

Boundary-condition problem in the Kane model

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The boundary conditions for a multicomponent effective wave function are obtained in the eight-band Kane model. The relations are established between boundary-condition matrix elements and the Kane Hamiltonian parameters in constitutive semiconductors. In general, these relations are incompatible with component-by-component continuity of the effective wave function, traditionally employed in multiband models. We show that the boundary conditions in the isotropic eight-band Kane model involve three linearly independent phenomenological parameters. Neglecting the spin-orbit interaction at the heterointerface, only two parameters are required to completely describe the matching conditions. These parameters do not depend on the energy of the charge carrier state, hence the nonparabolic regime is described in the most natural way. The boundary condition matrices are derived also for the most important approximate limits: the six-band Kane model, describing the energy spectrum of narrow-gap semiconductors, and the four-band Luttinger model, describing the valence-band top energy region in zinc-blende and diamondlike semiconductors.

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I. INTRODUCTION

In multiband effective mass theory an electric charge carrier state can be represented phenomenologically by a column of smoothly varying functions, $\Psi = \{\psi_n\}$, conventionally referred to as envelope functions. The number of these functions equals the number of energy bands explicitly considered in the model. In a homogeneous crystal, such a multicomponent wave function satisfies the Schrödinger equation with an effective matrix Hamiltonian \hat{H} . The general form of the effective Hamiltonian can be obtained by symmetry considerations alone,¹⁻³ while the values of the phenomenological parameters used in the Hamiltonian are determined primarily by the microscopic structure of the crystal. In the presence of an abrupt heterointerface it seems to be possible to also separate the *mesoscopic*, or quasiparticle, description of the charge carrier state (on the spatial scale of the quasiparticle de Broglie wavelength) from the *microscopic* description (on the characteristic scale of a lattice constant). Below we consider an abrupt heterointerface $z = 0$ between semiconductors *A* and *B*. The phenomenological description of an arbitrary mesoscopic state in the bulk of constitutive semiconductors by means of an effective Schrödinger equation should be accomplished with appropriate boundary conditions providing the matching procedure between the *A* and *B* parts of the effective wave function Ψ . Since the effective Hamiltonian is supposed to include terms quadratic in the momentum operator $\mathbf{p} = -i\hbar\nabla$, the required boundary conditions are of the form

$$\begin{pmatrix} \Psi_A \\ \Psi'_A \end{pmatrix}_{z=-0} = T_{AB} \begin{pmatrix} \Psi_B \\ \Psi'_B \end{pmatrix}_{z=+0}; \quad (1)$$

$$T_{AB} = \begin{pmatrix} \hat{F} & \hat{S} \\ \hat{R} & \hat{G} \end{pmatrix}; \quad \Psi = \begin{pmatrix} \psi_0 \\ \vdots \\ \psi_n \end{pmatrix}; \quad \Psi' = \frac{\partial \Psi}{\partial z}.$$

Boundary conditions for the effective wave function cannot be obtained by integrating the field equations across the interface, since the phenomenological equations of the effective mass theory are valid neither at the heterointerface nor inside any hypothetical transition layer.⁴ Nevertheless, the integration procedure is often used in multiband models that assume the continuity of wave-function envelopes, resulting in boundary conditions of the following type:⁵⁻⁷

$$\Psi_A = \Psi_B; \quad \hat{j}_z \Psi_A = \hat{j}_z \Psi_B; \quad \hat{j}_z = \frac{\partial \hat{H}}{\partial p_z}. \quad (2)$$

Here \hat{j}_z is the *z* component of an effective current operator. The assumption $\hat{F} = 1$, used in the latter form of boundary conditions, is not generally justified. It has been argued for a long time that more complete form of boundary conditions should be used, which includes some inherent parameters of the heterointerface.⁸⁻¹⁶ The most general boundary conditions of this kind consistent with the effective-mass approximation were suggested by Ando *et al.*,¹² and in this paper we extend their method to eight-band Kane model,² which is widely used for the description of electron energy spectra of direct-band-gap A_3B_5 and A_2B_6 semiconductor heterostructures. Boundary conditions in the general form (1) have not been obtained yet for this model, thus the simplified heuristic form (2) is still in use even for very subtle problems.^{17,18}

In this paper we follow the traditional effective-mass scheme and construct the effective quasiparticle wave function piecewise in the different materials, rather than use a more sophisticated technique developed recently by Burt,¹³ which requires some modifications of the Hamiltonian. No modification of the effective Hamiltonian is assumed in our approach, so we can keep the original eight-band bulk Kane Hamiltonian, which is usually well known for constitutive materials. In the proposed scheme the boundary condition matrix structure is determined only by the reduction of the symmetry group of the effective bulk Hamiltonian due to the presence of an abrupt heterointerface. In this reduced symmetry group the matrix representation of the multicomponent effective wave function also becomes reducible, and wave-function components associated with equivalent irreducible representations mix at the interface, resulting in a nontrivial structure of boundary condition submatrices in Eq. (1). We assume an isotropic bulk quasiparticle energy spectrum, which is a good approximation for most of the cubic A_3B_5 semiconductors. High-symmetry interface perpendicular to four-fold or three-fold axis is assumed between two adjacent crystals. This is equivalent to the reduced symmetry $C_{\infty v}$ of the electron energy spectrum of the heterostructure. Effects, resulting from the reduced symmetry of some particular heterointerfaces, such as the C_{2v} symmetry of a zinc-blende-based $\{001\}$ interface, can be included in our boundary conditions as additive terms.¹⁷ Luttinger model with anisotropic bulk quasiparticle energy spectrum is considered in the last section of the paper.

