General boundary conditions for the envelope function in the multiband k·p model

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We have derived general boundary conditions (BC's) for the multiband envelope functions (which do not contain spurious solutions) in semiconductor heterostructures with abrupt heterointerfaces. These BC require the conservation of the probability flux density normal to the interface and guarantee that the multiband Hamiltonian be self-adjoint. The BC are energy independent and are characteristic properties of the interface. Calculations have been performed of the effect of the general BC on the electron energy levels in a potential well with infinite potential barriers using a coupled two band model. The connection with other approaches to determining BC for the envelope function and to the spurious solution problem in the multiband **k·p** model are discussed.

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I. INTRODUCTION

It is impossible to overestimate the role of the multiband effective mass approximation (MEMA), which consists of the multiband **k·p** method together with the envelope function approximation (EFA), in the simulation of electronic and optical devices formed from various semiconductor heterostructures, such as those with type-I and -II heterointerfaces, quantum well structures and superlattices, and one and zero-dimensional semiconductor structures such as quantum wires and quantum dots. The calculations of energy bands and wave functions in such structures have often been considered as only being a matter of ''energy band engineering'' or ''wave function engineering.'' However, although such calculations successfully describe many heterostructures (see, for example, Ref. 1), a general theoretical description of structures with abrupt interfaces has yet to be developed.

The MEMA gives an accurate description of the energy band structure of bulk semiconductors near the extrema of the first Brillouin zone. In this approach the carrier wave functions are expanded in the band edge Bloch functions near an extremum with ''envelope function'' coefficients, or components, that are required to vary slowly over a distance on the scale of the unit cell a_0. The bulk MEMA Hamiltonian contains such parameters as band edge energies, interband momentum matrix elements and carrier effective masses. These material parameters are determined by fitting to independent experimental data or are obtained from first principles calculations. The MEMA is certainly appropriate for calculating the spectrum and carrier wave functions in the presence of any slowly varying potential.[2]

However, abrupt heterointerfaces in semiconductor heterostructures break the periodicity of the crystal potential.[3,4] The nonperiodic part of the potential varies rapidly in an interface region of size $a \approx a_0$. This may lead to such interface effects as the admixture of remote band states,[3] coupling of states with different symmetry,[5–8] and the formation of surface localized states.[4] Moreover, Bloch functions in dissimilar materials can be significantly different[9] and do not even exist in the boundary regions.[10] In light of the great success of the MEMA, it is important to develop an adequate description of semiconductor heterostructures with abrupt boundaries using the MEMA to describe each material in the heterostructure. Laikhtman[10] has shown that this is possible for heterostructures with a characteristic length $L \gg a$, provided that the boundaries are treated appropriately. The problem is then focused on the appropriate choice of boundary conditions (BC) for piece-wise defined envelope functions in these heterostructures.

Conservation of the current normal to the interface is an obvious requirement dictated by conservation of probability density. In the EFA this condition reduces to the continuity across the interface of the normal component of the probability flux density J_τ averaged over the unit cell.[3,11] In a heterostructure formed of semiconductors with parabolic bands, which can be described by a single band effective mass approximation (EMA) (the simplest MEMA), this condition can be expressed as the continuity across the interface of

$$J_\tau = -i\frac{\hbar}{2m}(f^* f' - f'^* f), \tag{1}$$

where $\vec{\tau}$ is a unit vector directed normal to the interface, m is the effective mass, and f is the single band envelope function

and the prime denotes the derivative along $\vec{\tau}$. The continuity of Eq. (1) is satisfied if

$$f_r = f_l, \quad \frac{f_r'}{m_r} = \frac{f_l'}{m_l}, \tag{2}$$

where the indices r and l refer to a point just to the right and just to the left, respectively, of the interface. These BC, expressing the separate continuity of the envelope function and the normal envelope velocity, f'/m, first suggested in Refs. 12,13, are referred to as ''conventional'' BC. However, the conventional BC of Eq. (2) were recognized almost 20 years ago[14] to be a special case of more general BC that conserve J_τ across the interface:[3,10,14–17]

$$\begin{pmatrix} f_r \\ f_r'/m_r \end{pmatrix} = T_{tr} \begin{pmatrix} f_l \\ f_l'/m_l \end{pmatrix}, \quad \det[T_{tr}] = t_{11}t_{22} - t_{12}t_{21} = 1, \tag{3}$$

where the elements t_{ij} of the transfer matrix T_{tr} are characteristic of the interface[10,3] and as seen from a more general derivation of Eq. (3),[16,17] based on the requirement for the EMA Hamiltonian to be self-adjoint,[18] do not depend on the particular states and are energy independent. For example, first principle calculations performed for GaAs/Al_xGa_{1-x}As heterostructures[15] show that the off diagonal elements t_{12} [which was shown to be always proportional to the small parameter a/L (Ref. 10)] and t_{21} are negligible for this interface. In this case the BC can be written in the form

$$m_r^\alpha f_r = m_l^\alpha f_l, \quad \frac{f_r'}{m_r^{\alpha+1}} = \frac{f_l'}{m_l^{\alpha+1}}, \tag{4}$$

similar to the general BC first suggested in Ref. 19. In general the parameters α and the off diagonal element t_{21} (which may be nonzero for other heterostructures[20]) strongly effect the penetration of the wave function into the barrier and the energy spectra in quantum wells (QW's). For example, this has been demonstrated in Ref. 21 by analyzing the experimental data for the exciton optical spectra in narrow GaAs/AlGaAs and InGaAs/InP QW's using the EMA with modified BC similar to those given by Eq. (4). However, the parabolic band approximation has a very narrow range of applicability and appropriate BC for the MEMA need to be developed for describing experimental data.

For the multiband analysis of heterostructures, a natural extension of the conventional BC of Eq. (2) is the continuity of each component of the N-component envelope function Ψ and of each component of the normal envelope velocity V_τ at each interface.[22–24] Taken together, these BC preserve the normal component of the envelope flux density J_τ averaged over a unit cell. The most general derivation of these BC, suggested by Baraff and Gershoni,[24] is based on the requirement for the MEMA Hamiltonian to be self-adjoint. A general form of the BC within the MEMA for the planar heterostructures was suggested by Kisin *et al.*[11] Those authors start from the conservation of J_τ at the interface, and introduce a transfer matrix connecting the components of the multiband envelope function Ψ and its normal derivative Ψ' on each side of the heterointerface. The general consideration of the 8×8 band model based on the symmetrical properties of the planar heterointerface[11] has allowed us to gain important information about the elements of the transfer matrices. However, the BC introduced in Ref. 11 may lead to an energy dependent connection between the components of Ψ and V_τ on the left and right sides of the heterointerface and, therefore, do not generally satisfy the requirement that the MEMA Hamiltonian be self-adjoint.

The MEMA that take band coupling into account have a significant theoretical problem when describing various semiconductor heterostructures. The full expansion of the N-band envelope function in the N independent plane wave solutions of the bulk Hamiltonian corresponding to the same energy ε includes solutions with a very large wave vector lying outside the first Brillouin zone.[25,26] Such ''wing'' (evanescent)[25] or ''spurious'' (oscillatory)[26] solutions must be rejected in the perturbation $\mathbf{k}\cdot\mathbf{p}$ theory; in the bulk they are rejected as being unphysical solutions.[27–29] However, their elimination from the multiband envelope function for heterostructures[30,31,28,11] leads to additional complications in the analysis of the BC. For example, the continuity of all N components of this truncated envelope function cannot be satisfied if the interband matrix elements of the momentum operator $\hat{\mathbf{p}}$ are not continuous across the interface.[11] The same problem remains for the alternative approach, based on modifying the MEMA Hamiltonian by discarding those terms responsible for the large k solutions.[25,26,32,33] The use of different BC for the conduction and valence band states (see, for example, Ref. 32) automatically results in the dependence of the BC on ε, and is justified only if band coupling in the MEMA Hamiltonian and bands nonparabolicity can be neglected.

In our paper we consider the boundary condition problem within the MEMA for heterostructures with abrupt boundaries. We show that the most general requirement for the MEMA Hamiltonian to be self-adjoint implies continuity at the interface of the normal component of the envelope flux density vector $J_\tau^{\alpha\beta}$. Here the indices α and β denote, in general, two arbitrarily chosen envelope functions Ψ_α and Ψ_β, respectively. This allows us to formulate general BC using a new *energy and state independent* transfer matrix connecting the components of the envelope functions and their normal velocities on each side of the interface. It also allows us to find a general way of eliminating the large-k solutions because these solutions make only a small (proportional to a/L) contribution to the envelope flux density. This procedure does not depend on the particular nature of the large-k solutions (which we shall hereafter call spurious) and can be applied to boundaries with either finite or infinite potential barriers. The elements of these transfer matrices can be considered as characteristic surface or interface parameters and are additional to the bulk energy band parameters in the multiband $\mathbf{k}\cdot\mathbf{p}$ approximation.

The paper is organized as follows. In Sec. II we derive the general form of BC for the multiband envelope function, that follows from the condition that the MEMA Hamiltonian be self-adjoint. In Sec. III we derive a truncated form of general BC for slowly varying envelope functions which do not al-

low spurious solutions. To clarify the general procedure, we first consider, in detail, the two band Kane model. Section IV gives analytical and numerical examples of the effect of the general BC on the quantum size energy levels in dots with infinite potential barriers. In Sec. V we discuss our results and compare them with those of other approaches to the BC problem within the MEMA and other **k·p** theories for heterostructures.

