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Connection rules for envelope functions at semiconductor-heterostructure interfaces

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Connection rules for envelope functions are formulated in terms of a transfer matrix, the elements of which are calculated using a scattering-matrix approach based on empirical pseudopotentials. We propose a 6×6 transfer matrix for the case when a four-band $\mathbf{k}\cdot\mathbf{p}$ model is used, contrary to the conventional 8×8 matrix. The transfer-matrix elements are calculated for a GaAs/AlAs interface, in which case the transfer matrix appears to be almost diagonal. The envelope functions are to a good approximation continuous at the GaAs/AlAs interface, whereas the first derivatives appear to be more or less discontinuous at the interfaces. However, we find no evidence for connection rules for the first derivatives of envelope functions involving effective-mass ratios, which is at variance with the rules as commonly used in the literature. For the InAs/GaSb interface the off-diagonal elements of the transfer matrix appear to be nonzero, whereas the diagonal elements are negligibly small.

I. INTRODUCTION

A frequently used approach for the calculation of the electronic and optical properties of heterostructures is the so-called envelope-function or $\mathbf{k}\cdot\mathbf{p}$ model approach (see, for instance, Refs. 1–7). This method is used to attempt to deal with the slowly varying envelopes of electronic wave functions only, omitting details of the additional rapid microscopic variations. The main advantage of the envelope-function approach is the simplicity of the method which makes it relatively easy to incorporate effects of external potentials, magnetic fields, doping, charging effects, etc. Another strong point is that, by concentrating on small but relevant parts of the involved band structures only, a relatively high accuracy can be reached in accounting for these parts in the theoretical description. There are, however, two serious drawbacks. The first one is the restriction to wave vectors lying close to particular band extrema, i.e., to envelopes varying slowly over unit-cell distances. Only if this restriction is made is it allowable to deal with relatively simple envelope-function equations. The second drawback has to do with the question of how to match envelope functions at heterostructure interfaces. Whereas an electronic wave function as well as its first derivative obviously have to be continuous at a heterostructure interface, this does not imply that its slowly varying envelope (and the first derivative of the envelope function) is also continuous at the abrupt interface. The problem of matching envelope functions at heterostructure interfaces has been the subject of several papers,[8–14] but has not yet been settled satisfactorily, the reason being the difficulty of translating the connection rules for real wave functions into rules for envelope functions without making an explicit appeal on those real wave functions themselves.

An alternative manner to describe electronic properties of heterostructures is to use a model based on empirical pseudopotentials.[15–17] In this theory the pseudo wave functions are properly matched at the heterostructure interfaces. Proper matching implies continuity of both the pseudo wave function and its first derivative in each point of the interface. In view of the well-known relation between the actual wave function and the pseudo wave function[18] the matching of pseudo wave functions implies proper matching of the actual wave function to a very high extent. The method is, contrary to the envelope-function approach, valid for wave vectors throughout the first Brillouin zone. A disadvantage of the method, also present in the more common $\mathbf{k}\cdot\mathbf{p}$ method approaches, is its restriction to the flat-band approximation in which the heterostructure layers are assumed to be entirely bulklike. A more serious drawback is that the matrices involved in the calculation have a dimension that is much larger than the dimension of the matrices involved in a simple envelope-function approach, thus drastically increasing computing time. It will be shown, however, how the results of a pseudo-wave-function approach can be used in formulating a much more reliable envelope-function approach.

The object of this paper is the following: From the *exact* treatment of the scattering of an electron at a heterostructure interface (based on empirical pseudopotentials) we can derive what the related envelope functions are, simply by rewriting our results for pseudo wave functions in the heterostructure in terms of envelope functions. We are then left with envelope functions which are what they ought to be. We are thus in the position to verify whether proposed boundary conditions for envelope functions at interfaces are valid or should be replaced by more appropriate ones. In this manner we are able to resolve, for a number of important cases, the ambiguities which exist in matching prescriptions for envelope functions at heterostructure interfaces, thus eliminating one of the major drawbacks in envelope-function theory.

The outline of the paper is as follows. We will first give a brief description of the scattering-matrix method, which uses empirical pseudopotentials, in Sec. II. In Sec. III a transfer matrix is introduced, connecting envelope functions and their first derivatives at a heterostructure interface. In this section we will explain the method to calculate the transfer-matrix elements using the scattering-matrix approach based on empirical pseudopotentials. The transfer-matrix elements will be calculated for a GaAs/$Al_xGa_{1-x}As$ interface in Sec. IV A. An important issue in the matter of connecting envelopes at heterostructure interfaces is the conservation of flux at an interface, which we deal with in Sec. IV B. For the InAs/GaSb interface the transfer-matrix elements are presented in Sec. IV C. We summarize our results and include some additional remarks in Sec. V.

II. SCATTERING-MATRIX APPROACH

The scattering-matrix approach for the calculation of electronic states in heterostructures using empirical pseudopotentials is extensively discussed in a previous paper.[15] We will therefore recall only the ingredients which are necessary for the understanding of this paper.