We show that in the eight-band Kane model the boundary condition set includes only three independent phenomenological parameters and, therefore, the boundary condition matrix, T_{AB} , assumes a rather simple form in a wide variety of applications. These parameters, being determined by the microscopic structure of the heterointerface, do not depend explicitly on the quasiparticle energy, thus the nonparabolicity of the energy spectrum can be treated in the most simple and effective way. We show also that in the framework of multiband effective-mass theory the number of boundary conditions implied on the smooth envelope functions does not necessarily equal the number of bands explicitly considered in the model. A simple and unambiguous truncation procedure for boundary conditions is defined in this paper to avoid the problem of spurious solutions.^{19–22} No independent matrix invariant in the effective Hamiltonian has been rejected in our scheme for this purpose in contrast to the last approach.²² Finally, we derive the truncated boundary condition systems for smooth effective wave function in the six-band Kane model,² describing narrow-band semiconductors, and in the four-band Luttinger model,¹ corresponding to the valence-band top energy region.

II. BASIC RELATIONS AND THE KANE MODEL WITHOUT SPIN

The boundary condition problem can be more clearly illustrated if we first consider the simplest isotropic four-band Kane model without spin. This model phenomenologically describes kp mixing between two close groups of basis electron states with opposite parities, $\{u_0\}$ and $\{u_1, u_2, u_3\}$,

(states of s - and p -type symmetry, respectively). The effective wave function of an arbitrary mesoscopic state is represented in this basis by the four-component column Ψ , which consists of scalar U and vector $\bar{\mathbf{V}}$ parts (with allowance for spin, these become, respectively, one even and three odd spinors):

$$\Psi = \begin{pmatrix} U \\ \bar{\mathbf{V}} \end{pmatrix}. \quad (3)$$

The overlined vector quantities will be considered below as three-component columns. Particular representation of the components of these columns depends on the choice of the vector part of the basis function set $\{u_n\}_{n=1,2,3}$. Apparently, the simplest (canonical) form of the boundary condition matrix can be obtained in the basis corresponding to the direct sum of irreducible representations of the reduced symmetry group of the heterostructure energy spectrum. In the presence of an interface, the full spherical group of the isotropic bulk energy spectrum reduces to the axial symmetry group $C_{\infty v}$, thus the canonical basis may be written in the form

$$\{u_n\}_{A,B} = \left\{ S; Z; \frac{X+iY}{\sqrt{2}}; \frac{X-iY}{\sqrt{2}} \right\}_{A,B}; \quad n=0,1,2,3. \quad (4)$$

It is worthy to emphasize that in the proposed phenomenological approach we neither deal with the microscopic wave function of the system nor refer to any particular form of the basis functions u_n of different irreducible representations of the effective Hamiltonian symmetry group. The irreducible representations for explicitly treated bands are supposed to be the same in constitutive semiconductors; however, we make no specific assumptions about the basis functions on each side of the heterointerface (A and B). The vector part of the basis (4) consists of the eigenfunctions of operator J_z corresponding to the z component of the angular momentum $J=1$. First two basis functions, u_0 and u_1 , transform under all symmetry operations $\omega \in C_{\infty v}$ according to the equivalent unit representations. The last pair of functions, u_2 and u_3 , form the basis of a two-dimensional representation. Symmetry considerations³ require the boundary condition submatrices in Eq. (1) to be partitioned into blocks linking only the wave-function components, which transform according to the equivalent representations. All other blocks should vanish identically. As a result, we have

$$\hat{F} = \begin{bmatrix} F_0 & F_{01} & 0 & 0 \\ F_{10} & F_1 & 0 & 0 \\ 0 & 0 & F_2 & F_{23} \\ 0 & 0 & F_{32} & F_3 \end{bmatrix},$$

$$\hat{G} = \begin{bmatrix} G_0 & G_{01} & 0 & 0 \\ G_{10} & G_1 & 0 & 0 \\ 0 & 0 & G_2 & G_{23} \\ 0 & 0 & G_{32} & G_3 \end{bmatrix}, \quad \dots \quad (5)$$

Since all one-dimensional representations in the canonical basis (4) are equivalent, we cannot further elaborate on the structure of the upper left 2×2 blocks in the boundary condition submatrices. On the other hand, the internal structure of the lower right 2×2 blocks is quite severely restricted by symmetry. Let us consider a certain spatial transformation ω from the reduced group $C_{\infty v}$ of the heterostructure energy spectrum. It may be a rotation $\omega_{z\phi}$ of the coordinate system xyz through an angle ϕ about the main symmetry axis z of the heterostructure, or the reflection operation, for certainty, in xz plane, ω_{xz} . The matrix $\hat{\omega}_{mn}$ of the corresponding unitary transformation describes the transition from a basis $\{u_n\}$ to a basis set $\{\tilde{u}_n\}$ in the new coordinate system $\tilde{x}\tilde{y}\tilde{z}$: $u_n = \hat{\omega}_{mn}\tilde{u}_m$. The invariance of the boundary conditions upon a symmetry operation ω means that relation (1), with the same boundary condition matrix, can be applied to the A and B parts of the transformed wave function

$$\tilde{\Psi}(\tilde{\mathbf{r}}) = \omega \Psi(\mathbf{r}) = \hat{\omega} \Psi(\omega^{-1}\tilde{\mathbf{r}}). \quad (6)$$