II. GENERAL FORM OF MULTIBAND BOUNDARY CONDITIONS IN HETEROSTRUCTURES WITH ABRUPT BOUNDARIES

Let us consider a semiconductor heterostructure made of M arbitrary shaped semiconductor layers with a characteristic length L. Single-electron wave functions $\Phi(\mathbf{r})$ in these structures are solutions of the Schrödinger equation with the microscopic Hamiltonian $\hat{H}_{\rm micr}$ containing a crystal potential. This potential is ''periodic'' inside each of the bulklike semiconductor layers, but it varies rapidly in the boundary regions with width $a \approx a_0$. Assuming that a/L is small, we neglect the exact behavior of $\Phi(\mathbf{r})$ in the boundary regions and expand $\Phi^j \equiv \Phi(\mathbf{r} \in \mathbf{R}_j)$ in the bulklike interior region $\mathbf{R}_j$ of the jth layer in the Bloch functions $u^j_{nk_{0j}}$ at a critical point k_{0j} of the bulk energy band structure for the material in that layer:

$$\Phi^j(\mathbf{r}) = \sum_{n=1}^{N_j} \Psi^j_n(\mathbf{r}) u^j_{nk_{0j}}, \quad j = 1,2,\ldots,M, \tag{5}$$

where N_j is the number of bands that describe the band-edge bulk properties of the material in the jth layer, and M is the number of layers. The symmetry of the material and the number of bands can be different in each region. The N_j component envelope function $\Psi^j(\mathbf{r}) = \{\Psi^j_n(\mathbf{r})\}_{n=1}^{N_j}$ is slowly varying in the bulklike region $\mathbf{r} \in \mathbf{R}_j$, where it satisfies the **k·p** Schrödinger equation

$$\hat{H}^j(\hat{\mathbf{k}})\Psi^j(\mathbf{r}) = \varepsilon \Psi^j(\mathbf{r}), \quad \mathbf{r} \in \mathbf{R}_j. \tag{6}$$

The $N_j \times N_j$ Hamiltonians $\hat{H}^j$ are obtained after averaging of the perturbed microscopic Hamiltonian $\hat{H}_{\rm micr}(\hat{\mathbf{p}} + \hbar\hat{\mathbf{k}})$ over a unit cell in each bulklike region[2] and includes terms up to the second order in the wave vector operator $\hat{\mathbf{k}} = -i\boldsymbol{\nabla}$. The boundary regions, however, are excluded from the averaging procedure, and the parameters of the resulting heterostructure MEMA Hamiltonians $\hat{H}^j$ may have abrupt jumps from one layer to another.

In what follows we study in detail the boundary conditions imposed on the wave functions $\Psi(\mathbf{r}) \equiv \Psi^j(\mathbf{r})$ for $\mathbf{r} \in \mathbf{R}_j$ at the interfaces. The microscopic Hamiltonian $\hat{H}_{\rm micr}$ acting on $\Phi(\mathbf{r})$ is a self-adjoint operator.[18] This is equivalent to the conservation of charge in the full heterostructure region Ω:

$$\frac{d}{dt}\int_\Omega \mathbf{d}^3\mathbf{r}|\Phi|^2 = 0. \tag{7}$$

If a/L is small, the contribution from the boundary regions can be neglected. Therefore, Eq. (7), within the accuracy of the MEMA, is replaced by $d/dt\langle\Psi,\Psi\rangle = 0$, where Ψ is the corresponding envelope function satisfying the BC and the inner product is now defined as

$$\langle \Psi_\alpha, \Psi_\beta \rangle = \sum_j \int_{\mathbf{R}_j} \mathbf{d}^3\mathbf{r}(\Psi^j_\alpha, \Psi^j_\beta),$$

$$(\Psi^j_\alpha, \Psi^j_\beta) = \sum_{n=1}^{N_j} \Psi^{j*}_{\alpha n}\Psi^j_{\beta n}. \tag{8}$$

This implies, in turn, that the heterostructure MEMA Hamiltonian $\hat{H} \equiv \hat{H}^j$ for $\mathbf{r} \in \mathbf{R}_j$, acting on Ψ has to be a self-adjoint operator. Therefore for any two arbitrarily chosen functions Ψ_α and Ψ_β, the condition

$$\langle \hat{H}\Psi_\alpha, \Psi_\beta \rangle = \langle \Psi_\alpha, \hat{H}\Psi_\beta \rangle \tag{9}$$

must be satisfied if the same BC is imposed on Ψ_α as well as on Ψ_β (see, for example, Ref. 34). The MEMA Hamiltonians $\hat{H}^j$, when defined for the ideally infinite homogenous bulk semiconductor, are self-adjoint, but when one adds the abrupt boundaries, the condition of Eq. (9) may be violated by boundary terms. The requirement for $\hat{H}$ to be self-adjoint limits the choice of the boundary conditions that may occur, but there is an ample variety of BC that satisfy it. We shall see that any self-adjoint MEMA Hamiltonian preserves the normal component of the envelope flux density for an arbitrary state of the system.

The MEMA Hamiltonians for the N_j component envelope wave functions have terms of first and second order in $\hat{\mathbf{k}}$:

$$\hat{H}^j = \hat{C}^j + \hbar\hat{B}^j_\mu\hat{k}_\mu + \hbar^2\hat{D}^j_{\mu\nu}\hat{k}_\mu\hat{k}_\nu, \tag{10}$$

where $\hat{C}^j$, each $\hat{B}^j_\mu$ $(\mu = x,y,z)$ and $\hat{D}^j_{\mu\nu}$ $(\mu,\nu = x,y,z)$ are Hermitian $N_j \times N_j$ tensors of rank 0, 1, and 2, respectively. They contain the energy band parameters for the material in $\mathbf{R}_j$ and are defined only in these bulk-like regions. Using Eq. (10) we can write a velocity operator $\hat{\mathbf{V}} \equiv \hat{\mathbf{V}}^j$ for $\mathbf{r} \in \mathbf{R}_j$ which acts on the heterostructure envelope functions

$$\hat{\mathbf{V}}^j = \frac{1}{\hbar}\frac{\partial \hat{H}^j}{\partial \mathbf{k}} = \hat{\mathbf{B}}^j + \hbar\frac{\partial \hat{D}^j_{\mu\nu}\hat{k}_\mu\hat{k}_\nu}{\partial \mathbf{k}}. \tag{11}$$

A general envelope flux density matrix can be written

$$\mathbf{J}^{\alpha\beta}(\mathbf{r}) = \frac{1}{2}[(\Psi_\alpha, \hat{\mathbf{V}}\Psi_\beta) + (\hat{\mathbf{V}}\Psi_\alpha, \Psi_\beta)], \quad \mathbf{r} \in \mathbf{R}_j, \tag{12}$$

where Ψ_α and Ψ_β are two arbitrarily chosen solutions $\Psi^j_\alpha \equiv \Psi_\alpha(\mathbf{r} \in \mathbf{R}_j), \Psi^j_\beta \equiv \Psi_\beta(\mathbf{r} \in \mathbf{R}_j)$ of the Schrödinger equation Eq. (6), defined in each bulklike region, with energies ε_α and ε_β, respectively. Noting that

$$\mathrm{div}\mathbf{J}^{\alpha\beta}(\mathbf{r}) = -\frac{i}{2}[(\hat{\mathbf{k}}\Psi_\alpha, \hat{\mathbf{V}}\Psi_\beta) - (\Psi_\alpha, \hat{\mathbf{k}}\cdot\hat{\mathbf{V}}\Psi_\beta)$$

$$-(\hat{\mathbf{V}}\Psi_\alpha, \hat{\mathbf{k}}\Psi_\beta) + (\hat{\mathbf{k}}\cdot\hat{\mathbf{V}}\Psi_\alpha, \Psi_\beta)], \quad \mathbf{r} \in \mathbf{R}_j,$$

and using Eqs. (10),(11) we arrive at the identity

$$(\Psi_\alpha,\hat{H}\Psi_\beta)-(\hat{H}\Psi_\alpha,\Psi_\beta)=\frac{\hbar}{i}\,\mathrm{div}\mathbf{J}^{\alpha\beta}(\mathbf{r}),\quad \mathbf{r}\in\mathbf{R}_j\,. \tag{13}$$

Thus, for the MEMA Hamiltonian $\hat{H}$ to be self-adjoint with BC imposed on Ψ_α and Ψ_β, Eq. (9) requires

$$\sum_j \int_{\mathbf{R}_j} d^3\mathbf{r}\cdot\mathrm{div}\mathbf{J}^{\alpha\beta}=\sum_j \int_{\mathbf{R}_j} d\mathbf{S}_j\cdot\mathbf{J}^{\alpha\beta}=0, \tag{14}$$

where $d\mathbf{S}_j$ is an element of the surface bounding $\mathbf{R}_j$. Noting that Eq. (14) holds for arbitrary surface shape, we find that local continuity of the normal envelope flux density matrix across each interface must hold:

$$J_\tau^{\alpha\beta}=\vec{\tau}\cdot\mathbf{J}^{\alpha\beta}=\frac{1}{2}[(\Psi_\alpha,\vec{\tau}\cdot\hat{\mathbf{V}}\Psi_\beta)+(\vec{\tau}\cdot\hat{\mathbf{V}}\Psi_\alpha,\Psi_\beta)]=\mathrm{const}. \tag{15}$$

Equation (15) is a generalization of the normal flux density conservation law, $J_\tau\equiv J_\tau^{\alpha\alpha}=\mathrm{const}$, that is often used as the starting point for deriving BC.[3,11] The condition $J_\tau^{\alpha\beta}=\mathrm{const}$ is a very general and strong requirement on the envelope functions at each point of the interface. For an unpenetratable interface, or a semiconductor/vacuum surface it reduces to $J_\tau^{\alpha\beta}=0$. We will consider this case only in Sec. IV, and shall assume, for now, that $J_\tau^{\alpha\beta}\neq 0$ at the semicondutor heterointerface.