In the scattering-matrix approach each material layer of a heterostructure is assumed to be entirely bulklike. The general wave-function solution in a heterostructure layer j, at given energy and parallel wave vector $\mathbf{k}_\parallel$, may then be expressed as a linear combination of Bloch and evanescent waves which are characterized by a (real or complex) wave vector k_z^{js}, where s labels each individual Bloch or evanescent wave and where the z direction is taken to be perpendicular to the interface planes. A calculation of the complex band structure of the layer material using empirical pseudopotentials,[19] at given $\mathbf{k}_\parallel$, gives the k_z^{js} values with corresponding wave functions $\psi_{\mathbf{k}_\parallel}^{js}(\mathbf{r})$. In Fig. 1 we have plotted the complex band structure of GaAs and AlAs at $\mathbf{k}_\parallel=\mathbf{0}$. Using N plane waves in the pseudopotential calculation, it can be shown[15,20] that the number of in-zone k_z^{js} solutions equals $2M$, where M is the number of projected reciprocal-lattice vectors $\mathbf{K}_\parallel$ on the interface plane. The general wave function in a material layer is therefore written as a linear combination of $2M$ Bloch and evanescent waves:

$$\psi_{\mathbf{k}_\parallel}^{j}(\mathbf{r})=\sum_{s=1}^{2M}\alpha^{js}\psi_{\mathbf{k}_\parallel}^{js}(\mathbf{r}) \ . \tag{1}$$

The α^{js} coefficients in Eq. (1) have to follow from the boundary conditions, which are the continuity of the pseudo wave function and its first derivative at every xy point of the interface plane.[15] The boundary conditions at the interfaces may be reformulated in terms of a scattering matrix relating all outgoing waves, which travel or decay away from the interface, to all incoming ones:[15,16]

$$\boldsymbol{\alpha}_{\rm out}=\boldsymbol{S}\boldsymbol{\alpha}_{\rm in} \ , \tag{2}$$

where $\boldsymbol{\alpha}_{\rm out}$ and $\boldsymbol{\alpha}_{\rm in}$ are $2M$-dimensional vectors, the elements of which are the α^{js} coefficients of the outgoing and incoming channels, respectively. Note that there are M outgoing and M incoming channels in each material layer. Choosing a particular incoming channel relation (2) will give all outgoing channels.

For each Bloch or evanescent wave $\psi_{\mathbf{k}_\parallel}^{js}(\mathbf{r})$ there is a set of corresponding envelope functions $f_n^{js}(z)$. These are related to $\psi_{\mathbf{k}_\parallel}^{js}(\mathbf{r})$ by means of

$$\psi_{\mathbf{k}_\parallel}^{js}(\mathbf{r})=e^{i\mathbf{k}_\parallel\cdot\rho}\sum_{n}^{N}f_n^{js}(z)\psi_{n0}^{j}(\mathbf{r}) \ , \tag{3}$$

in which $\psi_{n0}^{j}(\mathbf{r})$ are the Bloch eigenfunctions of the unperturbed bulk crystal of material j with a band index n at $\mathbf{k}=\mathbf{0}$ and where we assume that $\mathbf{k}_\parallel$ lies in the area in which only one envelope function per band index is needed.[21] The number N is equal to the number of plane waves taken into account in our pseudopotential calculation. The envelope functions of the final wave-function solution in layer j, given by Eq. (1), are then expressed as

$$\mathcal{F}_n^{j}(z)=\sum_{s}^{2M}\alpha^{js}f_n^{js}(z) \ . \tag{4}$$

III. TRANSFER MATRIX FOR ENVELOPE FUNCTIONS

It should be realized that the number N of energy bands taken into account in Eq. (3) will generally be large, say, equal to 27 or 59. On the other hand, the number of band-indexed envelope functions taken into account in *practical* applications of the envelope-function formalism is much lower, and may vary between one and four (or eight if spin states are explicitly dealt with). This reduction is generally justified by the application of a Löwdin-renormalization procedure.[22] In the Löwdin procedure a small number of bands (belonging to class $\mathcal{A}$), lying close together in energy, is taken into account exactly, whereas all other bands (belonging to class $\mathcal{B}$) are accounted for in a perturbative way. Typically for states in the energy region around the conduction-band minimum only one energy band in class $\mathcal{A}$ could be sufficient. For such a case the Löwdin-renormalized envelope-function equations reduce to the widely used effective-mass equation in which the normal electron mass, due to the influence of states in class $\mathcal{B}$, is renormalized to the effective mass. For holelike states, on the other hand, we have at least to include heavy- and light-hole bands in $\mathcal{A}$. In that case a more sophisticated mod-

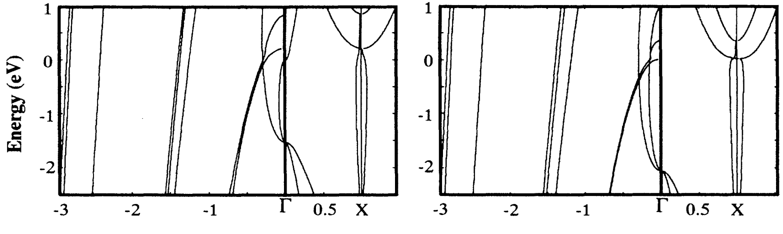

FIG. 1. The complex band structures of GaAs and AlAs at $\mathbf{k}_\parallel=\mathbf{0}$. The conduction-band minimum of AlAs at the Γ point has an offset of approximately 1.0 eV with respect to the GaAs minimum.

el, such as the four-band **k**·**p** model in which class $\mathcal{A}$ consists of the three valence bands and the lowest conduction band (which form, in fact, eight bands if the spin-orbit interaction is included), is frequently used.[4,5]

The $\mathcal{N}$-band Löwdin-renormalized envelope-function equations for a perfect bulk material, which form a set of $\mathcal{N}$ coupled second-order differential equations, give rise to $2\mathcal{N}$ k_z^{js} solutions, where $\mathcal{N}$ is the number of energy bands in class $\mathcal{A}$.[4,5] (We use the script notation to distinguish numbers in the Löwdin-renormalized scheme from those mentioned in the previous section.) The number of *in-zone* solutions k_z^{js} will generally be smaller and will be denoted by $2\mathcal{M}$. In case of the simple one-band effective-mass approximation we obviously obtain two in-zone k_z^{js} solutions only, corresponding to $\mathcal{M}=1$ (so here $\mathcal{M}=\mathcal{N}$). In the case of the four-band **k**·**p** model for the heavy-hole, light-hole, and conduction bands six different in-zone k_z^{js} solutions are obtained. Two k_z^{js} solutions are always such that they are out zone. In the valence-band energy region four of these six in-zone k_z^{js} solutions correspond with the two heavy-hole bands (see Fig. 1) and two k_z^{js} solutions correspond to the light-hole band. At energies in the conduction-band region we find two Γ-point conduction band k_z^{js} solutions and four solutions corresponding to branches of imaginary k_z^{js} values which are connected with the two heavy-hole bands (see Fig. 1). For energies in the energy gap again four heavy-hole type imaginary k_z^{js} solutions are obtained as well as two imaginary k_z^{js} solutions corresponding to the branches connecting the light-hole band with the conduction band. The six k_z^{js} solutions correspond with $\mathcal{M}=3$, so for the four-band model $\mathcal{M}<\mathcal{N}$.