Let us consider, for instance, the first matrix row in Eq. (1):

$$\begin{aligned} \tilde{\Psi}_A(\tilde{\mathbf{r}}) &= \omega \Psi_A(\mathbf{r}) = \omega [\hat{F}_{AB} \Psi_B(\mathbf{r}) + \hat{S}_{AB} \Psi'_B(\mathbf{r})] \\ &= \hat{\omega} [\hat{F}_{AB} \Psi_B(\omega^{-1}\tilde{\mathbf{r}}) + \hat{S}_{AB} \Psi'_B(\omega^{-1}\tilde{\mathbf{r}})] \\ &= \hat{\omega} \hat{F}_{AB} \hat{\omega}^{-1} \tilde{\Psi}_B(\tilde{\mathbf{r}}) + \hat{\omega} \hat{S}_{AB} \hat{\omega}^{-1} \tilde{\Psi}'_B(\tilde{\mathbf{r}}) \\ &= \hat{F}_{AB} \tilde{\Psi}_B(\tilde{\mathbf{r}}) + \hat{S}_{AB} \tilde{\Psi}'_B(\tilde{\mathbf{r}}). \end{aligned} \quad (7)$$

Therefore, the invariance condition, for example for submatrix \hat{F} , has the form

$$\hat{F} = \hat{\omega} \hat{F} \hat{\omega}^{-1}. \quad (8)$$

The time-reversal operation $\tau \Psi(t) = \hat{\tau} \Psi^*(-t)$ can also be included in the symmetry group of the effective Hamiltonian, leading to

$$\hat{F} = \hat{\tau} \hat{F} \hat{\tau}^{-1}. \quad (9)$$

In basis (4), the transformations $\omega_{z\phi}$, ω_{xz} , and the time-reversal operator, τ , are represented, respectively, by 4×4 matrices

$$\hat{\omega}_{z,\phi} = e^{i\phi \hat{J}_z} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{i\phi} & 0 \\ 0 & 0 & 0 & e^{-i\phi} \end{bmatrix};$$

$$\hat{\omega}_{xz} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}; \quad \hat{\tau} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \mathcal{K}. \quad (10)$$

Here \mathcal{K} is the complex conjugation operator. Note that $\hat{\omega}_{xz}^2 = \hat{\tau}^2 = 1$, as it should be in a spinless model. Substituting Eq. (10) into Eqs. (8) and (9), we readily obtain the following additional restrictions on the matrix elements:

$$F_{23} = F_{32} = 0; \quad F_2 = F_3; \quad F_{mn} = F_{mn}^*. \quad (11)$$

All the restrictions, which have been imposed above on the matrix elements of submatrix \hat{F} , hold true also for the matrix elements of all other boundary condition submatrices.

We can extend this general analysis, considering the structure of spinless Kane model eigenfunctions in greater detail. The free-quasiparticle Hamiltonian includes first- and second-order terms in the momentum operator \mathbf{p} and can be constructed as a superposition of invariants in the form:^{1,3}

$$\hat{H} = E_g \hat{B}_0 + P(\mathbf{p}\hat{\mathbf{A}}) + \gamma_0 p^2 \hat{B}_0 - \gamma_3 p^2 \hat{B}_3 - \gamma_2 (\mathbf{p}\hat{\mathbf{J}})^2. \quad (12)$$

Spherical symmetry is assumed here for the quasiparticle energy spectrum, therefore, only three second-order invariants are included in the Hamiltonian. The structure of the bulk Hamiltonian is similar on both sides of the interface, but at least some of the parameters involved in Eq. (12) are different in the half-crystals A and B . All hatted operators are represented in the four-band model by square 4×4 matrices. The matrices $\hat{B}_0(\hat{B}_3)$ are diagonal unit matrices for scalar (vector) subspaces, revealing the intraband nature of corresponding operators, while the nondiagonal matrix operator $\hat{\mathbf{A}}$ represents the matrix structure of interband kp -mixing, characterized by Kane's velocity P . For the sake of a uniform description of the model, we also introduce square 4×4 matrices \hat{J}_i which have nonzero elements only in the vector subspace, where they coincide with ordinary 3×3 matrices J_i of angular momentum $J = 1$. Operator $\hat{\mathbf{J}}$ plays the part of the quasiparticle spin operator, because it compensates the commutator of the Hamiltonian with the orbital angular momentum operator $\hbar \hat{\mathbf{L}} = (\hat{B}_1 + \hat{B}_3)(\mathbf{r} \times \mathbf{p})$, and guarantees the conservation of the total angular momentum of the quasiparticle $\hat{\mathbf{L}} + \hat{\mathbf{J}}$:

$$[\hat{H}, (\hat{\mathbf{L}} + \hat{\mathbf{J}})]_- = 0; \quad [\hat{H}, \hat{\mathbf{J}}]_- = -[\hat{H}, \hat{\mathbf{L}}]_- = iP(\hat{\mathbf{A}} \times \mathbf{p}). \quad (13)$$

