}}$) and bonding ($\Gamma_{15\mathrm{v}}$) p states at the zone center. α_{X} is the ratio of the $\Gamma_{15\mathrm{c}}$ and $\Gamma_{15\mathrm{v}}$ band offsets. F', G, and H_1 are the Kane parameters. The second of these should not be confused with the profile function $G(z)$.

Parameter	8×8	6×6
L'	$F'+2G+\hbar^2/2m_0$	
M	$H_1+\hbar^2/2m_0$	
N	$F'-G+H_1$	
A'	$(\hbar^2/2m_0)(m_0/m_c-E_P(E_G+\Delta/3)/\{(E_G-\Delta/3)(E_G+2\Delta/3)\})$	
F'	$-(3\hbar^2/m_0)\sigma+(\hbar^2/2m_0)(E_P/E_G)$	$-(3\hbar^2/m_0)\sigma$
G	$-(3\hbar^2/m_0)\delta$	
H_1	$-(3\hbar^2/m_0)\pi$	
σ	$-(1+\gamma_1-8\gamma_2-12\gamma_3)/18$	
δ	$(1+\gamma_1+\gamma_2-3\gamma_3)/9$	
π	$(1+\gamma_1-2\gamma_2)/6$	
E_P	$2m_0P^2/\hbar^2$	
r	$\dfrac{\alpha_{\mathrm{X}}-0.5}{\alpha_{\mathrm{X}}-1}$	$\dfrac{\frac{1}{2}\left\{\{2\alpha_{\mathrm{X}}-1\}\frac{E_G}{E_{\mathrm{X}'}-E_{\mathrm{X}}}\frac{H_1}{F'}-1\right\}\frac{\delta E_V}{\Delta E_G}}{1-2(1-f^z_{\mathrm{Z}\sigma})\frac{P_z}{F'}\frac{\delta P^{(lc)}_z}{\Delta E_G}-\{1-\alpha_{\mathrm{X}}\}\frac{H_1}{F}\frac{E_G}{E_{\mathrm{X}'}-E_{\mathrm{X}}}\frac{\delta E_V}{\Delta E_G}}$
η_{Z}		$-(F'/2E_G)\delta E_V$
η_{X}	$-(H_1/2\{E_{\mathrm{X}'}-E_{\mathrm{X}}\})\delta E_V$	

zero in the presence of inversion symmetry), as are contributions from f, or more remote states. The coefficients in Eq. (27) and (29) which come from the symmetric part of $G'(z)$ are $\kappa_0 = i(\hbar/m_0)D^s_{0,\mathrm{YX}'}p^y_{\mathrm{X}'\mathrm{Z}}/(E_{\mathrm{X}'}-E_{\mathrm{X}})$, $\kappa_2 = i(\hbar/m_0)\Sigma_{s=\Gamma_{12}^{\pm}}p^y_{\mathrm{Y}s}D^s_{0,s\mathrm{Z}}/(E_s-E_{\mathrm{X}})$, and $\kappa_1 = i(\hbar/m_0)D^s_{0,\sigma\mathrm{Z}'}p^y_{\mathrm{Z}'\mathrm{X}}/(E_{\mathrm{X}'}-E_{\mathrm{X}}+E_G/2)$. In deriving the terms proportional to κ_0 or κ_1 in Eq. (27), symmetry relations between momentum matrix elements of the form $p^x_{\mathrm{Y}'\mathrm{Z}}$ are applied, as given in Ref. 28, and the following symmetry relations for the D_0 operator are used: $D^s_{0,\mathrm{XY}'}=D^s_{0,\mathrm{YX}'}=D^s_{0,\mathrm{Y}'\mathrm{X}}$ and $D^s_{0,\mathrm{YZ}'}=D^s_{0,\mathrm{XZ}'}=0$. The other terms in Eq. (27) are directly related to the D_0 operator: $\alpha=D^s_{0,\mathrm{XY}}$ and $\beta=D^s_{0,\sigma\mathrm{Z}}$. The coefficients in Eqs. (28) and (30) which come from the antisymmetric part of $G'(z)$, as defined in Appendix B, are $\chi_0 = i(\hbar/m_0)[p^y_{\mathrm{XZ}'}D^a_{0,\mathrm{Z}'\mathrm{Z}}+D^a_{0,\mathrm{XX}'}p^y_{\mathrm{X}'\mathrm{Z}}]/(E_{\mathrm{X}'}-E_{\mathrm{X}})$, $\chi_1 = i(\hbar/m_0)\Sigma_{s=\Gamma_{12}^{\pm}}D^a_{0,\sigma s}p^z_{s\mathrm{Z}}/(E_s-E_{\mathrm{X}})$, and $\chi_2 = i(\hbar/m_0)p^z_{\mathrm{XY}'}D^a_{0,\mathrm{Y}'\mathrm{Y}}/(E_{\mathrm{X}'}-E_{\mathrm{X}})$. The diagonal terms: $D^a_{0,\sigma\sigma}$, $D^a_{0,\mathrm{XX}}=D^a_{0,\mathrm{YY}}$, and $D^a_{0,\mathrm{ZZ}}$ in Eq. (28) were introduced in Sec. III and are due to the D_0 operator. Similarly $\bar{\alpha}=-iD^a_{1,\mathrm{XY}}$ and $\bar{\beta}=-iD^a_{1,\sigma\mathrm{Z}}$ in Eq. (30) are due to the D_1 operator and are analogous to the α, β coefficients of the D_0 operator.

The appearance of χ_1 in Eq. (30) ensures Hermiticity when combined with Eq. (28). Note, however, that the terms in χ_1 and κ_2 are probably quite small relative to the other χ_i and κ_i terms in the interface matrices since they are due to fairly remote antibonding d states (the contributions due to bonding d states are negligible since they would be zero in the presence of inversion symmetry). These terms might be considered to be smaller than $\delta\bar{V}\cdot(\bar{k}a)^2$ and ignored, thereby simplifying the interface matrices for no common atom superlattices quite significantly.

In Eq. (29), the η_{X} term is related to $\mu^{\mathrm{XX}}_{\alpha,zz}$, which was discussed after Eq. (16). It is given by $\eta_{\mathrm{X}}=(\hbar^2/4)\mu^{\mathrm{XX}}_{\alpha,zz}$. Corresponding terms $\eta_\sigma=(\hbar^2/4)\mu^{\sigma\sigma}_{\alpha,zz}$ and $\eta_{\mathrm{Z}}=(\hbar^2/4)\mu^{\mathrm{ZZ}}_{\alpha,zz}$ contain two Γ_{12} d states and are taken to be negligible: $\mu^{\sigma\sigma}_{\alpha,zz} = (2/m_0^2)\Sigma_{s=\Gamma_{12}^{\pm}}\delta U_{\sigma s}p^z_{s\mathrm{Z}}p^z_{\mathrm{Z}\sigma}/(E_s-E_V)(E_s-E_C)$ and $\mu^{\mathrm{ZZ}}_{\alpha,zz}\approx -G(4/\hbar^2)(E_d-E_V)\delta E_V$, where E_d is a typical d-state energy. The $d_{1,nn}$ terms in Eq. (29) are due to the D_1 operator, where $d_{1,nn}=-iD_{1,nn}$ is real. These terms may be small enough to be ignored, according to the values estimated for $d_{1,nn}$ in Sec. III. In fact, all the terms in Eqs. (29) and (30) should be comparable in size to the $d_{1,nn}$ terms, so it is probably a reasonable approximation to omit $\bar{\bar{M}}'_{IF_1}$ and $\bar{\bar{M}}'_{IF_2}$ altogether.