The general envelope-function solutions of the Löwdin-renormalized envelope-function equations in a material layer j at given energy and $\mathbf{k}_\parallel$ and with $n\in\mathcal{A}$ are linear combinations of all $2\mathcal{M}$ in-zone solutions $f_n^{js}(z)$, i.e.,

$$\mathcal{F}_n^j(z)=\sum_s^{2\mathcal{M}}\alpha^{js}f_n^{js}(z)\ . \tag{5}$$

In the previous section we already dealt with an expression of this form [see (4)] in which n was not exclusively in $\mathcal{A}$ and in which the summation over s ran from 1 to $2M$, where M was the number of two-dimensional reciprocal-lattice vectors taken into account. Here, in the Löwdin-renormalized approach, we consider the envelope functions (5) as truncated approximations of the more general expression (4), with $n\in\mathcal{A}$ and with s running from 1 to $2\mathcal{M}$ instead of from 1 to $2M$. In the scattering-matrix approach described previously the α^{js} coefficients followed from the continuity of the full electronic wave function and its first derivative [reformulated into Eq. (2)]. However, in Löwdin-renormalized envelope-function approaches one does not want to appeal explicitly to the electronic wave function itself. Instead, an appropriate set of boundary conditions for the envelope functions $\mathcal{F}_n^j$ and their first derivatives is sought. The most general (linear) relation between envelope functions $\mathcal{F}_n^j$ and their first derivatives at interfaces can be written in the form

$$\begin{bmatrix}\boldsymbol{\mathcal{F}}^{j+1}\\ \dfrac{\partial\boldsymbol{\mathcal{F}}^{j+1}}{\partial z}\end{bmatrix}=T\begin{bmatrix}\boldsymbol{\mathcal{F}}^{j}\\ \dfrac{\partial\boldsymbol{\mathcal{F}}^{j}}{\partial z}\end{bmatrix}\ , \tag{6}$$

where $\boldsymbol{\mathcal{F}}^j$ stands for a vector with components $\mathcal{F}_n^j(z_0)$, z_0 is the position of the interface, and T is the transfer matrix. Including all envelope functions with $n\in\mathcal{A}$ in Eq. (6) implies in fact that we are then dealing with $2\mathcal{N}$ boundary conditions, where in the above two examples we have either $\mathcal{N}=1$ or $\mathcal{N}=4$. As mentioned before, a uniform and generally accepted set of boundary conditions is not available.

In order to fix the $2\mathcal{M}$ unknown coefficients α^{js} in expression (5) in each material layer j there are $2\mathcal{M}$ conditions needed at each interface, together with $2\mathcal{M}$ conditions in $z=\pm\infty$. In the effective-mass approximation, (6) involves two boundary conditions ($\mathcal{N}=1$) which is sufficient to fix the two α^{js} coefficients in each layer ($\mathcal{M}=\mathcal{N}=1$). For the four-band **k**·**p** model, Eq. (6) constitutes eight boundary conditions ($\mathcal{N}=4$). There are, however, only six α^{js} coefficients which are to be determined in each layer, since $\mathcal{M}=3$. So here Eqs. (6) form too many equations for the determination of the α coefficients ($\mathcal{N}>\mathcal{M}$). This inconsistency can be resolved in the following way. At a given energy, we always obtain k_z^{js} solutions which are related to three bands only, although there are four bands involved in the calculation of the complex band structure: At energies in the valence-band regime we find two light-hole and four heavy-hole band k_z^{js} solutions and in the conduction-band energy region we find two conduction-band and four heavy-hole band k_z^{js} solutions, the latter corresponding to evanescent waves. In the energy gap the branches connecting the light-hole band and the conduction band must be attributed a band index either belonging to the conduction band or the light-hole band, depending on which one is closest in energy. So at each fixed energy it is sufficient to incorporate three band-indexed envelope functions only in (6). Consequently, the T matrix (6) becomes a 6×6 matrix, which is consistent with the number of equations required to fix the six unknown α^{js} coefficients in each material layer.

Our scattering-matrix calculations based on empirical pseudopotentials enable us to determine the actual values of the T-matrix elements as a function of energy. We derive the proper electronic wave function for a heterostructure first, as previously described. Once we have calculated the α^{js} coefficients, we are able to calculate the envelope functions $\mathcal{F}_n^j(z)$ using Eq. (4) in which the envelope functions $f_n^{js}(z)$ are calculated using relation (3). Envelope functions obtained in that manner contain terms corresponding to a large number of $2M$ solutions k_z^{js} which may have a real part not only close to $\mathbf{k}_0=\mathbf{0}$ (the Γ extremum) but close to $\mathbf{k}_0=(2\pi/a)\mathbf{e}_z$ (the X extremum) as well. In a Löwdin-renormalized scheme only a limited number of $2\mathcal{M}$ solutions k_z^{js}, which lie close to one particular $\mathbf{k}_0$ value, are taken into account. In order to obtain envelope functions using the empirical pseudopotential method which are as close as possible to envelope functions obtained in Löwdin-renormalized schemes we restrict the summation over s in Eq. (5) to the reduced number $2\mathcal{M}$. This implies that we have to be aware of shortcomings in the Löwdin-renormalized scheme which have to do with the neglect of possibly participating channels.