Quasispin $\hat{\mathbf{J}}$ is determined by the microscopic orbital motion of the electron and, hence, is nonrelativistic by nature. Finally, in basis (4) the Hamiltonian (12) is represented by the matrix

$$\hat{H} = \begin{bmatrix} E_g + \gamma_0 p^2 & P p_z & P p_+ & P p_- \\ P p_z & -\gamma_3 p^2 - 2\gamma_2 p_+ p_- & \gamma_2 p_z p_+ & \gamma_2 p_z p_- \\ P p_- & \gamma_2 p_z p_- & -\gamma_3 p^2 - \gamma_2(p_z^2 + p_+ p_-) & \gamma_2 p_-^2 \\ P p_+ & \gamma_2 p_z p_+ & \gamma_2 p_+^2 & -\gamma_3 p^2 - \gamma_2(p_z^2 + p_+ p_-) \end{bmatrix}; \quad p_{\pm} = \frac{1}{\sqrt{2}}(p_x \pm i p_y). \quad (14)$$

It is convenient to classify the bulk eigenfunctions of the Kane model into the ‘‘light’’ and the ‘‘heavy’’ states.²³ Since the spherical symmetry of the free quasiparticle energy spectrum has been assumed, the only distinguished spacial direction is the direction of the quasiparticle momentum \mathbf{k} . Under the rotation of the coordinate system about this direction, all the wave-function components must transform in the same way and get the same phase shift. Two different situation can be considered in spinless model and used to establish the classification scheme. First, there should be two purely vector eigenfunctions with vector parts orthogonal to the vector \mathbf{k} and to each other. Under rotations of the coordinate system about the \mathbf{k} direction, these functions transform into each other, hence in the bulk they relate to a double degenerate band. We shall refer to these eigenfunctions as ‘‘heavy’’ states

$$\Psi_{h1,2} = \begin{pmatrix} 0 \\ \bar{\mathbf{V}}_h \end{pmatrix}_{1,2}; \quad (\mathbf{V}_{h1,2}\mathbf{k})=0; \quad (\mathbf{V}_{h1}\mathbf{V}_{h2})=0. \quad (15)$$

Matrices J_i of angular momentum $J=1$ allow us to express the vector multiplication operation in convenient matrix form $i\mathbf{k} \times \bar{\mathbf{V}} \equiv (\mathbf{k}\mathbf{J})\bar{\mathbf{V}}$, hence a projection operator onto the subspace of two-fold ‘‘heavy’’ states can be readily defined

$$\hat{\Lambda}_h = (\mathbf{m}\hat{\mathbf{J}})^2; \quad \mathbf{m} = \mathbf{k}/k; \quad \hat{\Lambda}_h^2 = \hat{\Lambda}_h; \quad \text{Sp}\hat{\Lambda}_h = 2; \\ \bar{\mathbf{V}}_h = (\mathbf{m}\mathbf{J})^2\bar{\mathbf{V}} = -\overline{\mathbf{m} \times (\mathbf{m} \times \mathbf{V})} = (\bar{\mathbf{V}} - (\mathbf{m}\mathbf{V})\bar{\mathbf{m}})_{\perp} \mathbf{m}. \quad (16)$$

Since the total dispersion equation in four-band Kane model is fourth order in k^2 , then, besides two ‘‘heavy’’ states, there should be two independent ‘‘light’’ states with different values of k^2 . For ‘‘light’’ eigenfunctions consisting of the kp mixture of scalar U and vector \mathbf{V} components, the vector part of the wave function must transform like a scalar under the rotations about the quasiparticle momentum direction, thus for these states one has $\mathbf{V}_i \parallel \mathbf{k}$. Due to relation $(\mathbf{k}\mathbf{J})^2\mathbf{k} \equiv 0$ (or $\hat{\Lambda}_h\Psi_i \equiv 0$), the Schrödinger equation for ‘‘light’’ eigenstates leads to the form

$$\Psi_{l1,2} = \begin{pmatrix} U_l \\ \bar{\mathbf{V}}_l \end{pmatrix}_{1,2}; \quad \bar{\mathbf{V}}_l = \frac{P\bar{\mathbf{k}}_{1,2}}{E + \gamma_3 k^2} U_l, \quad (17)$$

and gives the dispersion equation

$$\det\{(E_g + \gamma_0 k^2 - E)\hat{B}_0 + P(\hat{\mathbf{A}}\mathbf{k}) - (E + \gamma_3 k^2)\hat{B}_3\} \\ = (E + \gamma_3 k^2)(E_g + \gamma_0 k^2 - E) + P^2 k^2 = 0. \quad (18)$$

If $\gamma_0, \gamma_3 \ll P^2/E_g$, which is usually the case, this dispersion relation gives

$$k_1^2 \approx \frac{(E - E_g)E}{P^2}; \quad k_2^2 \approx -\frac{P^2}{\gamma_0 \gamma_3}. \quad (19)$$