The condition of Eq. (15) must be fulfilled independently of whether the number of the envelope function components on the two sides of interface is the same. For clarity in the following we will only consider heterostructures formed of semiconductors whose energy band structures are described by multiband Hamiltonians $\hat{H}^j$ of same symmetry and with $N_j=N$ in each region. For the more general case, a more complicated procedure similar to that suggested in Ref. 10 is needed. The appropriate number of boundary conditions depends on the number of independent components of the envelope function Ψ and normal envelope velocity $V_\tau=\tau\cdot\mathbf{V}\Psi$. If all the components of Ψ and V_τ, are linearly independent on each side of the interface, the most general BC one can impose on the envelope functions are of the form

$$\begin{pmatrix}\Psi^+\\ iV_\tau^+\end{pmatrix}=T_{2N}\begin{pmatrix}\Psi^-\\ iV_\tau^-\end{pmatrix}, \tag{16}$$

where the indices "$-$" and "$+$" refer to neighboring points on neighboring bounding surfaces S_j and S_{j+1}, respectively, and T_{2N} is the $2N\times 2N$ transfer matrix. In the BC described by Eq. (16) the material parameters of the MEMA Hamiltonian are included in the vectors of the normal envelope velocity. Equation (15) is satisfied for all arbitrarily chosen α and β if and only if the BC of Eq. (16) are imposed on all Ψ_α as well as on all Ψ_β with the same T_{2N} and

$$T_{2N}^\dagger\begin{pmatrix}0 & I_N\\ -I_N & 0\end{pmatrix}T_{2N}=\begin{pmatrix}0 & I_N\\ -I_N & 0\end{pmatrix}, \tag{17}$$

where I_N is the $N\times N$ unit matrix and the dagger denotes the Hermitian conjugate. Therefore, T_{2N} must be state independent and characteristic only of the interface. For the conventional BC, $\Psi^+=\Psi^-, V_\tau^+=V_\tau^-$, the transfer matrix reduces to the unit matrix, $T_{2N}=I_{2N}$.

In the "pure" Kane models ($\hat{D}_{\mu\nu}\equiv 0$ and $\hat{H}$ only contains terms linear in $\hat{\mathbf{k}}$) the N components of $V_\tau=\vec{\tau}\cdot\hat{\mathbf{B}}\Psi$ depend linearly on the N components of Ψ. In this case, the general BC can be written

$$\Psi^+=T_N\Psi^-,\quad T_N^\dagger B_\tau^+ T_N=B_\tau^-\,. \tag{18}$$

Here $B_\tau=\vec{\tau}\cdot\hat{\mathbf{B}}$ and T_N is an $N\times N$ state independent transfer matrix. One can see that if $B_\tau^+\neq B_\tau^-$, the transfer matrix T_N cannot be the unit matrix I_N. The number of independent equations in Eq. (18) is determined by the rank of the matrices B_τ and can be less then N.

The elements of the state independent transfer matrix may depend on such properties of the heterojunction as band offsets and surface crystal symmetry due to, e.g., its reconstructions. Additional restrictions on the components of the transfer matrix can be obtained from symmetry consideration of the bulk and surface properties[11,7] in particular cases. For heterostructures which geometrical shape has some elements of symmetry one can expect the boundary parameters to be the same at the symmetrical points of the interface. For example, in a QW the parameters of the transfer matrix are the same along the plane, and in the spherically shaped heterostructure, the parameters of the transfer matrix are the same anywhere on the surface.

III. ELIMINATION OF SPURIOUS SOLUTIONS FROM MULTIBAND k·p MODEL: TRUNCATED BOUNDARY CONDITIONS

Consider a heterostructure with a single heterointerface described by a piece-wise $N\times N$ Hamiltonian of Eq. (10), and with nonzero energy dispersion matrices $D_{\mu\nu}$. The envelope functions can be expanded in a complete set of N plane wave eigenfunctions, $\Psi_i(k_i)$, of the $N\times N$ MEMA Hamiltonian

$$\Psi=\sum_{i=1}^{N} C_i\Psi_i(k_i), \tag{19}$$

where the N values of k_i^2 are the roots of the bulk energy dispersion equation $\det[H(k)-\varepsilon]=0$, and C_i are numerical coefficients. The set of $2N$ boundary condition equation in Eq. (17) can be solved only if the expansion in Eq. (19), for both sides of the interface, includes all N of the plane wave eigenfunctions. If any, say m roots $|k_i|$ $(i=N-m+1,\ldots N)$ lie outside the first Brillouin zone, the corresponding spurious solutions must be excluded from the wave function. In this case, $2m$ components of the envelope wave function and their velocities are linearly dependent on the other components, and only $2(N-m)$ independent BC can be imposed on the truncated function $\tilde{\Psi}=\Sigma_{i=1}^{N-m}C_i\Psi_i(k_i)$. In this section we suggest an approximate procedure which allows us to derive a truncated set of general BC that must be

imposed on the envelope function in order to satisfy $J_\tau^{\alpha\beta}=\text{const}$. For the sake of clarity, we first consider a two band model ($N=2$, $m=1$) and a planar heterointerface. We then generalize it to arbitrary N and m and an arbitrarily shaped heterointerface.

The Hamiltonian of the two band Kane model is written

$$\hat{H}=\begin{pmatrix} E_c & 0 \\ 0 & E_v \end{pmatrix}+\hat{H}_K, \quad \hat{H}_K=\frac{\hbar^2}{2m_0}\begin{pmatrix} \alpha_c\hat{k}_z^2 & i\frac{2P}{\hbar}\hat{k}_z \\ -i\frac{2P}{\hbar}\hat{k}_z & -\alpha_v\hat{k}_z^2 \end{pmatrix}, \tag{20}$$

where $\hat{k}_z=-id/dz$ is the wave vector along the normal to the interface, m_0 is the free electron mass, P is the Kane interband matrix element, α_c and α_v describe the contribution of the remote bands to the electron m_c and hole m_v effective masses, respectively, and the distance between the bottom of conduction band E_c and the top of the valence band E_v is the energy gap $E_g=E_c-E_v$. The band edge effective masses can be written as $m_0/m_{c,v}=\alpha_{c,v}+E_p/E_g$. Here $E_p=2P^2/m_0$ is the Kane energy which also characterizes the nonparabolicity of the electron and hole bulk energy spectra. Although this two band model completely neglects spin-orbit interactions, it describes the electron and light hole band coupling in real semiconductors and is often used in one dimensional heterojunctions[11] and spherical dots.[35,29,36] For most semiconductors, $|\alpha_c|\sim|\alpha_v|\sim 1$ (they can be either positive or negative) and $E_p\approx 20\pm 5$ eV. In the "pure" Kane model $\alpha_c=\alpha_v=0$.

For a planar heterointerface, the general normal flux density continuity condition, Eq. (15), takes the form

$$J_\tau^{\Psi\,\Phi}(z)=\frac{1}{2}[(\Psi,V_\Phi)+(V_\Psi,\Phi)]=\text{const}, \tag{21}$$

where Ψ and Φ are two arbitrary chosen eigenfunctions of the Hamiltonian in Eq. (20), $V_\Psi=\hat{V}_z\Psi$ and $V_\Phi=\hat{V}_z\Phi$ are the respective normal velocities calculated with the two band Kane model velocity operator $\hat{V}_z$

$$\hat{V}_z=\frac{\hbar}{m_0}\begin{pmatrix} \alpha_c\hat{k}_z & i\frac{P}{\hbar} \\ -i\frac{P}{\hbar} & -\alpha_v\hat{k}_z \end{pmatrix}. \tag{22}$$

The general BC, Eqs. (16),(17), now reduce to

$$\begin{pmatrix} \Psi^r \\ iV_\Psi^r \end{pmatrix}=T_{tr}\begin{pmatrix} \Psi^l \\ iV_\Psi^l \end{pmatrix}, \quad T_{tr}^\dagger\begin{pmatrix} 0 & I_2 \\ -I_2 & 0 \end{pmatrix}T_{tr}=\begin{pmatrix} 0 & \hat{I}_2 \\ -\hat{I}_2 & 0 \end{pmatrix}, \tag{23}$$

where T_{tr} is an energy independent 4×4 transfer matrix, and r (l) refers to a point to the right (left) side of the planar interface. The conventional BC ($\Psi^r=\Psi^l$ and $V_\Psi^r=V_\Psi^l$) are described by the unite transfer matrix $T_{tr}\equiv I_4$. In the general case, $\alpha_c\alpha_v\neq 0$, the BC of Eq. (23) represent four linear independent equations for two (conduction and valence band) wave function components Ψ_c,Ψ_v and two normal velocity components $V_{\Psi c},V_{\Psi v}$. In order to solve them, the envelope function of a state with energy ε is written as a linear superposition of two plane wave eigenfunctions of the Hamiltonian, Eq. (20): $\Psi=C_1\Psi_1(k_1)+C_2\Psi_2(k_2)$, where $k_{1,2}^2$ are the solutions of the bulk energy dispersion equation

$$\left(\frac{\hbar^2k^2}{2m_0}\alpha_c+E_c-\varepsilon\right)\left(\frac{\hbar^2k^2}{2m_0}\alpha_v-E_v+\varepsilon\right)+\frac{\hbar^2k^2}{2m_0}E_p=0. \tag{24}$$