In the case of the scattering of an electron at a GaAs/AlAs single interface the procedure is that we choose one particular incoming channel, for instance corresponding to an incoming conduction-band electron, and determine the α coefficients of all outgoing waves using the S-matrix description (2). For this configuration the values of $\mathcal{M}$ band-indexed envelope functions and their first derivatives at both sides of the interface can then be calculated in the manner described above. Substituting these values in Eqs. (6) gives $2\mathcal{M}$ equations for the $2\mathcal{M}\times 2\mathcal{M}$ unknown T-matrix elements. In each material layer there are $2\mathcal{M}$ k_z^{js} solutions which we have taken into account in the calculation of the envelope functions, $\mathcal{M}$ of which correspond to incoming channels. There are therefore $2\mathcal{M}-1$ other independent possibilities for choosing the incoming channel, namely, $\mathcal{M}-1$ channels which are incident from the GaAs side and another $\mathcal{M}$ which are incident from the AlAs side. Each choice for an incoming channel leads to $2\mathcal{M}$ equations for the T-matrix elements. The total number of equations will therefore be equal to $2\mathcal{M}\times 2\mathcal{M}$ which fixes each T-matrix element.

IV. RESULTS

A. The GaAs/Al$_x$Ga$_{1-x}$As interface

1. Conduction-band energy region

We will focus here on the energy region above the Γ-point conduction-band minimum in GaAs. At these energies the most important α^{js} coefficients, for the case of an incident electron with $\mathbf{k}_{\parallel}=\mathbf{0}$, are the ones which correspond to the transmitted and reflected electron.[15] In view of the fact that the important α^{js} coefficients in each layer correspond to two k_z^{js} solutions which both have real parts close to the Γ point, we take $\mathcal{M}=1$ and $\mathbf{k}_0=\mathbf{0}$ in the calculation of the envelope functions. The calculation procedure provides us with expressions for $f_n^{js}(z)$ functions with varying n. Obviously, the conduction-band ($n=c$) envelope functions $f_c^{js}(z)$ are important at energies in the conduction-band regime. However, we find that also the light-hole band ($n=\mathrm{lh}$) envelope functions $f_{\mathrm{lh}}^{js}(z)$ are significant. In Fig. 2 we have plotted the values of the envelope functions $\mathcal{F}_c$ and $\mathcal{F}_{\mathrm{lh}}$ at the interface position z_0, constructed according to (5). Values of $\mathcal{F}_n$ for all other n values appear to be negligible. In most applications of the effective-mass approximation, in which class $\mathcal{A}$ consists of the conduction band only, the light-hole band envelope function lying in class $\mathcal{B}$ is entirely neglected. The wave function $\psi_{\mathbf{k}_{\parallel}}^j(\mathbf{r})$ is then simply approximated by $\exp(i\mathbf{k}_{\parallel}\cdot\rho)\mathcal{F}_c^j(z)\psi_{c0}^j(\mathbf{r})$ [see Eq. (3)]. Charge densities, for instance, are thus expressed in terms of conduction-band envelope functions only. This is at least not justified for our case dealing with GaAs and AlAs since the absolute value of the light-hole band envelope function may take values as large as 50% of the value of the conduction-band envelope function. Note in this connection that if the class $\mathcal{A}$ is reduced to the conduction band only, we may express the value of the light-hole band envelope function $\mathcal{F}_{\mathrm{lh}}^j(z)$ approximately in terms of $\nabla_z\mathcal{F}_c$.[22] For a zinc-blende structure we find with $\mathbf{k}_0=\mathbf{0}$

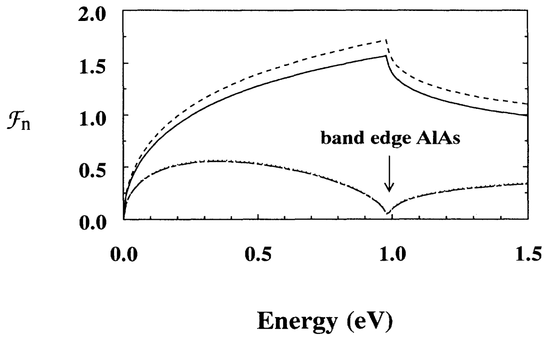

FIG. 2. The absolute value of the conduction-band envelope function at the right-hand side (solid line) and left-hand side (dashed line) of the GaAs/AlAs interface in case of the scattering of an electron at a single interface. Also the light-hole band envelope functions at the right- and left-hand sides are depicted (long-short dashed and dotted lines). The zero of energy lies at the GaAs conduction-band edge. The conduction-band edge of AlAs lies at 0.98 eV.

$$\mathcal{F}_{\mathrm{lh}}^j(z)\approx\frac{P^j}{E_{\mathrm{gap}}^j}\frac{\partial}{\partial z}\mathcal{F}_c^j(z)\ , \tag{7}$$

where we define $P^j=(\hbar/m)\langle\psi_{\mathrm{lh},0}^j|(\hbar/i)(\partial/\partial z)|\psi_{c,0}^j\rangle$. For GaAs and AlAs we find from our empirical-pseudopotential calculations the values 0.95 and 0.48 for P^j/aE_{gap}^j, respectively (a is the lattice constant).