As a result, for each energy value and for given quasiparticle momentum direction we have four independent eigenfunctions, two ‘‘heavy’’ and two ‘‘light.’’ Therefore, in the bulk of constitutive semiconductors any arbitrary mesoscopic state, Ψ , may be represented as a superposition of four wave packets $\Psi = \Psi_{l1} + \Psi_{l2} + \Psi_{h1} + \Psi_{h2}$. This fact is of principal importance for the boundary condition analysis, because it allows us to consider all four components of the arbitrary column Ψ as independent variables. This can be further used in the analysis of the current continuity at a heterointerface. The current operator in the four-band spinless Kane model has the form

$$\hat{\mathbf{j}} = \frac{\partial \hat{H}}{\partial \mathbf{p}} = P\hat{\mathbf{A}} + 2\mathbf{p}(\gamma_0\hat{B}_0 - \gamma_3\hat{B}_3) - \gamma_2(\hat{\mathbf{J}}(\mathbf{p}\hat{\mathbf{J}}) + (\mathbf{p}\hat{\mathbf{J}})\hat{\mathbf{J}}). \quad (20)$$

In the canonical basis (4), z component of this operator is represented by the matrix

$$\hat{j}_z = \begin{bmatrix} 2\gamma_0 p_z & P & 0 & 0 \\ P & -2\gamma_3 p_z & -\gamma_2 p_+ & -\gamma_2 p_- \\ 0 & -\gamma_2 p_- & -2(\gamma_2 + \gamma_3)p_z & 0 \\ 0 & -\gamma_2 p_+ & 0 & -2(\gamma_2 + \gamma_3)p_z \end{bmatrix}. \quad (21)$$

Accordingly, we have the current continuity condition

$$\langle j_z \rangle_A = \langle j_z \rangle_B; \quad (22)$$

$$\langle j_z \rangle_{A,B} = \{P(\psi_0^* \psi_1 + \text{c.c.}) - \gamma_2[\psi_1^*(p_+ \psi_2 + p_- \psi_3) + \text{c.c.}] \\ - i\gamma_0(\psi_0^* \psi'_0 - \text{c.c.}) + i\gamma_3(\psi_1^* \psi'_1 - \text{c.c.}) \\ + i(\gamma_2 + \gamma_3)(\psi_2^* \psi'_2 + \psi_3^* \psi'_3 - \text{c.c.})\}_{A,B}.$$

Since all of the wave-function components are treated as independent quantities, the component combinations in parentheses in the last expression are also independent. Expressing all Ψ_A components in the left-hand side of Eq. (22) through Ψ_B components by means of boundary conditions (1) and equating the coefficients at independent combinations of Ψ_B components, we can continue the analysis of boundary condition matrix structure and impose additional restrictions on the matrix elements. First, we notice that due to the boundary mixing some combinations of Ψ_B compo-

nents can appear in the left-hand side of current continuity Eq. (22), which are incompatible with the matrix structure of the current operator \hat{j}_{zB} or, equally, with the matrix structure of the bulk Hamiltonian \hat{H}_B . For example, the mixing between the scalar, ψ_0 , and the vector, ψ_1 , wave-function components induces the appearance of the combinations like $(\psi_1^* \psi_1 + \text{c.c.})_B$, which would require the presence of linear in p_z terms on the main diagonal of the Hamiltonian \hat{H}_B . Analogously, the mixing between wave-function components and their derivatives, induced by the boundary condition submatrix \hat{S} , leads to the combinations $(\psi_1^* \psi_1' + \text{c.c.})_B$, which would correspond to the nonhermitian terms in current and Hamiltonian operators. The coefficients at such combinations must equal zero. As a result we have

$$\hat{S} \equiv 0; \quad F_{01} = F_{10} = 0; \quad G_{01} = G_{10} = 0; \quad R_{01} = R_{10} = 0, \quad (23)$$

so that in the spinless Kane model all the boundary condition submatrices become diagonal. Finally, the following canonical relations between nonzero boundary condition matrix elements can be readily obtained from current continuity condition:

$$F_0 F_1 = \frac{P_B}{P_A}; \quad F_1 F_3 = \frac{\gamma_{2B}}{\gamma_{2A}}; \quad F_2 = F_3; \quad G_2 = G_3; \quad (24)$$

$$F_0 G_0 = \frac{\gamma_{0B}}{\gamma_{0A}}; \quad F_1 G_1 = \frac{\gamma_{3B}}{\gamma_{3A}}; \quad F_3 G_3 = \frac{(\gamma_2 + \gamma_3)_B}{(\gamma_2 + \gamma_3)_A}.$$

The diagonal elements of the submatrix \hat{R} do not enter the current continuity equation Eq. (22) because they cancel in component combinations $(\psi_1^* \psi_1' - \text{c.c.})$. These elements can be found from the reciprocity relation for the boundary conditions. To relate the boundary condition matrix T_{AB} for AB heterointerface with the boundary condition matrix T_{BA} for BA interface, let us consider a narrow double heterostructure $A-B-A$ with small width 2δ of the B -type semiconductor. Since the reflection operation

$$\omega_{xy} \Psi(x, y, z) = \hat{\omega}_{xy} \Psi(x, y, -z) \quad (25)$$

is included into the symmetry group of the double heterostructure, we have

$$\begin{aligned} \bar{\Psi}_A(-\delta) &= T_{AB} \bar{\Psi}_B(-\delta) = T_{AB} \Omega_{xy} \bar{\Psi}_B(+\delta) \\ &= T_{AB} \Omega_{xy} T_{BA} \bar{\Psi}_A(+\delta) = \Omega_{xy} \bar{\Psi}_A(+\delta), \end{aligned} \quad (26)$$

where the shorthand notations have been introduced:

$$\bar{\Psi} = \begin{pmatrix} \Psi \\ \Psi' \end{pmatrix}; \quad \Omega_{xy} = \begin{bmatrix} \hat{\omega}_{xy} & 0 \\ 0 & \hat{\omega}_{xy} \end{bmatrix}. \quad (27)$$