Generally we are only interested in states whose energy is either on the order of or smaller than the semiconductor energy gap. Using the condition $E_p/|\alpha_c\alpha_v|\gg E_g,|\varepsilon-E_c|,|\varepsilon-E_v|$, we find for the two roots of the dispersion equation

$$\hbar^2k_1^2\approx\frac{2(\varepsilon-E_v)(\varepsilon-E_c)m_0}{(\varepsilon-E_v)\alpha_c+(E_c-\varepsilon)\alpha_v+E_p}, \quad \hbar^2k_2^2\approx-\frac{2E_pm_0}{\alpha_c\alpha_v}. \tag{25}$$

For typical values of the bulk energy band parameters, the second wave vector $|k_2|\sim 1$ Å^{-1} lies beyond the first Brillouin zone in which the MEMA is valid. The corresponding eigenvector, $\Psi_2(k_2)$ is a spurious solution [either evanescent or propagating, depending on the sign of the product $(\alpha_c\alpha_v)$[27]] and must be excluded from the expansion of the total wave function. The continuity of the normal flux density, Eq. (21), is now limited to slowly varying functions of $k_1,\Psi=\Psi_1(k_1)$ and $\Phi=\Phi_1(k_1)$, and leads to $J_{\tau,1}^{\Psi\Phi}(z)\equiv J_\tau^{\Psi_1\Phi_1}(z)$:

$$\begin{aligned} J_{\tau,1}^{\Psi\Phi}(z)=\frac{iP}{m_0}\Bigg[&\Psi_c^*\Phi_v\Bigg(1+\alpha_c\frac{\varepsilon_\Phi-E_v}{E_p}+\alpha_v\frac{E_c-\varepsilon_\Psi}{E_p} \\ &+\alpha_c\alpha_v\frac{\hbar^2}{2m_0E_p}[k_1^2(\varepsilon_\Phi)+k_1^2(\varepsilon_\Psi)]\Bigg) \\ &-\Psi_v^*\Phi_c\Bigg(1+\alpha_c\frac{\varepsilon_\Psi-E_v}{E_p}+\alpha_v\frac{E_c-\varepsilon_\Phi}{E_p} \\ &+\alpha_c\alpha_v\frac{\hbar^2}{2m_0E_p}[k_1^2(\varepsilon_\Phi)+k_1^2(\varepsilon_\Psi)]\Bigg)\Bigg] \\ =&\,\text{const}. \end{aligned} \tag{26}$$

Here ε_Ψ and ε_Φ are the energies of the states described by the two component envelope functions $\Psi_1(k_1)\equiv[\Psi_c=\Psi_c(k_1),\Psi_v=\Psi_v(k_1)]$ and $\Phi_1(k_1)\equiv[\Phi_c=\Phi_c(k_1),\Phi_v=\Phi_v(k_1)]$, respectively. The two components of the normal velocities $V_{\Psi c}$ ($V_{\Phi c}$) and $V_{\Psi v}$ ($V_{\Phi v}$) are expressed through the wave function components Ψ_c (Φ_c) and Ψ_v (Φ_v). Since the envelope functions Ψ and Φ are now truncated, the normal velocity and envelope function components are no longer linearly independent. Therefore, the Eq. (26) cannot be fulfilled if $\alpha_c\alpha_v\neq 0$. [For the case $\alpha_c\alpha_v=0$ the spurious solution k_2 does not arise, and Ψ_1 is then the full solution of the Hamiltonian (20)]. However we shall see below that we can impose an alternative set of the state independent BC that retain the continuity of the normal flux density $J_{\tau,1}^{\Psi\Phi}$ for truncated wave functions within an accuracy consistent with

the MEMA. We consider a $\tilde{J}_{\tau,1}$ that differs from $J_{\tau,1}$ of Eq. (26) only by the terms $\tilde{\gamma}^2 \sim \alpha_c \alpha_v$ which are small: $\tilde{\gamma}^2 = \alpha_c \alpha_v (\varepsilon - E_c)(\varepsilon - E_v)/E_p^2 \approx (k_1/k_2)^2$. A typical value of the momentum k_1 in a heterostructure with size L is $k_1 \sim 1/L$. Substituting the value of k_2 from Eq. (22) into $\tilde{\gamma}$ we find that $\tilde{\gamma}^2 \sim (a_0/L)^2 \ll 1$. We can write then the approximate condition

$$\tilde{J}_{\tau,1}^{\Psi\Phi}(z) = \frac{iP}{m_0}\left[\Psi_c^* \Phi_v \left(1 + \alpha_c \frac{\varepsilon_\Phi - E_v}{E_p}\right)\left(1 + \alpha_v \frac{E_c - \varepsilon_\Psi}{E_p}\right) - \Psi_v^* \Phi_c \left(1 + \alpha_c \frac{\varepsilon_\Psi - E_v}{E_p}\right)\left(1 + \alpha_v \frac{E_c - \varepsilon_\Phi}{E_p}\right)\right] = \text{const}, \tag{27}$$

which is fulfilled exactly if the envelope functions Ψ and Φ satisfy the truncated set of BC:

$$\begin{pmatrix} \Psi_c^r \left(1 + \alpha_v^r \dfrac{E_c^r - \varepsilon}{E_p^r}\right) \\ P^r \Psi_v^r \left(1 + \alpha_c^r \dfrac{\varepsilon - E_v^r}{E_p^r}\right) \end{pmatrix} = \tilde{T}_{tr} \begin{pmatrix} \Psi_c^l \left(1 + \alpha_v^l \dfrac{E_c^l - \varepsilon}{E_p^l}\right) \\ P^l \Psi_v^l \left(1 + \alpha_c^l \dfrac{\varepsilon - E_v^l}{E_p^l}\right) \end{pmatrix}, \tag{28}$$

where the components of the 2×2 transfer matrix $\tilde{T}_{tr}$ are real and state independent and $\det[\tilde{T}_{tr}] = 1$. One can see that the connection between the left and right hand side components of Ψ_c and Ψ_v has now energy dependent coefficients. This is a consequence of the linear dependence of the components of the truncated wave function and its normal velocity on the same side of the interface. However, the new energy independent transfer matrix $\tilde{T}_{tr}$ is still characteristic of the interface only. The truncated general BC of Eq. (28) no longer allow the simultaneous continuity of the both envelope function components $\Psi_c(k_1)$ and $\Psi_v(k_1)$ at the interface. For the case where the off diagonal matrix elements of $\tilde{T}_{tr}$ are negligibly small, $\tilde{t}_{12} \approx \tilde{t}_{21} \approx 0$, the general BC reduce to

$$P^\alpha \left(1 + \alpha_v \frac{E_c - \varepsilon}{E_p}\right)\Psi_c = \text{const},$$

$$P^{1-\alpha}\left(1 + \alpha_c \frac{\varepsilon - E_v}{E_p}\right)\Psi_v = \text{const}, \tag{29}$$

which is similar to the BC of Eq. (4) for heterostructures with parabolic bands.

Equations (28),(29) are general BC for the truncated smooth wave functions in semiconductor heterostructures with nonzero $\alpha_c \alpha_v$. These BC do not depend on the sign of $\alpha_c \alpha_v$ (i.e., whether the spurious solution is evanescent or propagating). They are also valid for any Kane model with $\alpha_c \alpha_v = 0$, in which Eqs. (21),(26) are satisfied exactly. The boundary condition Eq. (29) was first discussed in Ref. 3 for the "pure" Kane model with $\alpha_c = \alpha_v = 0$; also the model with $\alpha_c = 0, \alpha_v \neq 0$ was considered in Ref. 33.