Note that α, β and $D^a_{0,\sigma\sigma}$, $D^a_{0,\mathrm{XX}}$, and $D^a_{0,\mathrm{ZZ}}$ in Eq. (27) and (28) are of order $\ell=1$ in $\delta\bar{V}\cdot(\bar{k}a)^\ell$ while the rest of the terms in Eqs. (27)–(30) are of order $\ell=2$. Note also that the diagonal $\ell=1$ terms in Eq. (28) couple the same states as the diagonal $\ell=2$ terms in Eq. (29) and that the off-diagonal $\ell=1$ terms in Eq. (27) couple the same states as the off-diagonal $\ell=2$ terms in Eq. (30). Therefore, in no common atom superlattices, the omission of $\bar{\bar{M}}'_{IF_1}$ and $\bar{\bar{M}}'_{IF_2}$ can be justified, not only on the grounds that they are very small but also because their contributions can simply be considered to renormalize the values of the $\ell=1$ terms.

In the 6×6 Hamiltonian, $\bar{\bar{M}}_1$, $\bar{\bar{M}}_{IF_2}$, and $\bar{\bar{M}}'_{IF_2}$ are given by the lower right-hand 3×3 block for the X↑, Y↑, and Z↑ states in Eqs. (26), (28), and (30), respectively, with the r parameter in Eq. (26) defined for the 6×6 case in Table I. The other interface matrices are as follows:

$$\bar{\bar{M}}_{IF_1} = \sum_i \pi_i\delta(z-z_i)\begin{bmatrix} 0 & \alpha & i(P\beta/E_G+\kappa_0+\kappa_2)k_x \\ \alpha & 0 & i(P\beta/E_G+\kappa_0+\kappa_2)k_y \\ -i(P\beta/E_G+\kappa_0+\kappa_2)k_x & -i(P\beta/E_G+\kappa_0+\kappa_2)k_y & 0 \end{bmatrix} \tag{31}$$

and

$$\bar{\bar{M}}'_{IF_1} = \sum_i \pi_i\delta'(z-z_i)\begin{bmatrix} \eta_{\mathrm{X}}-\kappa_0+d_{1,\mathrm{XX}} & 0 & 0 \\ 0 & \eta_{\mathrm{X}}-\kappa_0+d_{1,\mathrm{XX}} & 0 \\ 0 & 0 & P\beta/E_G+\eta_{\mathrm{Z}}+\kappa_2+d_{1,\mathrm{ZZ}} \end{bmatrix}. \tag{32}$$

The appearance of $P\beta/E_G$ in Eq. (31) is due to expressions like $\{Q^y_{L,\mathrm{YZ}}+Q^y_{R,\mathrm{YZ}}\}$ which can now include a term $i(\hbar/m_0)p^y_{\mathrm{Y}\sigma}D_{0,\sigma\mathrm{Z}}/(E_\sigma-E_{\mathrm{X}})$ in addition to $i\kappa_0$. A similar term appears in $Q^z_{L,\mathrm{ZZ}}$ and hence in Eq. (32) due to the remote antibonding s band (which was not remote in the 8×8 formulation). This band also contributes to $\eta_{\mathrm{Z}}=(\hbar^2/4)\mu^{\mathrm{ZZ}}_{\alpha,zz}$ which had only weak d-band contributions in the 8×8 case. The expression for $\mu^{\mathrm{ZZ}}_{\alpha,zz}$ is given in Eq. (16). Unlike the 8×8 case, $\bar{\bar{M}}'_{IF_1}$ cannot be totally ignored since, as shown below, the η_{Z} term can be quite large in some superlattices.

VII. NUMERICAL ESTIMATES OF r, η_{X}, and η_{Z}

In this section the parameters r, η_{X}, and η_{Z} which depend on bulk Kane parameters, and which give rise to interface contributions in the Hamiltonian, are estimated. Table II shows the values of r, η_{X}, and η_{Z} for four rather different heterojunction systems: GaAs/$Al_{0.3}Ga_{0.7}$As, $Al_{0.7}Ga_{0.3}$As/AlAs, $In_{0.53}Ga_{0.47}$As/InP, and InAs/GaSb. In the last case, only results appropriate to the 8×8 Hamiltonian are listed because the valence band of GaSb overlaps with the conduction band of InAs, making the 6×6 treat-

ment inappropriate. Values are compared using both well and barrier parameters, in order to show the sensitivity of the result to a change in the reference crystal from the well to the barrier material.

Luttinger parameters and band-gap data were taken from Refs. 29–32 as indicated in the table. The $\Gamma_{15}^{+}-\Gamma_{1}^{-}$ band gap, E_G, was set equal to $E_0+\Delta_0/3$, where $E_0=E_{\Gamma_{6c}}-E_{\Gamma_{8v}}$ is the fundamental band gap of the material and Δ_0 is the spin-orbit splitting energy. In $In_{0.53}Ga_{0.47}As$ and $Al_xGa_{1-x}As$ alloys, the procedure outlined by Vurgaftman *et al.*[31] was used to determine E_0, using the bowing parameters in Ref. 31. In $Al_xGa_{1-x}As$, a linear interpolation was also performed for heavy and light hole masses, E_P, Δ_0, and $\gamma_3-\gamma_2$. The Luttinger parameters for the alloy were then calculated from the mass values and the interpolated value for $\gamma_3-\gamma_2$.

The $\Gamma_{15c}-\Gamma_{15v}$ band gap, $E_{X'}-E_X$, between bonding and antibonding p states, is set equal to $E_{\Gamma_{7c}}-E_{\Gamma_{8v}}+(2/3)\Delta_0'+(1/3)\Delta_0$, where $\Delta_0'=E_{\Gamma_{8c}}-E_{\Gamma_{7c}}$. For the alloys, a linear interpolation was performed. This band gap is fairly constant among III-V materials with the same lattice constant. However, even small variations in the value of $E_{X'}-E_X$ can affect the value of the parameter α_X quite significantly. Fortunately, this only has a very small effect on the values of r (6×6) and η_X, except for superlattice systems with a large band gap, where E_0 and $E_{X'}-E_X$ are comparable in size, as discussed below. Although r (8×8) is sensitive to the value of α_X, the product $r\Delta N^{(lc)}$ is much less so, and this is what determines any interface contribution. Such contributions are, in any case, quite small.

As discussed after Eq. (22), $\Delta H_1\approx\{1-\alpha_X\}(H_1/E_{X'}-E_X)\delta E_V$ and $\Delta G\approx0$. In addition, $F'(8\times8)\approx0$, since only the bonding s states (σ') contribute to this Kane parameter, and their contribution is very small, due both to their large energy separation from the valence-band edge ($\geq$10 eV), and to the small value of the momentum matrix element $p^x_{\sigma'X}$, the squared modulus of which appears in the numerator of F' and which vanishes in the presence of inversion symmetry. These last two conditions can be written, $E_0/E_{\sigma'X}\leq(\bar{k}a)$, where $E_{\sigma'X}=E_V-E_{\sigma'}$ and $P'\sim(\bar{k}a)P$, where $P'=(\hbar/im_0)p^x_{\sigma'X}$ (see Ref. 26). Thus $F'(8\times8)\cdot\bar{k}^2=[(\hbar^2/2m_0)E_{P'}/E_{\sigma'X}]\bar{k}^2\sim(\bar{k}a)^3\times|[(\hbar^2/2m_0)(E_{P'}/E_{\sigma'X}-E_P/E_0)]\bar{k}^2|$. Since the square bracket in the last term is just $|F'(6\times6)|$ and $|F'(6\times6)\cdot\bar{k}^2|\sim\delta\bar{V}$, this shows that $|F'(8\times8)\cdot\bar{k}^2|<\delta\bar{V}\cdot(\bar{k}a)^2$. Hence, $F'(8\times8)\approx0$ is consistent with our accuracy limit of $\delta\bar{V}\cdot(\bar{k}a)^2$. These constraints on F', H_1, and G, together lead to the following relations:

$$1+\gamma_1-8\gamma_2-12\gamma_3+3\gamma_4\approx0, \tag{33a}$$

$$\Delta\gamma_2-\Delta\gamma_3\approx-\frac{\chi}{3}(1+\gamma_1^A-2\gamma_2^A) \tag{33b}$$

$$\Delta\gamma_2+\Delta\gamma_3\approx\frac{\Delta\gamma_4}{3} \tag{33c}$$

where $\gamma_4=E_P/E_G$, $\chi=\{1-\alpha_X\}\delta E_V/(E^A_{X'}-E^A_X)$, $\delta E_V=E^B_V-E^A_V$, $\Delta\gamma_2=\gamma_2^B-\gamma_2^A$, etc., in which A and B are the well and barrier materials and A is the reference crystal. As a result, the number of band-structure fitting parameters can, in principle, be reduced from 8 (γ_1, γ_2, γ_3 and γ_4 for each material of the superlattice) to just 4 (e.g., γ_1, γ_2, and γ_4 for the well material and γ_4 for the barrier material). Note that Eq. (33) refers to materials, A and B, which are perfectly lattice matched. Thus Luttinger parameters deduced using Eq. (33), may differ by a small amount from bulk values, if material B has a slightly different lattice parameter than material A. Of the superlattice materials in Table II, InAs/GaSb has a significantly larger lattice mismatch ($\sim$0.6%) than the others and so might be expected to show the most significant deviation from the bulk values.

In Table II, the band-structure parameters taken from the literature have been slightly modified in some instances, in order to achieve consistency with Eq. (33). It is not claimed that they are more accurate in each case than the literature values since no attempt has been made to fit them to experimental data or to include strain effects. The purpose is only to provide typical estimates for the magnitudes of r, η_X, and η_Z, which are presented *both* with the original literature parameters and with the adjusted parameters, for comparison. Where the parameters are not the same, the literature values are shown in square brackets. It should be noted that the literature parameters sometimes lead to inconsistencies, such as a value for $|F'(6\times6)|$ in both InAs and GaSb which is about 25% greater than $(\hbar^2/2m_0)(E_P/E_G)$, when in fact it must be very slightly smaller.

The operator ordering parameter $r(6\times6)$, calculated in Table II, depends on the second operator ordering parameter, f, which is defined in Eq. (11). Its value is not known, so the r values given in Table II are computed for $f=0.5$. For comparison with the r value, the equivalent result for the operator ordering in the Burt formulation, $r_{Burt}=\Delta H_1/(\Delta D+\Delta H_1)$, is also included in Table II, where $D=F'(6\times6)-G$. It can be seen from the table that r is fairly insensitive to the choice of reference crystal and is also quite different from the Burt value. This is true, regardless of the value chosen for f. Note that both in $GaAs/Al_{0.3}Ga_{0.7}As$ and $In_{0.53}Ga_{0.47}As/InP$, r takes a value quite close to minus half the valence-band offset ratio, $\delta E_V/\Delta E_G\sim\delta E_{V0}/\Delta E_0$. The reason for this was discussed earlier. For $Al_{0.7}Ga_{0.3}As/AlAs$, r appears to be much more sensitive to the parameters f and a_X. Presumably this is because $E_G=E_\sigma-E_X$ is no longer substantially smaller than $E_{X'}-E_X$, so the second term in the numerator and the first term in the denominator of Eq. (23), which are due only to the antibonding s states (σ), are no longer dominant. However, even in this case the error in r is less than $\sim(\bar{k}a)$, which will only introduce an error of order $\delta\bar{V}\cdot(\bar{k}a)^3$ into the interface term due to $\Delta N^{(lc)}$. Thus simply setting r equal to minus half the valence-band offset ratio in all cases is an acceptable simplification.

In the 8×8 case, the operator ordering parameter, $r(8\times8)$, and the Burt value, $r_{Burt}=\Delta H_1/(\Delta D+\Delta H_1)$, are again generally different for most of the heterojunctions. In this case $D=F'(8\times8)-G$. An exception appears to be InAs/GaSb, but the near agreement for this heterojunction is likely to be coincidental, for the reasons discussed after Eq. (18). In fact, for the 8×8 case, $\Delta N=\Delta D+\Delta H_1\sim\Delta H_1$ is quite small,

TABLE II. Values of the operator ordering parameter r determined in the 6×6 (with $f=0.5$) and 8×8 Hamiltonians, and the equivalent Burt parameter $r_{\mathrm{Burt}}=\Delta H_1/\Delta D+\Delta H_1$, calculated for different heterojunction combinations. Values are also calculated for the η_Z parameter in the 6×6 Hamiltonian, and the η_X parameter appropriate to both the 6×6 and 8×8 Hamiltonians. The source of each band-structure parameter is indicated by a letter as follows: *a*= Ref. 29, *b*= Ref. 30, *c*= Ref. 31, and *d*= Ref. 32. The parameter values for $Al_xGa_{1-x}As$ alloys are determined from the parameter values of the binary materials, as described in the text. In cases where γ_1, γ_2, or γ_3 have been changed, for reasons given in the text, the original literature values, and the computed results based on the literature values, are given in square brackets.

	Parameters								6×6			Both	8×8	
Reference crystals	γ_1	γ_2	γ_3	E_P (eV)	E_0 (eV)	Δ_0 (eV)	$E_{X'}-E_X$ (eV)	$\frac{\delta E_{V0}}{\Delta E_0}$	r_{Burt}	r	η_Z (eV Å^2)	η_X (eV Å^2)	r_{Burt}	r
			3.19							0.19	−3.1	−0.24		2.2
GaAs	6.84[a]	2.10[a]	[2.9[a]]	25.7[a]	1.52[c]	0.34[b]	4.73[a]		−0.01	[0.19]	[−2.8]	[−0.24]	1.0	[2.2]
	5.58	1.44	2.55					−0.4	[0.04]	0.18	−1.8	−0.25	[0.25]	2.2
$Al_{0.3}Ga_{0.7}As$	[5.2]	[1.38]	[2.12]	24.3	1.94	0.33	4.66			[0.18]	[−1.6]	[−0.23]		[2.2]
			2.01							0.17	−1.7	−0.34		2.8
$Al_{0.7}Ga_{0.3}As$	4.0	0.89	[1.56]	22.5	2.46	0.33	4.57		−0.02	[0.15]	[−1.3]	[−0.34]	1.0	[2.8]
	3.31	0.52	1.66					−0.4	[0.08]	0.12	−1.0	−0.35	[0.24]	2.8
AlAs	[3.45[a]]	[0.68[a]]	[1.29[a]]	21.1[a]	3.10[c]	0.32[b]	4.50[a]			[0.10]	[−0.8]	[−0.33]		[2.8]
			4.97							0.32	−15.5	−0.41		0.0
$In_{0.53}Ga_{0.47}As$	11.01[d]	4.18[d]	[4.84[d]]	25.3[d]	0.816[c]	0.36[a]	4.75[a]		0.01	[0.33]	[−15.2]	[−0.41]	1.0	[0.0]
	6.58	2.02	2.78					−0.6	[0.07]	0.38	−5.1	−0.39	[0.53]	0.0
InP	[4.95[a]]	[1.65[a]]	[2.35[a]]	20.4[a]	1.424[c]	0.11[c]	4.88[a]			[0.42]	[−4.3]	[−0.29]		[0.0]
			6.33									0.62		0.8
InAs	19.7[a]	8.37[a]	[9.29[a]]	22.2[a]	0.418[a]	0.38[c]	4.76[a]					[0.62]	1.0	[0.8]
	13.72	4.95	3.20					1.3				0.96	[0.88]	0.8
GaSb	[11.8[a]]	[4.02[a]]	[5.26[a]]	22.4[a]	0.812[a]	0.75[c]	3.72[a]					[0.95]		[0.8]

as is the parameter, $\overline{\Delta N}$, defined before Eq. (24), which determines the interface contribution to the Hamiltonian due to operator ordering. Thus, operator ordering in the 8×8 case is probably less important than in the 6×6.