In a Löwdin-renormalized scheme in which only two k_z^{js} solutions are taken into account ($\mathcal{M}=1$), the T matrix at the interface reduces to a 2×2 matrix, as described earlier in Sec. III. This T matrix relates the envelope function $\mathcal{F}_c^{j+1}(z)$ and $(\partial/\partial z)\mathcal{F}_c^{j+1}(z)\equiv\mathcal{F}_{c'}^{j+1}(z)$ for AlAs to the ones for GaAs. We remark that most, if not all, connection prescriptions in the literature for electron states in the considered energy region are formulated in terms of a *diagonal* 2×2 T matrix. Our calculations, for $\mathbf{k}_{\parallel}=\mathbf{0}$, show that the values of the off-diagonal elements of T, i.e., the ones connecting $\mathcal{F}_c(z)$ to $\mathcal{F}_{c'}(z)$, are smaller than 10^{-4} so that they indeed appear to be negligibly small and to support the diagonal T-matrix model. The absolute value of the diagonal T-matrix elements T_{cc}, connecting the functions $\mathcal{F}_c(z)$, and the absolute value of $T_{c'c'}$, which connects the derivatives $\mathcal{F}_{c'}(z)$, are given in Fig. 3 as a function of energy. (Note that T_{cc} can be chosen to be real.) A striking feature is that T_{cc} is almost constant and close to unity $(0.9<T_{cc}<0.92)$ in a relatively large energy interval (1.5 eV) above the Γ-point conduction-band minimum in GaAs. This implies that the envelope function $\mathcal{F}_c(z)$ is almost continuous at a GaAs/AlAs interface, which is only slightly at variance with the connection rule for the conduction-band en-

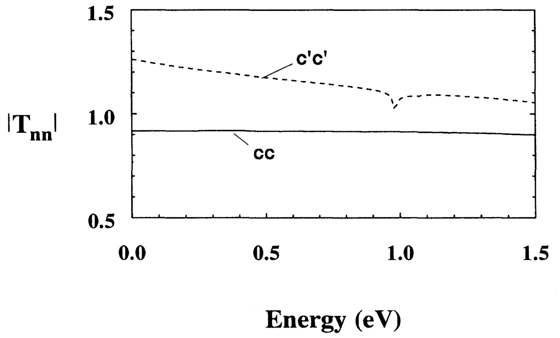

FIG. 3. The absolute value of the matrix elements T_{cc} (solid line) and $T_{c'c'}$ (dashed line) which connect the conduction-band envelope function and its first derivative at a GaAs/AlAs interface, respectively. The zero of energy lies at the conduction-band minimum of GaAs (this will be so in all the following figures). The Γ-point conduction-band minimum of AlAs is located at 0.98 eV.

velope function as often used in the literature and which supposes continuous envelope functions. The first derivative $\mathcal{F}_{c'}(z)$ appears to be more or less discontinuous; we find $1.05 < |T_{c'c'}| < 1.26$. We also find that $T_{c'c'}$ is almost real valued, so that the phase of the first derivative does not change very much across the interface. The value of $|T_{c'c'}|$ is much closer to unity than to the often applied value of $|T_{c'c'}| = m_{j+1}^*/m_j^*$ which would be equal to about 1.8 for effective masses for a GaAs/AlAs based heterostructure, as obtained using empirical pseudopotentials. It is worthwhile to reemphasize that we did not assume the basis functions $\psi_{n0}^j(\mathbf{r})$ [see Eq. (3)] to be identical for both materials, as is a common Ansatz in the literature, but have taken the exact eigenfunctions of the Schrödinger equation at $\mathbf{k}_0 = \mathbf{0}$ for each material. We also want to stress that the envelope functions which have been used to obtain the T-matrix elements are the exact ones and are not obtained from an approximate set of Löwdin-renormalized envelope-function equations.

2. *Parallel wave vector* $\mathbf{k}_\parallel$ *unequal to zero*

In order to investigate whether the above result concerning the approximate continuity of the conduction-band envelope function and the slight discontinuity of its first derivative also holds for $\mathbf{k}_\parallel \neq \mathbf{0}$, we have calculated the T-matrix elements for $k_x = 0.1(2\pi/a)$. However, for this value of $\mathbf{k}_\parallel$ the coefficients α^{js} corresponding to k_z^{js} branches connected at the heavy-hole valence bands are not negligible anymore, due to the coupling between heavy holes and electrons at $\mathbf{k}_\parallel \neq \mathbf{0}$. The number $\mathcal{M}$ therefore has then at least to be taken equal to 3 in order to incorporate the heavy-hole type k_z^{js} solutions. This implies that a simple one-band effective-mass model is not valid anymore, since it entirely neglects the heavy-hole type k_z^{js} solutions. Clearly, a four-band $\mathbf{k}\cdot\mathbf{p}$ model (in which $\mathcal{M} = 3$) should be used. The dimension of the T matrix then becomes 6×6, connecting the conduction-band and two heavy-hole band envelope functions and their first derivatives. We have calculated each of these T-matrix elements as a function of energy. The diagonal elements of T at $k_x = 0.1(2\pi/a)$ are plotted in Fig. 4. We again find approximate continuity for the conduction-band envelope function, as well as for the two heavy-hole envelope functions. The first derivative of the conduction-band envelope function is also for this case slightly discontinuous, in accordance with our previous results at $\mathbf{k}_\parallel = \mathbf{0}$. We remark that if we take $\mathcal{M} = 1$, despite the obvious importance of the heavy-hole type solutions, the conduction-band envelope function and its first derivative appear to be largely discontinuous. The first derivatives of the heavy-hole band envelope functions show rather sizable discontinuities. Note that the value of $|T_{\mathrm{hh}',\mathrm{hh}'}|$ lies between 0.6 and 0.8 which is much smaller than the ratio of the heavy-hole effective masses which equals 1.04 for effective masses obtained using empirical pseudopotentials. Also the largest off-diagonal element $T_{\mathrm{hh}1',\mathrm{lh}'}$, which has a value close to 0.1, has been depicted in Fig. 4. All other off-diagonal elements have smaller values.