To generalize this procedure and derive general BC for truncated slowly varying envelope functions for heterostructures described by an $N \times N$ Hamiltonian having m spurious solutions, it is important to trace from where these solutions arise. Examining Eqs. (17),(25) (and also see Ref. 11 which describes spurious solutions in the 8×8 model) we find that the spurious solutions $|k_i|$ $(i = N-m+1, \ldots, N)$ of the dispersion equations for the Hamiltonian of Eq. (10) are proportional to the large components of the matrices $\hat{\mathbf{B}}$ and inversely proportional to the square root of the product of the tensor $D_{\mu\nu}$ conduction and valence band components. For the sake of definiteness,[37] let us assume that the matrices $\hat{\mathbf{B}}$ contain the submatrices $\hat{\mathbf{B}}' = \hat{\mathbf{B}}^\gamma/\gamma$ of rank $2m$, where $\gamma \sim a_0/L$ is a dimensionless small parameter responsible for the spurious solutions. For example, in the two band model considered above the normal component $B_\tau^\gamma = \vec{\tau} \cdot \hat{\mathbf{B}}^\gamma$ is

$$\hat{B}_\tau^\gamma = \frac{i\hbar}{m_0 L}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \gamma = \frac{\hbar}{PL} \sim \frac{a_0}{L}. \tag{30}$$

We can write the velocity operator of Eq. (11) as

$$\hat{\mathbf{V}} = \frac{1}{\gamma}\hat{\mathbf{B}}^\gamma + \hat{\mathbf{V}}_0, \tag{31}$$

and write the truncated slowly varying envelope function as the superposition of two linearly independent orthogonal wave functions $\tilde{\Psi} = \Psi_1 + \Psi_2$, such that the $2m$ component function Ψ_1 and $n = N - 2m$ component function Ψ_2 satisfy the condition

$$B_\tau^\gamma \Psi_1 \neq 0, \quad B_\tau^\gamma \Psi_2 = 0. \tag{32}$$

Furthermore, we can write the function $\vec{\tau} \cdot \hat{\mathbf{V}}_0 \tilde{\Psi} = V_1 + V_2$ as superposition of a $2m$ component function V_1 and an n component function V_2 belonging to the same subspaces as the functions Ψ_1 and Ψ_2, respectively, i.e., $(\Psi_1, V_2) = (\Psi_2, V_1) = 0$. Note that Ψ_2 is absent $(n = 0)$ in the two band model; Ψ_1 is the total slowly varying envelope function and $V_1 = \hat{V}_0 \Psi_1$ [$\hat{V}_0$ is the diagonal part of the velocity operator in Eq. (22)]. However, the functions V_1 and V_2 do not coincide with $\vec{\tau} \cdot \hat{\mathbf{V}}_0 \Psi_1$ and $\vec{\tau} \cdot \hat{\mathbf{V}}_0 \Psi_2$, respectively, for the general case $n \neq 0$. The flux density continuity of Eq. (15) can now be written as

$$J_\tau^{\alpha\beta} = J_{\tau,1}^{\alpha\beta} + J_{\tau,2}^{\alpha\beta} = \text{const}, \tag{33}$$

$$J_{\tau,1}^{\alpha\beta} = \frac{1}{\gamma}(\Psi_{1\alpha}, B_\tau^\gamma \Psi_{1\beta}) + \frac{1}{2}[(\Psi_{1\alpha}, V_{1\beta}) + (V_{1\alpha}, \Psi_{1\beta})], \tag{34}$$

$$J_{\tau,2}^{\alpha\beta} = \frac{1}{2}[(\Psi_{2\alpha}, V_{2\beta}) + (V_{2\alpha}, \Psi_{2\beta})]. \tag{35}$$

Neglecting terms of second order in γ, Eq. (34) can be expressed

$$\tilde{J}_{\tau,1}^{\alpha\beta} = \frac{1}{\gamma}(\tilde{\Psi}_{1\alpha}, B_\tau^\gamma \tilde{\Psi}_{1\beta}), \quad \tilde{\Psi}_1 = \Psi_1 + \frac{\gamma}{2} B_\tau^{\gamma-1} V_1, \tag{36}$$

where V_1 is, to this order, included in $\tilde{\Psi}_1$. Equations (34) and Eq. (36) are the multiband extension of Eqs. (26) and (27) obtained for the two band model. The vector $\{\tilde{\Psi}_1,\Psi_2,V_2\}$ has in total $2m+2n=2(N-m)$ independent components and the general boundary condition satisfying $J_\tau^{\alpha\beta}\approx\tilde{J}_\tau^{\alpha\beta}=\tilde{J}_{\tau,1}^{\alpha\beta}+J_{\tau,2}^{\alpha\beta}=\text{const}$ can be written as

$$\begin{pmatrix}\tilde{\Psi}_1^+\\ \Psi_2^+\\ iV_2^+\end{pmatrix}=T_{2(N-m)}\begin{pmatrix}\tilde{\Psi}_1^-\\ \Psi_2^-\\ iV_2^-\end{pmatrix},\quad T_{2(N-m)}=\begin{pmatrix}T_{2m} & T_{12}\\ T_{21} & T_{2n}\end{pmatrix}. \tag{37}$$

We shall neglect the off diagonal matrices, i.e., set $T_{12}=T_{21}=0$ (thus satisfying the stronger condition that both $\tilde{J}_1^{\alpha\beta}=\text{const}$ and $J_2^{\alpha\beta}=\text{const}$) and obtain the following restrictions on the elements of the energy independent transfer matrices T_{2m} and T_{2n}:

$$T_{2m}^\dagger\frac{1}{\gamma}B_\tau^\gamma\Big|_{\mathbf{s}_j+0}T_{2m}=\frac{1}{\gamma}B_\tau^\gamma\Big|_{\mathbf{s}_j-0},$$

$$T_{2n}^\dagger\begin{pmatrix}0 & I_{2n}\\ -I_{2n} & 0\end{pmatrix}T_{2n}=\begin{pmatrix}0 & I_{2n}\\ -I_{2n} & 0\end{pmatrix}. \tag{38}$$

Equations (37) and (38) represent $2(N-m)$ boundary condition equation for the truncated envelope wave function. These general BC do not allow the continuity of all envelope function components at the interface if B_τ^γ/γ is not continues. While the elements of T_{2m} and T_{2n} are state independent, the function $\tilde{\Psi}_1$ may be related to Ψ_1 by the energy dependent expression.

This procedure can be directly applied to heterostructures described by the 8×8 Pidgeon and Brown Hamiltonian.[38] The bulk energy dispersion equations for this Hamiltonian has eight solutions k_i^2 (taking spin degeneracy into account), for each energy ε; two of these are spurious, and proportional to the large interband Kane matrix element P (see, for example, Ref. 11). In the case of zero spin-orbit interaction, Ψ_1 must include coupled electron and light hole band envelope functions, while Ψ_2 includes the heavy hole band envelope functions only. For planar heterostructures Eqs. (37),(38) take into account the mixing of light and heavy holes for the states with finite in-plane momentum. However they neglect the effect of the ''low interface symmetry''[7] that mixes light and heavy hole plane waves normally incident on the interface (because we assume that $T_{12}=T_{21}=0$). The detailed application of our procedure to the 8×8 models for planar and spherical heterostructures will be presented elsewhere.

IV. ONE-DIMENSIONAL QUANTUM WELL WITH INFINITE POTENTIAL BARRIERS

Let us consider an effect of the general BC on the energy spectrum of a one-dimensional quantum well having infinite potential barriers. The conventional BC for structures with an impenetrable barrier require vanishing of the envelope wave function at the barrier surface, but this requirement has never been justified (see, for example, Ref. 39). In general, the self-adjointness of the MEMA Hamiltonian requires vanishing of the normal flux density at the boundaries

$$J_\tau^{\alpha\beta}(z=\pm L\mp0)=0, \tag{39}$$

where $2L$ is the thickness of the quantum well. If we assume that the two interfaces are completely identical, the quantum well possesses reflection symmetry about $z=0$ and all solutions of the Schrödinger equation are characterized by their parity according to whether their components are even or odd under reflection. However, the BC are local characteristics of each interface. Therefore, the Eq. (39) must be fulfilled at each interface independent of the symmetry of the functions Ψ_α and Ψ_β.

Now we consider the effect of the general BC for the case of the two band Kane model. In order to satisfy Eq. (39) in a quantum well with symmetric interfaces, one can write the general BC for the conduction Ψ_c and valence band Ψ_v components of the envelope wave function (which do not contain spurious solutions) as

$$\Psi_c(\pm L\mp0)\left(1-\alpha_v\frac{\varepsilon-E_c}{E_p}\right)=\mp\Theta\Psi_v(\pm L\mp0)\left(1+\alpha_c\frac{\varepsilon-E_v}{E_p}\right), \tag{40}$$

where Θ is a real number and the sign difference is due to the opposite parity of the conduction and valence band components of the envelope functions. The surface parameter Θ does not depend on the energy or symmetry of either state. Equation (40) can be derived directly from the general BC of Eq. (28) obtained in Sec. III for the case of a finite potential barrier. To do this one has to assume that $\Psi\equiv0$ outside the quantum well and use the state independent transfer matrices $\tilde{T}_{tr}^+$, for $z=L-0$, and $\tilde{T}_{tr}^-$, for $z=-L+0$ interfaces, which differ only by the sign (opposite) of the offdiagonal matrix elements and satisfy the condition $\det[\tilde{T}_{tr}^+]=\det[\tilde{T}_{tr}^-]=0$.