Values are given in Table II for the η_Z parameter in the 6×6 Hamiltonian and the η_X parameter appropriate to both the 6×6 and 8×8 Hamiltonians. The diagonal derivative of a delta-function parameter η_X is typically 0.1–1.3 eV Å^2. This should be comparable in size with the $d_{1,XX}$ parameter with which it appears in both the 6×6 and 8×8 Hamiltonians. However, the η_Z derivative of a delta-function parameter can be quite large and it exhibits a large sensitivity to the choice of the reference crystal, especially for narrow gap systems such as $In_{0.53}Ga_{0.47}As/InP$. In this case it can only be determined with an error of ~50% if a suitable virtual-crystal average is used as the reference crystal (e.g., 10 ± 5 eV Å^2). Even in $GaAs/Al_{0.3}Ga_{0.7}As$ it can only be determined with an error of ~25% (e.g., 2.4 ± 0.6 eV Å^2). Thus even if the correct operator ordering and all relevant interface contributions are taken into account, these uncertainties in η_Z will limit the ultimate accuracy of the 6×6 treatment. As an example, the matrix element of η_Z for the lowest light hole state in a quantum well of width L takes a value of approximately $2\pi\eta_Z/3L^2$. For $L=100$ Å and $\eta_Z=10$ eV Å^2, this corresponds to an energy of ~3 meV, which represents the expected level of precision. Since η_Z is proportional to the band offset, the precision will improve with a smaller band offset (smaller Δx in $Al_xGa_{1-x}As$). This is as anticipated since it reduces the value of $\delta\bar{V}/E_G$ and makes the 6×6 treatment a better approximation.

VIII. RELATIVISTIC CORRECTIONS

In this section the relativistic corrections to the preceding Hamiltonians are considered. Based on the treatment of Takhtamirov and Volkov[10] the spin-orbit interaction adds two important terms to the right-hand side of Eq. (3): $\Sigma_{n'}\{\hbar\langle n|\nabla U_A\times\mathbf{p}\cdot\boldsymbol{\sigma}|n'\rangle/4m_0^2c^2\}F_{n'}(\mathbf{k})$ and $\Sigma_{n'}\{\hbar\langle n|\nabla\delta U\times\mathbf{p}\cdot\boldsymbol{\sigma}|n'\rangle/4m_0^2c^2\}\times\int G(k_z-k_z')\delta(\mathbf{k}_\parallel-\mathbf{k}_\parallel')F_{n'}(\mathbf{k}')d\mathbf{k}'$ in which $\boldsymbol{\sigma}$ is the Pauli spin matrix vector. These terms introduce an extra term into Eq. (6): $\frac{1}{3}\Sigma_{n'}(\Delta_{nn'}+\tilde{G}(z)\delta\Delta_{nn'})F_{n'}(r)$ in which $\Delta_{nn'}=3\langle n|(\partial U_A/\partial r)\mathbf{L}\cdot\mathbf{S}/r|n'\rangle/2m_0^2c^2$ and $\delta\Delta_{nn'}=3\langle n|(\partial\{U_B-U_A\}/\partial r)\mathbf{L}\cdot\mathbf{S}/r|n'\rangle/2m_0^2c^2$ and $\mathbf{S}$ is the spin angular momentum operator. This leads to the addition of the familiar spin-orbit energy matrix to Eq. (25). It has the form

$$H_{SO}=\frac{\Delta(z)}{3}\begin{bmatrix}G_\Delta & \Gamma_\Delta\\ -\Gamma_\Delta^* & G_\Delta^*\end{bmatrix},\ \text{where}$$

$$G_\Delta = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \text{ and } \Gamma_\Delta = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -i \\ 0 & -1 & i & 0 \end{bmatrix} \tag{34}$$

with $\Delta(z)=\Delta_A+\tilde{G}(z)(\Delta_B-\Delta_A)$ and $\Delta_A=\Delta^A_{X\uparrow Z\downarrow}=-i(3\hbar/4m_0^2c^2)\langle X|[\nabla U_A\times\mathbf{p}]_y|Z\rangle$.

Takhtamirov and Volkov[10] also derived interface-band mixing terms $S_{l,nn'}$ which are analogous to the $D_{l,nn'}$ terms in Eq. (4) and also an additional interface contribution: $(1/2\pi)\int\delta(\mathbf{k}_\parallel-\mathbf{k}'_\parallel)B_{0,nn'}F_{n'}(\mathbf{k}')d^3k'$, all of which should be added to Eq. (3). For a symmetric interface in which $G'(z)|_a\approx 0$, $B_{0,nn'}$ is given by $B_{0,nn'}=\hbar\langle n|[\nabla(\Phi_0^s\delta U)\cdot(\hbar\mathbf{k}'\times\boldsymbol{\sigma})]|n'\rangle/4m_0^2c^2$ and the $S_{l,nn'}$ terms by $S_{0,nn'}=\chi^0_{nn'}$ and $S_{1,nn'}=i(\chi^1_{nn'}-\chi^0_{nn'})$, with $\chi^0_{nn'}=\hbar\langle n|[\nabla(\Phi_0^s\delta U)\times\mathbf{p}\cdot\boldsymbol{\sigma}]|n'\rangle/4m_0^2c^2$ and $\chi^1_{nn'}=\hbar\langle n|[\Phi_1^s\nabla(\delta U)\times\mathbf{p}\cdot\boldsymbol{\sigma}]|n'\rangle/4m_0^2c^2$. In principle, $S_{0,nn'}$ gives a contribution of order $\delta\bar{V}_{SO}\cdot(\bar{k}a)$ while the other two terms are of order $\delta\bar{V}_{SO}\cdot(\bar{k}a)^2$, where $\delta\bar{V}_{SO}$ is a typical band offset due to the spin-orbit energy: $\delta\bar{V}_{SO}\sim\Delta_B-\Delta_A$. However, since the difference in the spin-orbit splitting, $\Delta_B-\Delta_A=-i(3\hbar/4m_0^2c^2)\langle X|[\nabla(\delta U)\times\mathbf{p}]_y|Z\rangle$, is usually quite small in many common superlattice materials, it might be reasonable to suppose that the spin-orbit related interface-band mixing is substantially smaller than the interface-band mixing due to the $D_{0,nn'}$ and $D_{1,nn'}$ terms. An exception may be in InAs/GaSb, where the difference in the spin-orbit splitting is comparable with the valence-band offset. For this reason, the form of the S_0 and S_1 contributions has been evaluated below. For a symmetric interface, the complete spin-orbit related interface mixing takes a form analogous to Eq. (8): $\Sigma_{z_i}\pi_i\tilde{\delta}(z-z_i)\{\Omega_{11}^{SO}\tilde{F}_1(r)+\Omega_{12}^{SO}\tilde{F}_2(r)\}+\pi_i\tilde{\delta}'(z-z_i)\{\Upsilon_{11}^{SO}\tilde{F}_1(r)+\Upsilon_{12}^{SO}\tilde{F}_2(r)\}$ in which

$$\Omega_{11}^{SO}=S_{0,11}+B_{0,11}+F_{0,11}+\sum_{\mu=x,y,z}\{Q^{SO,\mu}_{L,11}+Q^{SO,\mu}_{R,11}\}k_\mu,$$

$$\Omega_{12}^{SO}=S_{0,12}+B_{0,12}+F_{0,12}+\sum_{\mu=x,y,z}\{Q^{SO,\mu}_{L,12}+Q^{SO,\mu}_{R,12}\}k_\mu,$$