3. *Valence-band energy region*

If we now focus on energies in the valence-band region we have to determine the matrix elements of the 6×6 T matrix which connect the light-hole and two heavy-hole band envelope functions and their first derivatives at the interface. For a GaAs/AlAs interface, with $\mathbf{k}_\parallel = \mathbf{0}$, we have plotted the diagonal T-matrix elements in Fig. 5. The envelope functions appear to be approximately continuous, with $0.991 < T_{\mathrm{lh},\mathrm{lh}} < 0.992$ and $1 < T_{\mathrm{hh}1,\mathrm{hh}1} = T_{\mathrm{hh}2,\mathrm{hh}2} < 1.009$. In contrast, the T-matrix elements connecting the first derivatives show rather large deviations from unity; we find $1.22 < T_{\mathrm{lh}',\mathrm{lh}'} < 1.47$ and $0.712 < T_{\mathrm{hh}1',\mathrm{hh}1'} = T_{\mathrm{hh}2',\mathrm{hh}2'} < 0.754$. The ratio of the effective masses in AlAs and GaAs for the light holes equals 1.8 and for the heavy holes 1.04, where the effective masses are obtained using an empirical-pseudopotential band-structure calculation. So also for this case we do not find that $(m^*)^{-1}\partial\mathcal{F}_n/\partial z$ is continuous at a GaAs/AlAs interface. The off-diagonal elements are all smaller than 0.08.

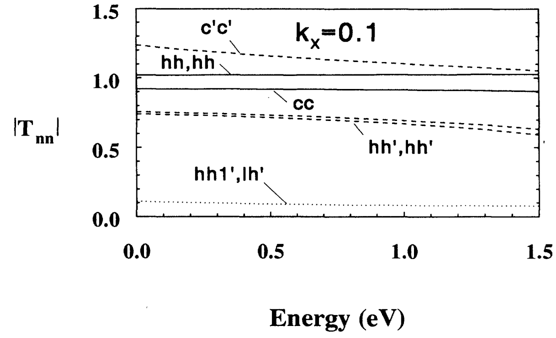

FIG. 4. The diagonal elements of the 6×6 T matrix connecting conduction-band and heavy-hole band envelope functions and their first derivatives at a GaAs/AlAs interface are given for $k_x = 0.1(2\pi/a)$. Also the largest off-diagonal element $|T_{\mathrm{hh}1',\mathrm{lh}}|$ is given.

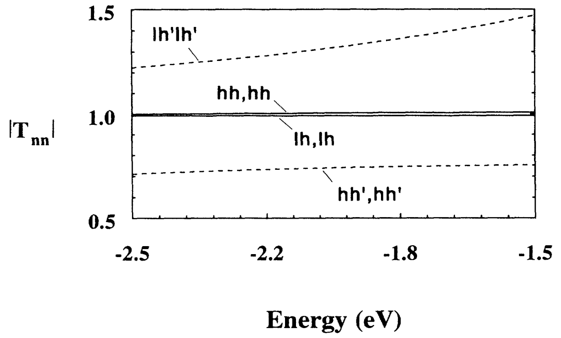

FIG. 5. The diagonal T-matrix elements between light-hole and heavy-hole band envelope functions for energies in the valence-band region, with $\mathbf{k}_{\parallel}=0$. The valence-band maxima of AlAs and GaAs lie at -2.06 and -1.53 eV, respectively.

Also for $\mathbf{k}_{\parallel}\neq 0$ we have calculated the T-matrix elements connecting the valence-band envelope functions. The diagonal T-matrix elements for $k_x=0.1(2\pi/a)$ are approximately the same as for $\mathbf{k}_{\parallel}=0$. The off-diagonal T-matrix elements which show appreciable values close to 0.1 or above have been depicted in Fig. 6. All other off-diagonal matrix elements are smaller.

In summary, in the valence-band energy regime the light-hole and heavy-hole band envelope functions are almost continuous. However, their first derivatives are discontinuous. Notably this discontinuity is not given by the ratio of the effective masses.

B. Conservation of flux

We want to emphasize again that the envelope functions are calculated starting from true electronic wave functions. These wave functions and their first derivatives are continuous at every (x,y) point of the interface. As a matter of course the charge density and density-current probability (or flux) will then be continuous as well. However, our results obtained above for the connection rules for conduction-band envelope functions and their first derivative seem at first sight to violate flux conservation at the interface, at least if the expression for the unit-cell averaged flux in the effective-mass approximation

$$\langle j \rangle_z \approx \frac{\hbar}{2im_j^*}\left[\mathcal{F}_c^{j*}(z_{\mathrm{uc}})\frac{\partial}{\partial z}\mathcal{F}_c^{j}(z_{\mathrm{uc}})-\mathrm{c.c.}\right] \tag{8}$$

is used.[23–25] Here the argument z_{uc} of the envelope function is some position within a unit cell. Since both the envelope function and its first derivative are approximately continuous, but the effective masses of both materials are largely different ($m^*_{\mathrm{AlAs}}/m^*_{\mathrm{GaAs}}\approx 1.8$ for effective masses as obtained with empirical pseudopotentials), this expression appears to be discontinuous across the interface. It is precisely because of the wish to have (8) continuous that a large variety of authors has urged to propose as obvious the connection rule that $(m_j^*)^{-1}\partial\mathcal{F}_c/\partial z$ should be continuous. This rule, together with continuous envelope functions $\mathcal{F}_c$, indeed provides a continuous density current, as given by expression (8). So there seems to be a contradiction between our approach in which the continuity of the density current within the scattering-matrix method is built in from the outset and the apparently discontinuous density current according to expression (8), in which the conduction-band envelope function obtained from pseudo-wave-functions and its first derivative are substituted.