Neglecting $\gamma^2\sim(a_0/L)^2$ terms, Eq. (40) can be written as two separate equations for the conduction and valence band components, respectively,

$$\Psi_c(\pm L\mp0)=\pm T_c a_0\frac{m_0}{m_c(E_e)}\Psi_c'(\pm L\mp0),\quad T_c a_0=\Theta\frac{\hbar}{2P}, \tag{41}$$

$$\Psi_v(\pm L\mp0)=\pm T_v a_0\frac{m_0}{m_v(E_h)}\Psi_v'(\pm L\mp0),$$

$$T_v a_0=\frac{1}{\Theta}\frac{\hbar}{2P}. \tag{42}$$

Here the energy-dependent effective masses in the conduction and valence bands are given by

$$\frac{m_0}{m_c(E_e)}=\alpha_c+\frac{E_p}{E_e+E_g},\quad \frac{m_0}{m_v(E_h)}=\alpha_v+\frac{E_p}{E_h+E_g}, \tag{43}$$

where the electron, E_e, and hole E_h energies are measured from the bottom of conduction and the top of the valence bands, respectively: $E_e=\varepsilon-E_c$ and $E_h=E_v-\varepsilon$. The even, $(+)$, and odd, $(-)$, solutions to Eqs. (38),(39) can be written

$$\Psi^{+}_{c(v)}(z)=A_{c(v)}\cos(\phi^{+}_{c(v)}z), \quad \Psi^{-}_{c(v)}(z)=A_{c(v)}\sin(\phi^{-}_{c(v)}z), \tag{44}$$

where $A_{c,v}$ are the normalization constants. We can derive equations for the energies of the even and odd electron and hole quantum size levels:

$$E_e^{\pm}=\frac{\hbar^2(\phi_c^{\pm})^2}{2m_0L^2}\frac{m_0}{m_c(E_e^{\pm})}\left(1-\alpha_v\frac{E_e^{\pm}}{E_p}\right),$$

$$E_h^{\pm}=\frac{\hbar^2(\phi_v^{\pm})^2}{2m_0L^2}\frac{m_0}{m_v(E_h^{\pm})}\left(1-\alpha_c\frac{E_h^{\pm}}{E_p}\right), \tag{45}$$

where $\phi_c^{\pm}$ and $\phi_v^{\pm}$ are the solutions of the equations

$$\phi_c^{\pm}[\tan(\phi_c^{\pm})]^{\pm 1}=\mp\frac{m_c(E_e^{\pm})}{m_0}\frac{L}{T_ca_0},$$

$$\phi_v^{\pm}[\tan(\phi_v^{\pm})]^{\pm 1}=\mp\frac{m_v(E_h^{\pm})}{m_0}\frac{L}{T_va_0}. \tag{46}$$

Figure 1 shows the dependence of the two lowest quantum size electron levels E_e^{+} and E_e^{-} on the well width L as a function of the surface parameter T_ca_0. In these calculations we use for m_c the electron effective mass at the bottom of the conduction band $m_c=0.1m_0$, and a band gap energy $E_g=1.7$ eV which are close to the parameters of CdSe and CdTe. We compare the effect of the general BC on the quantum size levels in the parabolic EMA [Fig. 1(a)], in the ''pure'' Kane model with $\alpha_c=\alpha_v=0$ [Fig. 1(b)], and in the ''full'' two band model with $\alpha_c\alpha_v\neq 0$ [Fig. 1(c)].

Equations (45),(46) describe the energy of the quantum size levels for coupled conduction and valence bands. However, the conduction and valence band energy spectra can be considered as being independent when the energies of the electron or hole levels are much less than the energy gap $|E_e|,|E_h|\ll E_g,E_p$. This limit case is realized in thick quantum wells and is described by the equations for the simple parabolic bands that one obtains by neglecting the energy dependence of the effective masses and the $E_{e,h}/E_p$ terms in Eqs. (45),(46). For this case the surface parameters T_ca_0 and T_va_0 can be chosen independently, and the conventional BC $\Psi_c(\pm L)=0$ are realized for $T_ca_0=0$. Figure 1(a) shows the effect of $T_ca_0\neq 0$ on the electron quantum size levels in the parabolic EMA. One sees that positive and negative values of T_ca_0 shift the quantum size levels energy up and down, respectively, from those obtained using conventional BC. The effect is negligible when $|T_ca_0|/L\ll\phi_c^{\pm}\,m_0/m_c$ but become noticeable in narrow wells and is greater for higher energy levels.

Figure 1(b) shows the effect of the general BC on the electron quantum size levels in the pure Kane model. One sees that the effect of $T_ca_0\neq 0$ is very similar to that in the parabolic EMA. The size dependence differs only in the nature of the nonlinear dependence on $1/L^2$. This is because the Kane model takes the nonparabolicity of the conduction band into account.

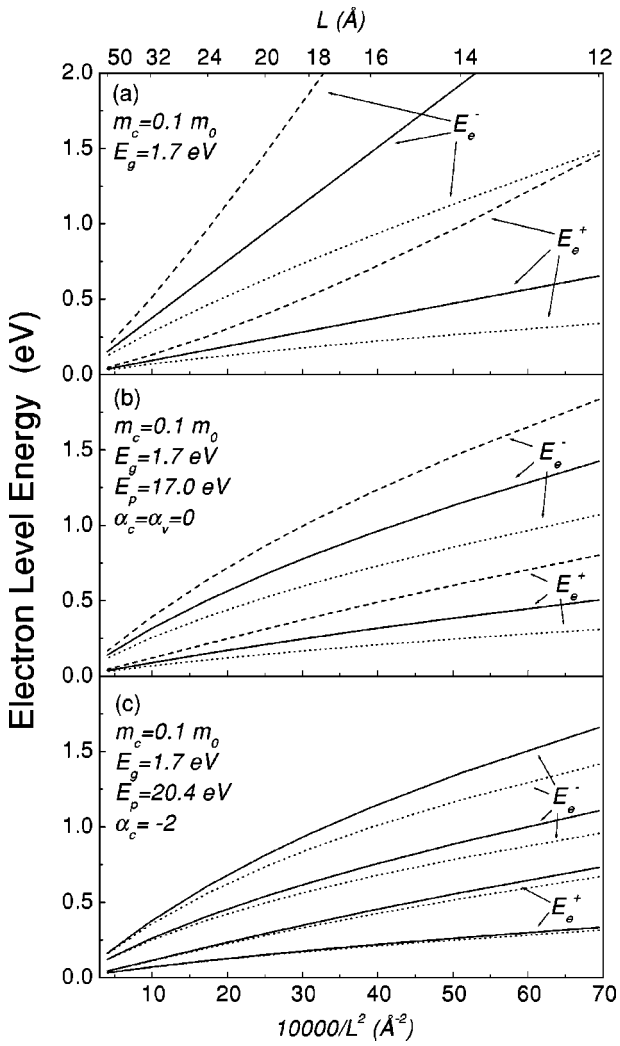

FIG. 1. The size dependence of the two lowest, even (E_e^{+}) and odd (E_e^{-}), electron quantum size levels in a well with infinite potential barriers calculated as a function of the surface parameter Ta_0: (a) in the parabolic EMA model; (b) in the pure Kane model ($\alpha_c=\alpha_v=0$); (c) in the full two band model ($\alpha_c\alpha_v\neq 0$). In (a) and (b), the solid, dashed, and dotted curves correspond to $Ta_0=0$, $Ta_0=0.5$ and $Ta_0=-0.5$ Å, respectively. In (c) the solid and dotted curves are calculated with $\alpha_v=-2$ and $\alpha_v=2$, respectively, upper curves for each level correspond to $Ta_0=0.43$ Å and lower curves to $Ta_0=-0.43$ Å. Other parameters used in calculations are shown in the figure.

The size dependence of the electron levels calculated with $T_ca_0=0$ is shown in Fig. 1(b) only for comparison. The conventional BC do not hold in the Kane model, because the surface parameters for coupled conduction and valence bands are related by $(T_ca_0)(T_va_0)=\hbar^2/2E_pm_0$. Choosing $T_ca_0=0$ for determining the electron energy levels corresponds to choosing $T_va_0\to\infty$, which does not describe the hole energy levels. The condition $|T_ca_0|=|T_va_0|=a^*$ realized for $|\Theta|=1$, describes a symmetric (relative to the center

of the band gap) structure of the electron and hole quantum size levels in semiconductors with $\alpha_c=\alpha_v$. Although these "symmetric semiconductor structures" do not exist in nature, the parameter $a^*=\hbar/2P\approx 0.45\pm 0.06$ Å gives a reasonable value of $|T_c a_0|$ and $|T_v a_0|$ in real semiconductor structures. If symmetric BC hold

$$\phi_c^{\pm}\frac{m_0}{m_c(E_e)}\frac{a^*}{L}\ll 1, \qquad \phi_v^{\pm}\frac{m_0}{m_v(E_h)}\frac{a^*}{L}\ll 1, \tag{47}$$

and the solutions of Eq. (46) for the lowest electron and hole quantum size levels, $\phi_{c,v}^{\pm}$, are close to those given by $T_{c,v}a_0=0$.

Figure 1(c) shows the size dependence of the electron levels calculated in the full two band model with the symmetric surface parameter $|Ta_0|=a^*=0.43$ Å. One can see that the term linear in α_v in Eq. (45) for the electron energy levels becomes important when they comparable with the band gap energy. On the other hand changing the sign of α_v leads only to small changes of the level energy.

The dependence of the lowest electron quantum size levels on the surface parameter $T_c a_0$ for the Kane and full two band models for wells with $L=30$ and 12 Å, respectively, is shown in Fig. 2. The surface parameter is varied from -3.0 to 3.0 Å for $L=30$ Å, and from -1.2 to 1.2 Å for $L=12$ Å, respectively, so that $|T_c a_0|\leqslant Lm_c/m_0$ is fulfilled. One can see that varying the surface parameter in this range produces a monotonic change of the first even and odd electron levels. The difference between models with different α_c and α_v (for the same m_c) is small for $L=30$ Å, but can be important for $L=12$ Å.