$$\Upsilon_{11}^{SO}=-i\{S_{1,11}+Q^{SO,z}_{L,11}\},$$

$$\Upsilon_{12}^{SO}=-i\{S_{1,12}+Q^{SO,z}_{L,12}\}. \tag{35}$$

In Eq. (35), $Q^{SO,\mu}_{L,12}=(\hbar/m_0)\Sigma_{s>2}\theta_{12,s}p^\mu_{1s}S_{0,s2}$ and $Q^{SO,\mu}_{R,12}=(\hbar/m_0)\Sigma_{s>2}\theta_{12,s}S_{0,1s}p^\mu_{s2}$. F_0 is a term due to Foreman,[33] which will be discussed below. The S_0 and F_0 terms are expressed in matrix form as

$$\bar{\bar{S}}_0+\bar{\bar{F}}_0=\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -A & iA & 0 \\ 0 & i\Delta C_4 & 0 & 0 & A & 0 & 0 & -i\Delta C_4 \\ 0 & 0 & -i\Delta C_4 & 0 & -iA & 0 & 0 & \Delta C_4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & A & iA & 0 & 0 & 0 & 0 & 0 \\ -A & 0 & 0 & -i\Delta C_4 & 0 & -i\Delta C_4 & 0 & 0 \\ -iA & 0 & 0 & -\Delta C_4 & 0 & 0 & i\Delta C_4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{36}$$

where the elements containing the parameter, A, are due to S_0, and the rest are due to F_0.

The S_1 term can be written

$$\bar{\bar{S}}_1=iS_{1a}\begin{bmatrix} G_\Delta & \Gamma_\Delta \\ -\Gamma^*_\Delta & G^*_\Delta \end{bmatrix}+iS_{1b}\begin{bmatrix} 0 & \Gamma_S \\ -\Gamma^*_S & 0 \end{bmatrix}$$

$$\text{with } \Gamma_S=\begin{bmatrix} 0 & 1 & -i & 0 \\ -1 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{37}$$

where S_{1a} and S_{1b} are real.

The parameter A in Eq. (36) is given by $A=(\hbar/4m^2c^2)\langle S\uparrow|(\delta U/r\partial r)\Phi_0^s(xp_z-zp_x)\sigma_y-\delta U\Phi_0^{s'}p_x\sigma_y|X\downarrow\rangle$. Similar expressions can be derived for the other parameters in Eqs. (36) and (37), apart from ΔC_4.

The F_0 terms are proportional to ΔC_4. They are of order $\delta\bar{V}_{SO}\cdot(\bar{k}a)$, and are analogous to the term

$$\tilde{F}_2(\hbar/m_0)\Sigma_\mu k_\mu\Sigma_{s>2}\theta_{12,s}\tilde{G}(z)p^\mu_{1s}\delta U_{s2}$$

in Eq. (10) in which δU_{s2} is replaced by the relativistic term $\{\hbar\langle s|\nabla\delta U\times\mathbf{p}\cdot\boldsymbol{\sigma}|2\rangle/4m_0^2c^2\}$. Foreman discusses this contribution in Ref. 33, where he shows it is stronger than the bulk linear-k mixing but it is still very weak. Not surprisingly, the superlattice combinations where it is strongest are InAs/

GaSb and InP/$In_{0.53}Ga_{0.47}As$ which have a relatively large difference in the value of Δ. In each case he estimates a value of $\Delta C_4 \sim 0.2$ eV Å. This however is much less than the first-order nonrelativistic interface-band mixing, which in InP/$In_{0.53}Ga_{0.47}As$ is estimated to be $D_{0,XY} \sim 2.9$ eV Å for InAs-like interfaces and 0.87 eV Å for InGaP-like interfaces.[23] In the case of GaAs/AlAs, where the materials have a very small difference in the value of Δ, the relativistic ΔC_4 interface contribution is an order of magnitude smaller,$\Delta C_4 \sim 0.02$ eV Å, and is again much less than the first-order nonrelativistic interface-band mixing, $D_{0,XY} \sim 0.2$ eV Å.

Contributions analogous to μ_α and μ_β in Eq. (14) or $r_{\mu\nu}\Delta N_{12}$ and $(1-r_{\mu\nu})\Delta N_{12}$ mixing in Eq. (17), in which the nonrelativistic matrix element $\delta U_{nn'}$ is again replaced by the equivalent relativistic term, will give rise to very complicated expressions. Fortunately such contributions will be a factor $\bar{k}a$ smaller than the ΔC_4 contribution and so can reasonably be ignored.

In the above expressions for the matrices $\bar{\bar{S}}_0$ and $\bar{\bar{S}}_1$, three parameters have been defined: A, S_{1a}, and S_{1b}. In the light of the discussion for ΔC_4, it may be assumed that the last two are generally extremely small since they should give contributions $\sim \bar{k}a$ smaller than the first, and this term should be smaller than the equivalent nonrelativistic D_0 term. The same goes for any additional parameters introduced in an evaluation of $\bar{\bar{B}}_0$. In addition the S_{1a} and S_{1b} terms have the same symmetry as the bulk SO mixing and the A-related mixing, respectively, which are significantly larger.

The matrices for the Q terms in Eq. (35) can be evaluated, based on the well-known properties of the momentum matrix elements and the symmetry of the S_0 term given above. However, since they will generally be smaller than the nonrelativistic $\delta\bar{V}\cdot(\bar{k}a)^2$ terms, they can probably be ignored, similar to the case of the S_1 and B_0 terms discussed above.

Finally, as for the nonrelativistic case, the effect of the antisymmetric contribution in the derivative of the interface profile function, $G'(z)|_a$, should be considered. If we assume, according to the previous argument, that only the A term is significant among those terms that depend on the details of the microscopic interface structure (ΔC_4 does not), then a similar treatment to the above for the symmetry of this term due to an antisymmetric profile function, shows that it will make a δ-function contribution (with no π_i factors) proportional to the spin-orbit matrix given in Eq. (34).

In summary, the relativistic contributions need only be considered in superlattices where the difference in the spin-orbit splitting energies is comparable with the valence-band offset. For these cases, a reasonably accurate approximation for the relativistic contribution might be given by Eq. (36). The effect of asymmetry in the derivative of the interface profile function may appear as a small interface contribution proportional to the spin-orbit matrix. It is likely that even then, all of the relativistic interface terms will have a weaker effect than the nonrelativistic D_0 term and so it may be possible to ignore them in many cases.

IX. SUMMARY AND CONCLUSIONS

A Kane-like Hamiltonian has been derived for lattice-matched semiconductor superlattice structures with metallurgically abrupt interfaces, which considers all terms of order $\delta\bar{V}\cdot(\bar{k}a)^2$ or larger. As pointed out by Takhtamirov and Volkov, terms of this order must be included, if differences in the mass parameters of the well and barrier materials are to be treated consistently. The basic approach that has been used here is based on Burt's original idea, of treating the crystal potential of the superlattice structure as a weak perturbation on that of a bulk reference crystal. However, since Burt did not include all terms of order $\delta\bar{V}\cdot(\bar{k}a)^2$, his result for the operator ordering of the mass terms has been revised in the present work. An operator ordering scheme has also been proposed for the linear-k P terms coupling Γ_1 conduction and Γ_{15} valence states, which was not considered in the Burt treatment. The aim of the present work has been to obtain a consistent Hamiltonian for the Γ_1 conduction and Γ_{15} valence states, which preserves the familiar form of the bulk Kane Hamiltonian, and which keeps the number of mass and interface related parameters as small as possible. This is intended to provide a practical and familiar envelope function equation with improved accuracy, which may be applied to the analysis of experimental data.