The discrepancy can be explained as follows: In Fig. 7 we have given the ratio of the unit-cell averaged flux, as given by (8) in which we have substituted the envelope function $\mathcal{F}_c$ and its first derivative which are calculated starting from the pseudo-wave-function and the "exact" flux as obtained within the scattering-matrix method using empirical pseudopotentials for a GaAs/$\mathrm{Al_{0.3}Ga_{0.7}As}$ single barrier structure ($\mathbf{k}_{\parallel}=0$). One conclusion to be drawn from this figure is that expression (8) apparently is a good approximation for the exact flux in GaAs at energies close to the conduction-band edge of GaAs. This is the energy region where the effective-mass approximation

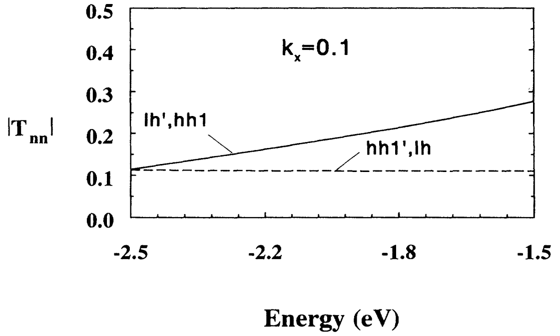

FIG. 6. The most important nonzero off-diagonal matrix elements of the 6×6 T matrix connecting light-hole band and heavy-hole band envelope functions and their first derivatives at a GaAs/AlAs interface are given for $k_x=0.1(2\pi/a)$.

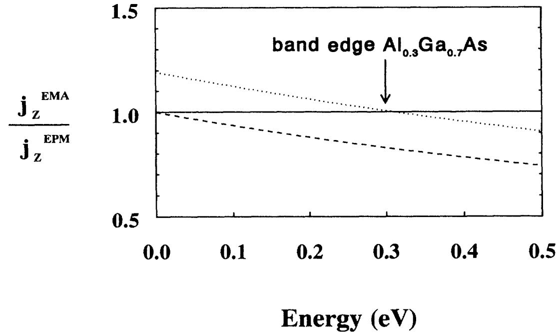

FIG. 7. The ratio between the unit-cell averaged flux j_z^{EMA} as calculated in the effective-mass approximation (in which the envelope function and its first derivative as obtained using the empirical-pusedopotential method are substituted) and the flux j_z^{EPM} as calculated exactly within the empirical-pseudopotential method in GaAs (dashed line) and $\mathrm{Al_{0.3}Ga_{0.7}As}$ (dotted line) for a single GaAs/$\mathrm{Al_{0.3}Ga_{0.7}As}$ barrier structure.

is valid. But at these energies the deviation of the flux in $Al_{0.3}Ga_{0.7}As$, given by (8), from the exact flux is rather larger (±20%). This is because the effective-mass approximation is rather poor at these energies in $Al_{0.3}Ga_{0.7}As$ since we are far from the conduction-band edge of $Al_{0.3}Ga_{0.7}As$. At energies close to the conduction-band edge in $Al_{0.3}Ga_{0.7}As$ the situation is reversed. At energies in between the conduction-band edges of both materials the deviations of the flux given by (8) from the exact flux are opposite in both material layers. Our conclusion therefore is that the flux, calculated with expression (8) in which we substitute the envelope functions obtained from the pseudo wave function obtained using the scattering-matrix method, indeed is discontinuous at the $GaAs/Al_{0.3}Ga_{0.7}As$ interface. This discontinuity is due to the poor approximation for the unit-cell averaged flux given by expression (8) in a material layer j at energies that are not close to the conduction-band edge of that material.

C. The InAs/GaSb interface

The $GaAs/Al_xGa_{1-x}As$ interface is a particularly favorable case: the materials are quite similar and the band lineup is such that, at a given energy, electron states are matched at interfaces which correspond to energy bands which have the same band index. For such a case it may be expected that a simple prescription for the connection rules for envelope functions can be obtained. The situation is less favorable for the case of an InAs/GaSb interface. Here the accepted value of the valence-band offset is such that the valence bands in GaSb are lined up with the conduction band in InAs. Whether it will still be possible to formulate simple connection rules for envelope functions can seriously be doubted for this case.

We have used the empirical-pseudopotential method to calculate the scattering amplitudes of an electron in InAs at an InAs/GaSb interface. The valence-band offset has been taken equal to 0.65 eV, so that the top of the valence bands of GaSb lies 0.15 eV above the minimum of the conduction band of InAs.[26] Spin-orbit interaction is neglected although actually this is not justified for these materials: The spin-orbit splitting of the valence bands at the Γ point equals 0.4 eV in InAs and 0.8 eV in GaSb. These values are comparable to the direct band gap, which is equal to 0.5 eV in InAs and equal to 1.0 eV in GaSb. However, we do not expect that spin-orbit interaction will qualitatively influence the results with respect to the connection rules for the envelope functions. At the InAs/GaSb interface there are two possible types of interfaces, one consisting of bonds between As and Ga and the other where the bonds are between Sb and In. Experiments show that the Ga-As interface is usually found.[27] We therefore consider an InAs/GaSb interface consisting of the As-Ga bonds. The precise interface position z_0, to be used in our scattering-matrix calculations, is to be chosen such that the difference between the total heterostructure potential and that of the bulk potential of material j shows antisymmetric behavior.[15] The results for the total self-consistent potential, averaged parallel to the interface plane, as given by Ihm, Lam, and Cohen,[27] indicate that the interface position where the difference potential satisfies this condition lies halfway between the Ga and As planes.

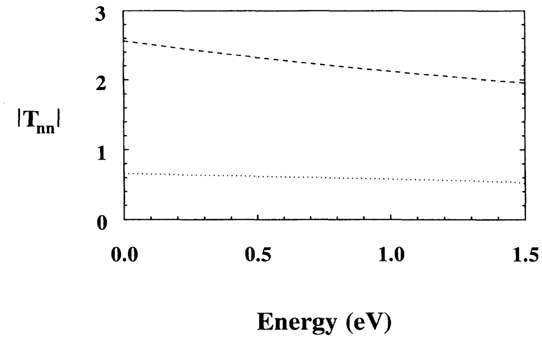

FIG. 8. The values of the matrix elements $|T_{c,lh'}|$ (dashed line), connecting the conduction-band envelope function in InAs at the first derivative of the light-hole band envelope function in GaSb, and $|T_{c',lh}|$ (dotted line), analogously defined, as a function of energy at $\mathbf{k}_{\parallel}=0$. The zero of energy lies at the conduction-band minimum of InAs.