In the limit $\delta \rightarrow 0$ it gives the reciprocity condition in the form

$$T_{AB} \Omega_{xy} T_{BA} = \Omega_{xy}. \quad (28)$$

In the canonical basis (4) the matrix representation of the reflection operation ω_{xy} is

$$\hat{\omega}_{xy} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad (29)$$

and (28) readily leads to the following relations between diagonal elements of boundary condition submatrices:

$$F_i \tilde{F}_i = 1; \quad G_i \tilde{G}_i = 1; \quad R_i \tilde{F}_i + G_i \tilde{R}_i = 0. \quad (30)$$

The elements of reciprocal matrix T_{BA} , which are marked here with tildes (\tilde{F}_i , \tilde{G}_i and \tilde{R}_i), should satisfy relations (24) with transposed indexes A and B . Combined with Eq. (30) this gives us the general form of the diagonal elements of submatrix \hat{R} :

$$R_i = |F_i G_i|^{1/2} \rho_i; \quad \rho_{AB} = -\rho_{BA}. \quad (31)$$

Here we introduce parameters ρ_i , which have the dimension of an inverse length and change sign upon reflection in the heterointerface. These parameters must vanish in a homogeneous material, so the dependence on the corresponding band offsets may be expected $\rho_{iAB} \sim (E_{iA} - E_{iB})$. Following Volkov and Pinsker,²⁴ we regard these parameters as mesoscopic in our classification scheme, that is $\rho_i \ll 1/a$, (a -lattice constant). Large value of ρ_i relates to an impenetrable interface for quasiparticle state near the band edge E_i .¹⁴

It should be noted that boundary conditions in the general form (1) can be used only if we consider the complete effective Hamiltonian including all possible independent matrix invariants. Correspondingly, all four independent eigenfunctions should be used in the wave-function expansion. Arbitrary discarding any solution unavoidably results in over-completeness of the boundary condition system (1). However, if the effective mass of one of the ‘‘light’’ eigenstate in Eq. (17), Ψ_{I1} , is formed mainly due to kp interaction of nearest bands, i.e., if $\gamma_0, \gamma_3 \ll 1/m_{I1} \sim P^2/E_g$, then the other ‘‘light’’ eigenstate, Ψ_{I2} , represents a spurious solution, evanescent or propagating, depending on the sign of the product $\gamma_0 \gamma_3$.^{19,20} An explicit treatment of the spurious solutions is beyond the applicability of the multiband effective-mass theory,^{21,22} thus we have to truncate the number of boundary conditions, providing them only for smooth part of the effective wave function. Rejected spurious solutions would then affect the values of the boundary condition parameters. Consider, for example, the evanescent solution Ψ_{I2} . The propagating spurious solutions can be treated in the same way. In the case of single heterointerface only decreasing exponentials are to be considered. From Eqs. (17) and (20) it follows that in canonical basis (4) the evanescent solution has the form

$$\Psi_{I2} \equiv \begin{pmatrix} 1 \\ \pm i \sqrt{\frac{\gamma_0}{\gamma_3}} \\ 0 \\ 0 \end{pmatrix} U_{I2} e^{\pm Pz/\sqrt{\gamma_0 \gamma_3}}. \quad (32)$$

The last two components of the column Ψ_{l_2} are of the order of $k_{\pm}/k_z \ll 1$ and can be neglected in the boundary conditions if U_{l_2} and U_{l_1} are of the same order of magnitude. Assuming $k_{l_2} \gg k_{l_1}, k_h, \rho$, we can show that $U_{l_2} \ll U_{l_1}$. To check this, let us write schematically the matching condition for the effective wave-function derivatives:

$$(k_{l_1}\Psi_{l_1} + k_{l_2}\Psi_{l_2} + k_{h1,2}\Psi_{h1,2})'_A \approx \hat{R}\Psi_B + \hat{G}(k_{l_1}\Psi_{l_1} + k_{l_2}\Psi_{l_2} + k_{h1,2}\Psi_{h1,2})'_B. \quad (33)$$

Here, k stands for z component of a wave vector. The ratio between the first two elements in column (32) is different in materials A and B , therefore, the first two rows of the boundary condition (33) can be fulfilled only if all terms in the parentheses are of the same order of magnitude. Thus,

$$U_{l_2} \sim (k_{l_1}/k_{l_2})U_{l_1} \ll U_{l_1}, \quad (34)$$

and we can lawfully omit the spurious solution Ψ_{l_2} in the following truncated boundary condition set:

$$\Psi_A = \hat{F}\Psi_B; \quad \begin{pmatrix} \psi'_2 \\ \psi'_3 \end{pmatrix}_A = G_3 \begin{pmatrix} \psi'_2 \\ \psi'_3 \end{pmatrix}_B + R_3 \begin{pmatrix} \psi_2 \\ \psi_3 \end{pmatrix}_B. \quad (35)$$

Here, the effective wave function of an arbitrary mesoscopic state $\Psi = \Psi_{l_2} + \Psi_{h1} + \Psi_{h2}$ includes only smooth components provided the ‘‘heavy’’ mass m_h is not too large. If $m_h \gg m_l$, the ‘‘heavy’’ states, $\Psi_{h1,2}$, should also be excluded from the effective wave-function expansion. In this case, Kane’s Hamiltonian becomes first order in the momentum operator \mathbf{p} , and boundary conditions are reduced simply to the relation $\Psi_A = \hat{F}\Psi_B$. This situation corresponds to a ‘‘flat-band’’ approximation for the ‘‘heavy’’-state dispersion and can be used only if the energy of the mesoscopic state under consideration is not too close to the valence-band top in either A or B material.