In the present work, the use of local, bulk, P and mass parameters has been justified in regions far from the interfaces. The operator ordering scheme deduced for the mass parameters has been compared with Burt's scheme, where it has been shown to give significantly different results for the off-diagonal terms. The two possible orderings of the off-diagonal mass terms are divided in the ratio r and $1-r$. In the 6×6 case (Γ_{1c} excluded), r is roughly equal to minus half the valence-band offset ratio, especially when the superlattice band gap is small. In the 8×8 case (Γ_{1c} included), r depends on the ratio between the band offsets for the antibonding and bonding p states, α_X. However, in this case the operator ordering should have a relatively insignificant effect due to the small change in the bulk mass parameter, N, with which r appears. For the diagonal mass terms, the familiar symmetrical operator ordering scheme has been obtained. However, additional derivative of a δ-function terms are introduced, which are quite significant for the 6×6 case. Nonparabolicity terms should also properly be included, especially in the 6×6 case.

Approximate constraints can be placed on the Kane parameters of perfectly lattice-matched superlattice materials: $\Delta H_1 \approx \{1-\alpha_X\}(H_1/E_{X'}-E_X)\delta E_V$, $\Delta G \approx 0$, and $F'(8\times8) \approx 0$. This is based on the assumption that the contributions to the Kane parameters, or their differences between the well and barrier materials, that come from momentum matrix elements which would be zero in the presence of inversion symmetry, or that come from energy denominators from sufficiently remote states, are significantly smaller than $\delta\bar{V}a^2$. In principle, this allows the number of *independent* Luttinger related fitting parameters to be reduced to just four, e.g., γ_1, γ_2, and γ_4 for the well material and γ_4 for the barrier material in the 8×8 case, where $\gamma_4=E_P/E_G$. If one of the superlattice materials, e.g., the barrier material, is not perfectly lattice matched, the above constraints apply to the material after it has been hydrostatically deformed to achieve a perfect lattice match. A change occurs in γ_4 that can be determined from the strain Hamiltonian, given for example in

Ref. 34, which modifies the values of both E_P and E_G. The Luttinger parameters of the deformed barrier material can then be deduced from the constraint equations, after which the strain Hamiltonian should be applied in the usual way to take any tetragonal deformation into account.[35]

A distinction can be made between superlattices made from materials with a common atom, such as $GaAs/Al_xGa_{1-x}As$, where the derivative of the profile function, $G'(z)$, is expected to be an essentially symmetric function on the common atom interface plane and superlattices with no common atom, such as InAs/GaSb, where $G'(z)$ exhibits a significant antisymmetric component on the atomic plane closest to the interface. A symmetric $G'(z)$ gives rise to relatively simple interface matrices, with off-diagonal δ-functionlike terms and diagonal derivative of a δ-functionlike terms, respectively. Compared with a simple piecewise approach in which the interfaces are not treated properly, essentially only four more parameters are needed in the present treatment of an 8×8 Hamiltonian for a common atom superlattice.[36] Of these, the three parameters which define the derivative of a δ-functionlike matrix can probably be omitted[37] since they couple to the same states as affected by a one monolayer variation in the layer thicknesses but their effect is much smaller. Unfortunately, six additional parameters are needed in a no common atom superlattice.[38] However, two of these make such a small contribution, relative to other interface contributions that couple to the same states, that they can probably also be omitted.[39,40]

In this work, off-diagonal linear-k interface terms have been introduced which depend on a combination of the microscopic interface potential and the $\mathbf{k}\cdot\mathbf{p}$ interaction. They result in terms proportional to $k_x \pm ik_y$ when the spin-orbit interaction is included (i.e., in the Luttinger Hamiltonian) and can introduce a small electric field dependence into the in-plane effective masses for fields applied parallel to the growth direction. However, they also compete with bulk terms which are significantly larger and which are also proportional to $k_x \pm ik_y$. The most important interface contributions are clearly the five k-independent δ-functionlike potentials, of order $\delta\bar{V}\cdot(\bar{k}a)$, which include the off-diagonal α and β terms. These off-diagonal terms provide a mechanism for zone-center band mixing that is totally absent from bulk $\mathbf{k}\cdot\mathbf{p}$ models. This can lead to some dramatic observable effects, such as in-plane anisotropy of both the optical and electrical properties when an electric field is applied along the superlattice growth direction. Some examples may be seen in Refs. 41–43. In contrast to the off-diagonal terms, the diagonal δ-functionlike potentials do not cause band mixing but simply modify the relative alignment of states at the zone center, such as heavy and light hole, somewhat analogous to the effect of an in-plane biaxial strain. However, while strain causes an effective change in well depth, the interface potentials cause an effective change in well width. For example, the energy shift of a superlattice heavy-hole state is given by $\delta E_{HH} \approx -(\partial E_{HH}/\partial L)(2D^a_{0,\mathrm{XX}}/\Delta V)$, where L is the width of the well layers and ΔV is their depth.[44] The heavy holes thus behave as if their well width is increased by an amount, $-2D^a_{0,\mathrm{XX}}/\Delta V$. The five k-independent interface potentials can be treated as fitting parameters, or they can be estimated using the functions Φ^s_0 and Φ^a_0 defined in this work, and model basis functions, deduced, for example, by the pseudopotential method.[11] The functions Φ^s_0 and Φ^a_0 are sensitive to the interface abruptness and so the effect of interface abruptness may also be included. However, it should be noted that according to Ref. 12, the results may become unreliable when the interface becomes significantly graded.

In superlattice combinations which exhibit a large difference in spin-orbit splitting energies, there can be additional weak relativistic interface contributions. The main common superlattice candidates for such contributions are InAs/GaSb and InP/InGaAs. Even here, the nonrelativistic contributions are expected to be larger. Part of the 8×8 interface matrix due to relativistic corrections has also been derived, which includes the most significant terms. However, in the interest of limiting the fitting parameters to a reasonable number, the relativistic interface contributions should most usually be omitted in any practical analysis of experimental data, unless symmetry considerations or other special arguments justify their inclusion.

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APPENDIX A: DERIVATION OF THE INTERFACE TERMS IN THE REAL-SPACE ENVELOPE FUNCTION EQUATION

Equation (3) is the envelope function equation in reciprocal space. It has been derived by Takhtamirov and Volkov[10] using the method of Luttinger and Kohn.[1] In the derivation of Eq. (3) the following normalization conditions are used: $\langle n|\hat{O}|n'\rangle = (2\pi)^3/\Omega \int_{cell} u_n^* \hat{O} u_{n'} d^3r$ and $\int_{cell} u_n^* u_{n'} d^3r = \delta_{nn'}\Omega/(2\pi)^3$, where Ω is the volume of the unit cell. Equation (3) contains an extra factor $\pi_i e^{-i(k-k'_z)z_i}$ that does not appear in Ref. 8 because the equivalent equation in Ref. 8 is for a representative interface at $z=0$ while here all the interfaces are included explicitly. Also the factor $\delta(k_\parallel - k'_\parallel + K_{j\parallel})$ has been replaced here by $\delta(k_\parallel - k'_\parallel)$ since it is shown in Ref. 8 that the only contribution is for $K_{j\parallel}=0$.