It is interesting to note that for positive values of the surface parameter Θ ($T_c a_0>0, T_v a_0>0$), Eqs. (45),(46) may have even and odd solutions with an energy in the forbidden gap $E_e<0, E_h<0$. In wide wells the energy of these gap levels do not depend on their symmetry $E^{+}_{(e,h),S}=E^{-}_{(e,h),S}=E_{(e,h),S}$ and can be found from

$$E_{e,S}=-\frac{\hbar^2}{2m_0}\frac{m_c(E_{e,S})}{m_0}\frac{1}{(T_c a_0)^2}\cdot\left(1-\alpha_v\frac{E_{e,S}}{E_p}\right), \tag{48}$$

$$E_{h,S}=-\frac{\hbar^2}{2m_0}\frac{m_v(E_{h,S})}{m_0}\frac{1}{(T_v a_0)^2}\cdot\left(1-\alpha_c\frac{E_{h,S}}{E_p}\right). \tag{49}$$

In wide "symmetric wells" these gap states have the same energy $E_{e,S}=E_{h,S}=-E_g/2$, and are localized within a layer of thickness $a_s=2a^*E_p/E_g$ near the surface. These solutions contain no contributions from the unphysical spurious solutions, and thus are not artifacts of the **k·p** model.

V. DISCUSSION AND COMPARISON WITH OTHER APPROACHES

The occurrence of discontinuities in the envelope wave functions at the heterointerface is one of the most important consequences of general BC. These discontinuities have a strong effect on the mathematical procedures often used for the calculation of various physical properties of heterostructures having finite potential barriers. In these procedures, the

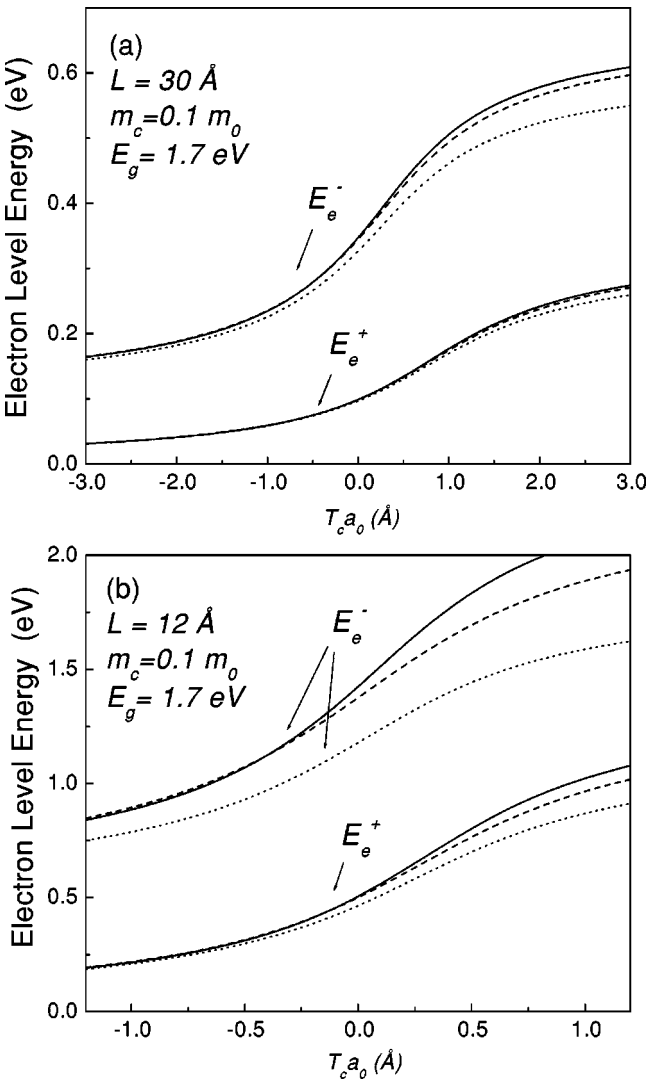

FIG. 2. The dependence of the two lowest , even (E_e^+) and odd (E_e^-), electron quantum size levels on the surface parameter $T_c a_0$ calculated in a well of width $2L$ surrounded by infinite potential barriers: (a) $L=30$ Å and (b) $L=12$ Å. The solid line is for the pure Kane model with $\alpha_c=\alpha_v=0$ and $E_p=17.0$ eV, the dashed line is for the symmetric two band model with $\alpha_c=\alpha_v=-2$ and $E_p=20.4$ eV, and the dotted line for the asymmetric two band model with $\alpha_c=-2$, $\alpha_v=2$, and $E_p=20.4$ eV. Other parameters used in the calculations are shown in the figure.

Schrödinger equation is integrated across the interface or a Fourier transformation is performed using the piece-wise spatially determined material parameters with the help of generalized step functions. However, the integration of terms such as products of $(1/m)\hat{k}_z^2$ or $P\hat{k}_z$ with envelope wave functions Ψ which are discontinuous across an interface may lead to mathematical uncertainties: integration of the product of a step function and a δ function is not well defined. To resolve this problem, a nonunique[40,30,16,17] symmetrized form of the kinetic energy operator $\hat{H}_k$ is used, and the BC for the envelope function Ψ are obtained by requiring that $\hat{H}_k\Psi$ be integrable across the interface.[40,24]

For example, in order to obtain the general BC of Eq. (4)

for parabolic bands, symmetrized kinetic energy operator of the form[40]

$$\hat{H}_K^{\alpha} = -\frac{\hbar^2}{2} m^{\alpha} \frac{d}{dz} \frac{1}{m^{1+2\alpha}} \frac{d}{dz} m^{\alpha} \tag{50}$$

is used. The case $\alpha=0$ then leads to the conventional BC of Eq. (2). The same symmetrized form $\hat{k}_z(1/m)\hat{k}_z$ is usually used for the diagonal terms of the multiband kinetic energy operator.[24,30] To derive the BC of Eq. (29) for the ''pure'' two band Kane model ($\alpha_c=\alpha_v=0$) that allow to integrate Schrödinger equation across the interface, one writes the kinetic energy operator as:

$$\hat{H}_K^{\alpha} = \frac{i\hbar}{m_0} \begin{pmatrix} 0 & P^{\alpha}\hat{k}_z P^{1-\alpha} \\ -P^{1-\alpha}\hat{k}_z P^{\alpha} & 0 \end{pmatrix}. \tag{51}$$

Here, now, there is no value of α that gives the symmetrized form $1/2(\hat{k}_z P + P\hat{k}_z)$, that is usually used for the off diagonal terms (linear in k) of the multiband Hamiltonian.[24,30] An asymmetric ordering, corresponding to $\alpha=1$ was suggested in Ref. 33 for the model with $\alpha_c=0$. The α dependence of Eqs. (50) and (51) clearly demonstrates that it is the BC that determine the integration across the abrupt heterointerface and not the other way round.

Fourier transforming the Schrödinger equation has been suggested by Winkler and Rössler[30] as an alternative approach to the MEMA problem for heterostructures with finite potential barriers. Then one does not deal explicitly with BC when solving the resulting integral equations for the momentum space envelope function, and avoids unphysical spurious solutions by restricting the range of integration to $|k| \ll 2\pi/a_0$. However, the resulting form of the momentum space MEMA Hamiltonian depends on the particular symmetrization procedure chosen for the kinetic energy operator in configuration space,[30] and, therefore, is again determined by the BC imposed on the envelope function. To illustrate this, we derive the explicit form of the momentum space Schrödinger equation for the one band EMA and the two band ''pure'' Kane model, using general BC. Fourier integration of the EMA Schrödinger equation with the kinetic energy operator of Eq. (50) leads to the following integral equation for the momentum space envelope function $F(k)$:

$$\frac{\hbar^2}{2}\int_{-\infty}^{\infty} q'k' M_{-\alpha}(k-q') M_{1+2\alpha}(q'-k') M_{-\alpha}(k'-q) F(q) \times dq'dk'\,dq + \int_{-\infty}^{\infty} F(q) V_c(k-q)dq = \varepsilon F(k), \tag{52}$$

where $F(k)$ satisfies the normalization condition $\int_{-\infty}^{\infty}|F(k)|^2 dk=1$ and

$$V_c(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} E_c(z)\exp(-ikz)dz,$$

$$M_{\nu}(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{1}{m^{\nu}(z)}\exp(-ikz)dz. \tag{53}$$

Here $E_c(z)$ and $m(z)$ are the energy of the bottom of the conduction band and the electron effective mass in each region of the one-dimensional heterostructure considered. The configuration space envelope function, in the jth region of the heterostructure, is now given by

$$f^j(z) = m_j^{-\alpha}\cdot\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F(q) M_{-\alpha}(k-q)\exp(ikz)dkdq, \tag{54}$$

and satisfies the general BC of Eq. (4). For the ''pure'' Kane model, Fourier transforming the Schrödinger equation, using the kinetic energy operator of Eq. (51), leads to the following coupled integral equations for the two component momentum space function $\{F_c(k),F_v(k)\}$:

$$\int_{-\infty}^{\infty} F_c(q)V_c(k-q)dq + i\frac{\hbar}{m_0}\int_{-\infty}^{\infty} q' G_{\alpha}(k-q') \times G_{1-\alpha}(q'-q)F_v(q)dqdq' = \varepsilon F_c(k), \tag{55}$$

$$-i\frac{\hbar}{m_0}\int_{-\infty}^{\infty} q' G_{1-\alpha}(k-q')G_{\alpha}(q'-q)F_c(q)dqdq' + \int_{-\infty}^{\infty} F_v(q)V_v(k-q)dq = \varepsilon F_v(k), \tag{56}$$

where $\int_{-\infty}^{\infty}(|F_c(k)|^2+|F_v(k)|^2)dk=1$ and

$$V_{c,v}(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} E_{c,v}(z)\exp(-ikz)dz,$$

$$G_{\nu}(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} P^{\nu}(z)\exp(-ikz)dz. \tag{57}$$

Here $E_v(z)$ and $P(z)$ are the energy of the top of the valence band and the Kane matrix element in each region, respectively. The configuration space envelope function $\Psi=\{\Psi_c,\Psi_v\}$ in the jth region of the one-dimensional heterostructure is now given by

$$\Psi_c^j(z) = P_j^{-\alpha}\cdot\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F_c(q) G_{\alpha}(k-q)\exp(ikz)dkdq, \tag{58}$$

$$\Psi_v^j(z) = P_j^{\alpha-1}\cdot\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} F_v(q) G_{1-\alpha}(k-q)\exp(ikz)dkdq, \tag{59}$$

and will satisfy the general BC of Eq. (29) with $\alpha_c=\alpha_v=0$.