Finally, we conclude that in the isotropic spinless four-band Kane model, the heterointerface is described by the boundary conditions (1) with only two independent phenomenological parameters. The existence of these two parameters in the spinless model and the absence of the submatrix \hat{S} in the total boundary condition matrix T_{AB} both confirm the assumptions used in preceding works.^{12,14} One independent parameter of the boundary conditions can be arbitrarily chosen from the parameter set (24). Depending on the choice, it relates to the matching condition at the corresponding band edge. It is interesting to derive the boundary conditions for an electron state near the nondegenerate conduction band edge characterized by the scalar effective wave function $\Psi \approx \psi_0$ (one-band effective-mass model). In this case, the Hamiltonian parameters $\gamma_{0A,B}$ should be renormalized to include the contribution from the basis \mathbf{V} states. Then, from the relations (24) and (31) the effective boundary conditions can be readily obtained. Omitting the unnecessary matrix indexes, we have

$$\psi_A = F\psi_B; \quad \psi'_A = G\psi'_B + R\psi_B; \quad (36)$$

$$FG = \frac{m_{cA}}{m_{cB}}; \quad R = \left(\frac{m_{cA}}{m_{cB}} \right)^{1/2} \rho.$$

Here quantities $m_{cA,B}$ represent conduction-band bulk effective masses in constitutive semiconductors. Relations (36) are the modified BenDaniel-Duke boundary conditions discussed in the Introduction. Parameter F can be chosen as the first independent phenomenological parameter describing the matching conditions at the conduction band edge. The second independent parameter, ρ , has the dimension of inverse length. Boundary condition parameter of this type have been discussed by Volkov and Pinsker,²⁴ Zhu and Kroemer,⁹ Ando *et al.*,¹² and Laikhtman.¹⁴

III. KANE MODEL WITH SPIN

For a correct description of valence-band states, spin of the electron, $\mathbf{s} = \frac{1}{2}\boldsymbol{\sigma}$, must be included in the Kane model. Assuming isotropic quasiparticle energy spectra in the constitutive semiconductors, we can write the effective bulk Hamiltonian in the following form:

$$\hat{H} = E_g \hat{B}_0 + \frac{\Delta}{3} (2\hat{\mathbf{J}}\hat{\mathbf{s}} - 1)\hat{B}_3 + P(\mathbf{p}\hat{\mathbf{A}}) + \gamma_0 p^2 \hat{B}_0 - \gamma_3 p^2 \hat{B}_3 - \frac{1}{2} \gamma_2 (\mathbf{p}\hat{\mathbf{J}})[\mathbf{p}(\hat{\mathbf{J}} + 2\hat{\mathbf{s}})]. \quad (37)$$

Since the spin states $\{\alpha, \beta\}$ are explicitly included in the basis set, the order of all matrix operators is now being doubled, for example, 4x4 unity matrices of the scalar and vector subspaces, B_0 and B_3 , are multiplied by the 2x2 unity matrix B_2 of the spin space, $\hat{B}_{0(3)} = B_{0(3)} \otimes B_2$. Operators with hats will refer in this section to the 8x8 matrices in the complete basis set. Second term of the Hamiltonian (37), \hat{H}_{so} , has no counterpart in the spinless model (12). This operator represents the spin-orbit splitting of the energy of the vector subspace basis states by the amount Δ and, simultaneously, allows us to keep the energy zero at the top of the valence band. The last term in Eq. (37) is formally analogous to the last term of the Hamiltonian (12), and has the matrix structure of the projection operator $\hat{\Lambda}_h$ onto the ‘‘heavy’’ state subspace (see Appendix). Phenomenological parameters γ_i used in our form of Kane Hamiltonian will be related below to the original Luttinger parameters γ^L .

For isotropic spin-including Kane model, the canonical basis is given by a set of four Kramers-conjugate pairs of states, representing the basis of coupled angular momenta:

$$\{u_n^v\} = \left\{ \begin{pmatrix} S\alpha \\ S\beta \end{pmatrix}; \frac{1}{\sqrt{6}} \begin{pmatrix} 2Z\alpha - (X+iY)\beta \\ 2Z\beta + (X-iY)\alpha \end{pmatrix}; \frac{1}{\sqrt{3}} \begin{pmatrix} Z\alpha + (X+iY)\beta \\ Z\beta - (X-iY)\alpha \end{pmatrix}; \frac{1}{\sqrt{2}} \begin{pmatrix} (X+iY)\alpha \\ (X-iY)\beta \end{pmatrix} \right\}. \quad (38)$$