In order to derive the envelope function Eq. (5), Eq. (3) must be transformed back to real space. Noting that the wave function in reciprocal space is written $F_{n'}(k') = F_{n'}(k'_z)\delta(k'_\parallel - q_\parallel)$, where $q_\parallel$ is the in-plane wave vector, this procedure is quite straightforward up to the term in $\delta U_{nn'}$ which is derived with a standard application of the convolution theorem. Writing the interface potential as $H^{IF}_{nn'} = H^{IF,0}_{nn'} + H^{IF,1}_{nn'}$, the next term transforms as follows:

$$\sum_{n'} H^{IF,0}_{nn'}\tilde{F}_{n'}(\boldsymbol{\rho},z_i) = \sum_{n'}\sum_{z_i} P(z_i)\frac{D_{0,nn'}}{2\pi}\int F_{n'}(k'_z)e^{ik'_z z_i}\delta(\mathbf{k}'_\parallel - \mathbf{q}_\parallel)dk'_z d^2k'_\parallel \int e^{ik_z z}e^{-ik_z z_i}e^{i\mathbf{k}_\parallel\cdot\boldsymbol{\rho}}dk_z d^2k_\parallel \delta(\mathbf{k}_\parallel - \mathbf{k}'_\parallel)$$

$$= \sum_{n'}\sum_{z_i}\pi_i\frac{D_{0,nn'}}{2\pi}\int F_{n'}(k'_z)e^{ik'_z z_i}dk'_z \int e^{ik_z z}e^{-ik_z z_i}e^{i\mathbf{k}_\parallel\cdot\boldsymbol{\rho}}dk_z d^2k_\parallel \delta(\mathbf{k}_\parallel - \mathbf{q}_\parallel)$$

$$= e^{i\mathbf{q}_\parallel\cdot\boldsymbol{\rho}}\sum_{n'}\sum_{z_i}\pi_i D_{0,nn'}\tilde{F}_{n'}(z_i)\tilde{\delta}(z-z_i) = \sum_{n'}\sum_{z_i}\pi_i D_{0,nn'}\tilde{F}_{n'}(\boldsymbol{\rho},z_i)\tilde{\delta}(z-z_i) \tag{A1}$$

where $\boldsymbol{\rho}=(x,y)$. Thus $H^{IF,0}_{nn'}=\pi_i\Sigma_{z_i}D_{0,nn'}\tilde{\delta}(z-z_i)$.

The last term transforms in a similar way,

$$\sum_{n'} H^{IF,1}_{nn'}\tilde{F}_{n'}(\boldsymbol{\rho},z_i) = \sum_{n'}\sum_{z_i}\pi_i e^{-i(k_z-k'_z)z_i}\frac{D_{1,nn'}}{2\pi}\int\int (k_z-k'_z)F_{n'}(\mathbf{k}')d^3k' e^{i\mathbf{k}.\mathbf{r}}d^3k\,\delta(\mathbf{k}_\parallel - \mathbf{k}'_\parallel)$$

$$= e^{i\mathbf{q}_\parallel\cdot\boldsymbol{\rho}}\sum_{n'}\sum_{z_i}\pi_i\frac{D_{1,nn'}}{2\pi}\frac{1}{i}\frac{\partial}{\partial z}\int e^{ik_z(z-z_i)}dk_z\tilde{F}_{n'}(z_i) - \pi_i D_{1,nn'}\frac{1}{i}\frac{\partial}{\partial z}\int F_{n'}(k'_z)e^{ik'_z z}dk'_z|_{z=z_i}\tilde{\delta}(z-z_i)$$

$$= iD_{1,nn'}\sum_{n'}\sum_{z_i}\pi_i\left\{\left.\frac{\partial\tilde{F}_{n'}(\boldsymbol{\rho},z)}{\partial z}\right|_{z=z_i}\tilde{\delta}(z-z_i) - \tilde{F}_{n'}(\boldsymbol{\rho},z_i)\tilde{\delta}'(z-z_i)\right\}. \tag{A2}$$

Using Eq. (A2) we can evaluate the matrix element,

$$\langle\tilde{F}_n(\boldsymbol{\rho},z)|H^{IF,1}_{nn'}|\tilde{F}_{n'}(\boldsymbol{\rho},z)\rangle = iD_{1,nn'}\sum_{z_i}\pi_i\int_{-\infty}^{\infty}\left\{\left.\frac{\partial\tilde{F}_{n'}(\boldsymbol{\rho},z)}{\partial z}\right|_{z=z_i}\tilde{F}^*_n(\boldsymbol{\rho},z)\tilde{\delta}(z-z_i) - \tilde{F}^*_n(\boldsymbol{\rho},z)\tilde{F}_{n'}(\boldsymbol{\rho},z_i)\tilde{\delta}'(z-z_i)\right\}dz$$

$$= iD_{1,nn'}\sum_{z_i}\pi_i\left\{\left.\frac{\partial\tilde{F}_{n'}(\boldsymbol{\rho},z)}{\partial z}\right|_{z=z_i}\tilde{F}^*_n(\boldsymbol{\rho},z_i) + \tilde{F}_{n'}(\boldsymbol{\rho},z_i)\left.\frac{\partial\tilde{F}^*_n(\boldsymbol{\rho},z)}{\partial z}\right|_{z=z_i}\right\}. \tag{A3}$$

Thus $H^{IF,1}_{nn'}=-iD_{1,nn'}\Sigma_{z_i}\pi_i\tilde{\delta}'(z-z_i)$.

In the above derivation, the following identities have been used:

$$\int\tilde{F}_{n'}(z)\tilde{\delta}(z)dz = \frac{1}{2\pi}\int_L\left\{\int_{1\text{st}\,BZ}F_{n'}(k')e^{ik'z}dk'\right\}\int_{1\text{st}\,BZ}e^{-ikz}dkdz = \frac{1}{2\pi}\int_L\left\{\int_{1\text{st}\,BZ}dk\int_{1\text{st}\,BZ}F_{n'}(k')e^{i(k'-k)z}dk'\right\}dz$$

$$= \int_{1\text{st}\,BZ}dk\int_{1\text{st}\,BZ}F_{n'}(k')\delta(k'-k)dk' = \int_{1\text{st}\,BZ}dkF_{n'}(k) = \left[\int_{1\text{st}\,BZ}F_{n'}(k_z)e^{ik_z z}dk\right]_{z=0} = [\tilde{F}_{n'}(z)]_{z=0} \tag{A4}$$

and

$$\int_{-\infty}^{\infty}\tilde{F}_{n'}(z)\tilde{\delta}'(z)dz = [\tilde{F}_{n'}(z)\tilde{\delta}(z)]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{\partial\tilde{F}_{n'}(z)}{\partial z}\tilde{\delta}(z)dz = \left[-\frac{\partial\tilde{F}_{n'}(z)}{\partial z}\right]_{z=0}. \tag{A5}$$

APPENDIX B: DEFINITION OF THE INTERFACE CELL IN SUPERLATTICES WITH NO COMMON ATOM

In this appendix the interface cell is defined for an idealized no common atom superlattice in which there are no strain effects, taking InAs/GaSb as an example. The metallurgical interface is located midway between the Sb and In atoms for an InSb-like interface and midway between the As and Ga atoms for a GaAs-like interface.

The cell used to calculate the D_0 and D_1 matrix elements, $\langle n|D_l|n'\rangle$, defined in Eq. (4), can be specified in several ways. If the origin of the cell ($z=0$) is defined as the metallurgical interface, then the atomic orbitals in the Bloch functions of the reference crystal, $|n\rangle$ and $|n'\rangle$, are located at positions $z=\pm a/4$, where a is the period of the Bloch functions and is also the size of the cell used to calculate $\langle n|D_l|n'\rangle$. In [001] superlattices, it is convenient to choose an

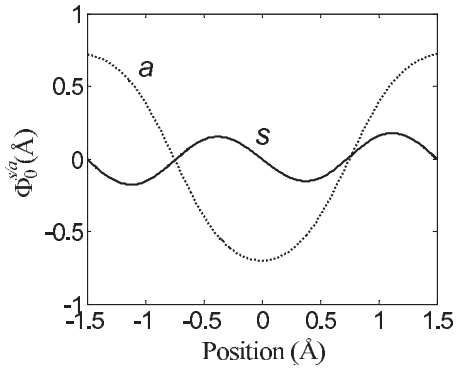

FIG. 3. Interface functions Φ_0^s (solid) and Φ_0^a (dashed) for a metallurgically abrupt InSb-like interface located at the plane of Sb atoms in an idealized InAs/GaSb superlattice with no strain effects. $G'(z)$ is a Gaussian with a full width at half maximum of 0.8 Å and a peak located half way between the Sb and In planes.