General BC, for heterostructures described by the MEMA Hamiltonian, that conserve the normal component of the envelope flux density J_{τ} have been suggested by Kisin *et al.*[11] We have shown that the general requirement that the heterostructure MEMA Hamiltonian be self-adjoint leads to the more general condition $J_{\tau}^{\alpha\beta}=\text{const}$. That is, that J_{τ} must be continuous for arbitrary chosen envelope functions $\Psi_{\alpha},\Psi_{\beta}$. This generalization to $\alpha\neq\beta$ is important, because it

shows that the components of the transfer matrix connecting the components of the envelope function Ψ and envelope normal velocity V_τ on the two sides of the interface, are state independent and are characteristic properties of the interface, not the states. This is not true for a transfer matrix which connects the components of Ψ and its derivatives Ψ' (see Ref. 11), because the relationship between the components of V_τ and Ψ, Ψ', on the same side of the interface, in the multiband model may depend on the symmetry (the value of the interface parallel momentum in planar heterostructures[11] and the total orbital angular momentum and parity in spherical dots[36]) or on the energy of the state.

An explicit treatment of ''interface'' effects can be seen in several **k·p** models of heterostructures that consider exact electron wave functions in the interface region.[8,9,41–44] Some of these models result in equations in addition to the bulk **k·p** equations that describe the interface.[43,44] The parameters of these ''interface'' Hamiltonians must be determined from microscopic wave functions or obtained from the comparison with experiment. However, these advanced models are generally much more complicated than the MEMA, completed by an appropriate choice of boundary conditions, which has already successfully described such interface effects as the Γ-X intervalley mixing in GaAs/AlAs heterostructures,[5,6] the heavy-light hole plane wave mixing at zinc blende interfaces under normal incidence[7] and the effect on the interband light absorption of the intervalley conversion of the electron at the surface of indirect-band-gap semiconductors.[45]

Heterostructures with abrupt heterointeface ($L \gg a$) are described by the MEMA models using energy independent transfer matrices which characterize the effects of the interfaces on the carrier wave functions within some energy interval. The energy of the state considered should be within the range of validity of the chosen bulk MEMA Hamiltonian in each layer. This means, that the energy should be smaller than the distance to the energy band extrema not explicitly included in the multiband model. In the appropriate energy interval, the elements of the transfer matrices can be treated as energy independent trial parameters in fitting the experimental data.

The number of independent transfer matrices required to ensure the flux continuity of Eq. (15), is determined by the number of physically nonequivalent interfaces of the heterostructure. Therefore, to write general BC, one must model the symmetry of the interface, i.e., the interface geometry and the symmetry of the material properties on the interface. On the other hand, this is true for any explicit determination of the full microscopic wave function near the interface.

In conclusion, we have derived a general form of state-independent BC for multicomponent envelope functions that are valid under the same conditions as the MEMA itself. Spurious components of the wave functions are eliminated by requiring that the envelope flux density be determined to the same order of approximation as the MEMA itself. The effect of the general BC on the electron and hole energy spectra has been demonstrated in the two band model for a potential well with infinite potential barriers. This procedure, using the general BC for truncated envelope wave functions, can be applied to any MEMA model containing any type of spurious solution and to heterostructures with finite or infinite potential barriers.

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[1] L. R. Ram-Mohan, D. Dossa, I. Vurgaftman, and J. R. Meyer, in *Handbook of Nanostructured Materials and Nanotechnolgy*, edited by H. S. Nalwa (Academic Press, New York, 1998), Chap. 109.

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

[3] E. I. Ivchenko and G. E. Pikus, *Superlattices and Other Heterostucture* (Springer, Berlin, 1995).

[4] W. Mönch, *Semiconductor Surfaces and Interfaces* (Springer, Berlin, 1995).

[5] T. Ando and H. Akera, Phys. Rev. B **40**, 11 619 (1989).

[6] Y. Fu, M. Willander, E.L. Ivchenko, and A.A. Kiselev, Phys. Rev. B **47**, 13 498 (1993).

[7] E.L. Ivchenko, A.Yu. Kaminski, and U. Rössler, Phys. Rev. B **54**, 5852 (1996).

[8] B.A. Foreman, Phys. Rev. Lett. **81**, 425 (1998).

[9] G.T. Einevoll and L.J. Sham, Phys. Rev. B **49**, 10 533 (1994).

[10] B. Laikhtman, Phys. Rev. B **46**, 4769 (1992).

[11] M.V. Kisin, B.L. Gelmont, and S. Luryi, Phys. Rev. B **58**, 4605 (1998).

[12] J.W. Conley, C.B. Duke, G.D. Mahan, and J.J. Tiemann, Phys. Rev. **150**, 466 (1966).

[13] D.J. Ben Daniel and C.B. Duke, Phys. Rev. **152**, 683 (1966).

[14] T. Ando and S. Mori, Surf. Sci. **113**, 124 (1982).

[15] T. Ando, S. Wakahara, and H. Akera, Phys. Rev. B **40**, 11 609 (1989).

[16] R. Balian, D. Bessis, and G.A. Mezincescu, Phys. Rev. B **51**, 17 624 (1995).

[17] M.-E. Pistol, Phys. Rev. B **60**, 14 269 (1999).

[18] M. Reed and B. Simon, *Methods of Modern Mathematical Physics* (Academic Press, New York, 1980), Vol. I: Functional Analysis, Sec. VIII.2.

[19] W.A. Harrison, Phys. Rev. **123**, 85 (1961).

[20] Q.-G. Zhu and H. Kroemer, Phys. Rev. B **27**, 3519 (1983).

[21] W. Trzeciakowski, Semicond. Sci. Technol. **10**, 768 (1995).

[22] G. Bastard, Phys. Rev. B **24**, 5693 (1981); **25**, 7584 (1982).

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

[24] G.A. Baraff and D. Gershoni, Phys. Rev. B **43**, 4011 (1991).

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

[26] M.F.H. Schuurmans and G.W. 't Hooft, Phys. Rev. B **31**, 8041 (1985).

[27] W. Trzeciakowski, Phys. Rev. B **38**, 12 493 (1988).

[28] M.J. Godfrey and A.M. Malik, Phys. Rev. B **53**, 16 504 (1996).
[29] L.-W. Wang, Phys. Rev. B **61**, 7241 (2000).
[30] R. Winkler and U. Rössler, Phys. Rev. B **48**, 8918 (1993).
[31] A.T. Meney, B. Gonul, and E.P. O'Reilly, Phys. Rev. B **50**, 10 893 (1994).
[32] R. Eppenga, M.F.H. Schuurmans, and S. Colak, Phys. Rev. B **36**, 1554 (1987).
[33] B.A. Foreman, Phys. Rev. B **56**, R12 748 (1997).
[34] A. Peres, *Quantum Theory: Concepts and Methods* (Kluwer Academic, Dordrecht, 1995), Ch. 4, pp. 86–88.
[35] P.C. Sercel and K.J. Vahala, Phys. Rev. B **42**, 3690 (1990).
[36] P.C. Sercel, Al.L. Efros, and M. Rosen, Phys. Rev. Lett. **83**, 2394 (1999).
[37] The case, where other small parameters are built into some elements of the tensor $D_{\mu\nu}$ may be treated in a similar way.
[38] C.R. Pidgeon and R.N. Brown, Phys. Rev. **146**, 575 (1966).
[39] L.S. Braginsky, Phys. Rev. B **60**, R13 970 (1999).
[40] R.A. Morrow and K.R. Brownstein, Phys. Rev. B **30**, 678 (1984).
[41] D.L. Smith and C. Mailhiot, Phys. Rev. B **33**, 8345 (1986).
[42] C. Aversa and J.E. Sipe, Phys. Rev. B **49**, 14 542 (1994).
[43] M.G. Burt, Phys. Rev. B **50**, 7518 (1994).
[44] B.A. Foreman, Phys. Rev. B **54**, 1909 (1996).
[45] L.S. Braginsky, Phys. Rev. B **57**, R6870 (1998).