At energies above the conduction-band edge in InAs, the light-hole band envelope functions are the dominant ones in GaSb. If we now, as a logical choice take the 2×2 T matrix such that it connects the light-hole band envelope function in GaSb with the conduction-band envelope function in InAs, we find that the diagonal elements of T are small; $T_{c,lh}\approx0.092$ and $T_{c',lh'}<0.008$, while the off-diagonal elements happen to be the larger ones in amplitude. This can be explained as follows: the GaSb light-hole band envelope function is, using relation (7), in first order proportional to the first derivative of the GaSb conduction-band envelope function. Vice versa, interchanging the conduction-band index and the light-hole band index in relation (7), the conduction-band envelope function in GaSb is in first order proportional to the first derivative of the light-hole band envelope function. Put otherwise we find, in first order, $\mathcal{F}_{lh}\propto\partial\mathcal{F}_c/\partial z$ and $\partial\mathcal{F}_{lh}/\partial z\propto\mathcal{F}_c$. The roles of the envelope function and its first derivative at the right-hand side of relation (6) have therefore effectively been interchanged. This implies that the previously diagonal elements of the T matrix for the GaAs/AlAs interface, connecting conduction-band envelope functions at both sides of the interface, now play their role on the off-diagonal positions. As a matter of course relation (7) is only approximate, the first-order approximation being poor since the energy generally is far from both the conduction-band edge of GaSb. In Fig. 8 we have printed the off-diagonal elements as a function of energy. The off-diagonal matrix element $T_{c,lh'}$ appears to be weakly dependent on energy, $2<|T_{c,lh'}|<2.6$ for energies between 0 and 1.5 eV above the conduction-band minimum of InAs. The matrix element $T_{c',lh}$ is almost constant. Its absolute value appears to be approximately equal to 0.8.

V. CONCLUSIONS

We have succeeded in calculating the T-matrix elements, connecting envelope functions at heterostructure interfaces, using the scattering-matrix method based on empirical pseudopotentials. We conclude from our scattering-matrix approach that the T matrix, for $\mathrm{GaAs/Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ interfaces and $\mathbf{k}_{\parallel}=0$, to be used in a 4-band envelope-function model is an almost diagonal 6×6 matrix, connecting two heavy-hole band envelope functions and either the light-hole band envelope function for energies in the valence-band region or the conduction-band envelope functions in the conduction-band energy region. The diagonal elements connecting the envelope functions appear to be close or even equal to unity. The first derivatives appear to be discontinuous. These discontinuities, however, have nothing to do with effective-mass ratios in contradiction with the often applied values for these matrix elements. For $\mathbf{k}_{\parallel}\neq0$ the diagonal T-matrix elements keep approximately the same values as for $\mathbf{k}_{\parallel}=0$, but now there are also off-diagonal elements which may take appreciable values. Only in the important energy region above the conduction-band minimum of GaAs and at $\mathbf{k}_{\parallel}=0$ the T matrix can be reduced to a 2×2 matrix connecting the conduction-band envelope function and its first derivative.

To give an indication of the errors due to the use of incorrect connection rules we have considered the lowest electron bound state in a 26.6-Å-wide AlAs/GaAs/AlAs quantum well. If we use envelope functions with wave vectors which follow from our empirical-pseudopotential calculations (so the conduction band is taken into account "exactly") and take the envelope function to be continuous and a first derivative divided by the effective mass to be continuous we find an error in the bound state energy of about 35 meV. In an effective-mass approximation, however, the conduction band is approximated by a parabolic band. This introduces an error which has nearly the same value but with the opposite sign. The final result in such an effective-mass approach therefore nearly coincides with the "exact" result. Note, however, that the errors due to the simple parabolic band approximation can easily be avoided by incorporating nonparabolic effects. The relative success of the effective-mass approach therefore certainly cannot be interpreted as a general plea for a connection rule for derivatives of envelope functions involving effective-mass ratios.

Given the results for the connection rules for the conduction-band envelope functions, the expression for the unit-cell averaged density-current probability in the effective-mass approximation gives a flux which is discontinuous at the interface. This discontinuity is due to a breakdown of this expression for the flux at energies which are far from the conduction-band edge in either one or the other material layer, rather than to erroneous connection rules for envelope functions.

For the InAs/GaSb interface, at which the conduction band in InAs is lined up with the valence bands in GaSb, the T matrix connecting the light-hole band envelope function and its first derivative in GaSb with the conduction-band envelope function and its first derivative in InAs appears to have diagonal matrix elements which are negligibly small. For this case the off-diagonal T-matrix elements are nonzero. These off-diagonal matrix elements have values which depend only weakly on energy.

Given the above results for T matrices, the envelope-function approach seems to be reasonably applicable for the description of the electronic properties of $\mathrm{GaAs/Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$-based heterostructures, at least for those cases in which the electronic properties are determined by the Γ-point Bloch waves in each material layer. Clearly it fails if states associated with other band extrema play an important role, as shown in Refs. 15 and 28 for the GaAs/AlAs single barrier case. For InAs/GaSb based heterostructures, in which case the conduction band and the valence bands are lined up close to each other, the envelope-function approach may be successfully used also, but now an off-diagonal transfer matrix must be used.

The connection rules for envelope functions as obtained using the scattering-matrix approach in principle apply to the special cases in which the flat-band approximation is valid only. The question is whether they will also be applicable to cases in which the flat-band approximation is not valid anymore such as in the presence of electric fields or potentials resulting from doping profiles. If these potentials are slowly varying over distances of the order of the size of a unit cell of a bulk material there will be, over distances of a few atomic layers near the interface, no difference with or without the additional potential. The connection rules at interfaces as obtained in the flat-band approximation will therefore be applicable to the cases in which slowly varying potentials are present also.

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