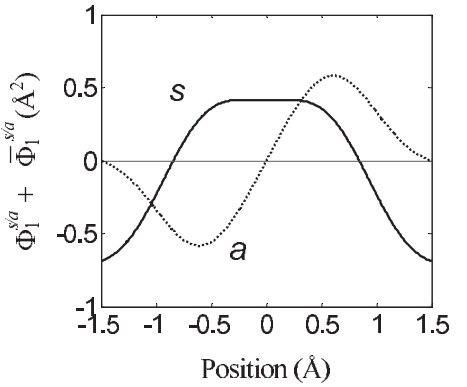

FIG. 4. Interface functions $\Phi_1^s+\bar{\Phi}_1^s$ (solid) and $\Phi_1^a+\bar{\Phi}_1^a$ (dashed) for the same interface as in Fig. 3.

a value equal to half the cubic lattice constant of the reference crystal. For a symmetric metallurgically abrupt interface located at $z=0$, as defined for Figs. 1 and 2, this arrangement gives nonzero diagonal D_0 terms such as $\langle Z|\delta U\cdot\Phi_0^s|Z\rangle$ and nonzero off-diagonal D_1 terms such as $\langle\sigma|\delta U\cdot\{\Phi_1^s+\bar{\Phi}_1^s\}|Z\rangle$. These terms have the *same* sign at GaSbIn and InSbGa interfaces. They should be comparable in size to the off-diagonal D_0 and diagonal D_1 terms, respectively, such as $\langle\sigma|\delta U\cdot\Phi_0^s|Z\rangle$ and $\langle Z|\delta U\cdot\{\Phi_1^s+\bar{\Phi}_1^s\}|Z\rangle$ which do change sign at opposite interfaces. Note that the following relations for the microscopic potential and the product of Bloch functions hold at opposite interfaces: $\delta U_{\mathrm{GaSbIn}}(z)=\delta U_{\mathrm{InSbGa}}(-z)$ and $u_Z(z)u_\sigma(z)|_{\mathrm{GaSbIn}}=-u_Z(-z)u_\sigma(-z)|_{\mathrm{InSbGa}}$.

As an alternative to the above, it is instructive to define the interface location, $z=0$, instead, as the anion or cation plane nearest to the metallurgical interface since this configuration is more directly comparable with the case of common atom superlattices such as GaAs/Al_xGa_{1-x}As, where the interface is located on an As plane. This definition changes the values of z_i which define the δ-function positions in Eq. (25) by $\pm a/4$, which is probably small enough to be ignored, but not the width of each layer which is still determined by $\Gamma(z)$ [defined after Eq. (7)]. Choosing the Sb plane at an InSb interface, the derivative of the profile function at neighboring interfaces can be expressed as $G'_{\mathrm{GaSbIn}}(z)=\delta(z-\varepsilon)=\rho(z)+\omega(z)$ and $G'_{\mathrm{InSbGa}}(z)=-\delta(z+\varepsilon)=-\rho(z)+\omega(z)$, where $\varepsilon=a/4$. The symmetric function $\rho(z)=[\delta(z-\varepsilon)+\delta(z+\varepsilon)]/2$ corresponds to $G'(z)|_s$ and the antisymmetric function $\omega(z)=[\delta(z-\varepsilon)-\delta(z+\varepsilon)]/2$ to $G'(z)|_a$. Only the contribution from the symmetric function changes sign at opposite interfaces and this gives rise to the factor π_i. that appears in Eq. (5) while there is no such factor for the antisymmetric contribution since it has the same sign at each interface.

Functions analogous to those in Sec. III can be defined for the $G'(z)|_a$ contribution as follows: $I_G^a(K_{zj})=-i\int_{-d}^{d}G'(z)|_a\sin(K_{zj}z)dz$ and $\bar{I}_G^a(K_{zj})=i\int_{-d}^{d}zG'(z)|_a\cos(K_{zj}z)dz$, where I_G^a is an odd function of K_{zj}, and $\bar{I}_G^a$ is an even function. Three real functions are also defined: $\Phi_0^a=\Sigma_{j\neq0}(e^{iK_{zj}z}/iK_{zj})I_G^a(K_{zj})$, $\Phi_1^a=\Sigma_{j\neq0}(e^{iK_{zj}z}/K_{zj}^2)I_G^a(K_{zj})$, and $\bar{\Phi}_1^a=\Sigma_{j\neq0}(e^{iK_{zj}z}/K_{zj})\bar{I}_G^a(K_{zj})$, where Φ_0^a is an even function of z, and Φ_1^a and $\bar{\Phi}_1^a$ are odd functions. Figures 3 and 4 show plots of Φ_0^s and Φ_0^a, and $\Phi_1^s+\bar{\Phi}_1^s$ and $\Phi_1^a+\bar{\Phi}_1^a$, respectively, for metallurgically abrupt interfaces in which the δ functions in $\rho(z)$ and $\omega(z)$ are replaced by Gaussians with a full width at half maximum of 0.8 Å (Ref. 45). Inspection of these functions shows that $G'(z)|_s$ and $G'(z)|_a$ make contributions of a similar magnitude at an interface in a no common atom superlattice and that there will thus be nonzero diagonal D_0 terms such as $\langle Z|\delta U\cdot\Phi_0^a|Z\rangle$ and nonzero off-diagonal D_1 terms such as $\langle\sigma|\delta U\cdot\{\Phi_1^a+\bar{\Phi}_1^a\}|Z\rangle$ comparable in size to $\langle\sigma|\delta U\cdot\Phi_0^s|Z\rangle$ and $\langle Z|\delta U\cdot\{\Phi_1^s+\bar{\Phi}_1^s\}|Z\rangle$, respectively.

The preceding, *one dimensional*, model treatment of a metallurgically abrupt interface contains the assumption that $G'(z)$ is symmetric about the plane $z=a/4$, i.e., that the average microscopic potential on a plane midway between the In and Sb atoms is equal to that for the virtual-crystal average of InAs and GaSb at that position. If this equality occurs on a plane at some other position between the In and Sb atoms, this can be taken into account by adjusting the value of ε in the functions $\rho(z)$ and $\omega(z)$. This will change the magnitudes of the matrix elements $\langle Z|\delta U\cdot\Phi_0^a|Z\rangle$, etc., but will make no qualitative change to the above conclusions, i.e., there will still be nonzero diagonal D_0 terms comparable in magnitude to the off-diagonal D_0 terms and nonzero off-diagonal D_1 terms comparable in magnitude to the diagonal D_1 terms.

*philip_k@scd.co.il

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[35] Formally, the Γ_{15c} deformation potential is also required in this procedure, in order to take the strain induced change in the $\Gamma_{15c}-\Gamma_{15v}$ band gap into account. However, it should only have a small effect.

[36] $d_{1,\sigma\sigma}$, $\eta_X-\kappa_0+d_{1,XX}$, $\kappa_2+d_{1,ZZ}$, κ_1, $\kappa_0+\kappa_2$, α, β, f but not γ_3^A, γ_1^B, γ_2^B, and γ_3^B.

[37] $d_{1,\sigma\sigma}$, $\eta_X-\kappa_0+d_{1,XX}$, and $\kappa_2+d_{1,ZZ}$.

[38] $\bar{\alpha}+\chi_2$, $\bar{\beta}$, χ_0, $D^a_{0,\sigma\sigma}$, $D^a_{0,XX}$, and $D^a_{0,ZZ}$.

[39] $\bar{\alpha}+\chi_2$ and $\bar{\beta}$.

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[45] Note that in evaluating these functions, d in Eq. (4) does not have to be limited to a value of $a/2$ but should be made large enough to achieve full convergence.