The first three doublets in Eq. (38), $\{u_n^v\}_{n=0,1,2}$, relate to three equivalent two-dimensional representations of the symmetry group of the heterostructure energy spectrum. The wave-function components corresponding to the equivalent irreducible representations can mix at the heterointerface, consequently, all the submatrices of the boundary conditions (1) should be sought in the form

$$\hat{F} = \begin{bmatrix} F_0 & F_{01} & F_{02} & 0 \\ F_{10} & F_1 & F_{12} & 0 \\ F_{20} & F_{21} & F_2 & 0 \\ 0 & 0 & 0 & F_3 \end{bmatrix},$$

$$\hat{G} = \begin{bmatrix} G_0 & G_{01} & G_{02} & 0 \\ G_{10} & G_1 & G_{12} & 0 \\ G_{20} & G_{21} & G_2 & 0 \\ 0 & 0 & 0 & G_3 \end{bmatrix}, \dots \quad (39)$$

All the considerations of the previous section remain valid. We need only to substitute the quasispin operator $\hat{\Sigma}$ for $\hat{\mathbf{J}}$ in space transformation operators (see the Appendix) and take into account the different form of the time-reversal operator $\hat{\tau}$

$$\hat{\omega}_{z,\phi} = e^{i\phi\hat{\Sigma}_z} = \begin{bmatrix} e^{(i/2)\phi\sigma_z} & 0 & 0 & 0 \\ 0 & e^{(i/2)\phi\sigma_z} & 0 & 0 \\ 0 & 0 & e^{(i/2)\phi\sigma_z} & 0 \\ 0 & 0 & 0 & e^{(3i/2)\phi\sigma_z} \end{bmatrix}; \quad (40)$$

$$\hat{\omega}_{xz} = (B_0 + B_3) \otimes i\sigma_y; \quad \hat{\tau} = (B_0 + B_3) \otimes i\sigma_y \mathcal{K}.$$

Here $\hat{\omega}_{xz}^2 = \hat{\tau}^2 = -1$, because now the fermionic nature of Kane quasiparticle is consistently included in the model. Relations (8) and (9) allow us to find the matrix structure of 2×2 blocks, linking the envelopes of Kramers conjugated basis states. Boundary condition invariance according to the rotations $\hat{\omega}_{z,\phi}$ provides the diagonal structure of each block, whereas the reflection operator $\hat{\omega}_{xz}$ exchanges the ‘‘upper’’ and ‘‘lower’’ components of basis Kramers doublets, thus making the diagonal elements equal. Taking into account time-reversal symmetry, we finally find that each elementary block in Eq. (39) is represented by a real number multiplied by 2×2 diagonal unity matrix B_2 . This structure of boundary condition submatrices means that in canonical representation the basis states with opposite sign of index ν do not mix at the interface, and we can analyze the mixing of the spinor components of the arbitrary mesoscopic wave-

function disregarding their particular ‘‘spin’’ structure. The effective wave function of the mesoscopic state should now be expanded into the wave packets, corresponding to different types of eigenfunctions of Schrödinger equation in the eight-band Kane model. One of these eigenfunctions has the matrix structure of ‘‘heavy’’ state and can be defined by means of the projection operator $\hat{\Lambda}_h$ (see the Appendix)

$$\Psi_h = \hat{\Lambda}_h \begin{pmatrix} U \\ \bar{\mathbf{V}} \end{pmatrix} = \begin{pmatrix} 0 \\ \bar{\mathbf{V}}_h \end{pmatrix}. \quad (41)$$

To find out the matrix structure of the ‘‘light’’ eigenstates in the spin-including Kane model, we have to take into account the existence of two linearly independent Hermitian operators exhibiting the transformation properties of a polar vector, specifically, \mathbf{p} and $\boldsymbol{\pi} = \mathbf{s} \times \mathbf{p}$.²⁵ Therefore, the vector part of the wave function Ψ_l should be thought of as a linear combination of both column $\bar{\mathbf{k}}$ and column $\bar{\mathbf{q}} = \mathbf{s} \times \bar{\mathbf{k}} = -i(\mathbf{J}\mathbf{s})\bar{\mathbf{k}}$

$$\Psi_l = \begin{pmatrix} U_l \\ \bar{\mathbf{V}}_l \end{pmatrix}; \quad \bar{\mathbf{V}}_l = P(a\bar{\mathbf{k}} + ib\bar{\mathbf{q}})U_l = P[a + b(\mathbf{J}\mathbf{s})]\bar{\mathbf{k}}U_l. \quad (42)$$

From the dispersion Eq. (A17) it follows that for a given energy E there exist three ‘‘light’’ eigenfunctions Ψ_l with different k^2 . As a result, the effective wave function of an arbitrary mesoscopic state, Ψ , can be expanded in four independent wave packets $\Psi = \Psi_{l1} + \Psi_{l2} + \Psi_{l3} + \Psi_h$, and all four spinor components ψ_n of the corresponding column can be considered as independent variables. The current continuity analysis developed in the previous section is still applicable and provides additional restrictions on the boundary condition matrix elements. In the eight-band Kane model with Hamiltonian (37), the current operator has the form

$$\hat{\mathbf{j}} = P\hat{\mathbf{A}} + 2\mathbf{p}(\gamma_0\hat{B}_0 - \gamma_3\hat{B}_3) - \frac{1}{2}\gamma_2\{[\hat{\mathbf{J}}(\mathbf{p}\hat{\mathbf{J}}) + \hat{\mathbf{s}}(\mathbf{p}\hat{\mathbf{J}}) + \hat{\mathbf{J}}(\mathbf{p}\hat{\mathbf{s}})] + \text{c.c.}\}, \quad (43)$$

and its z component in the coupled angular momenta basis is represented by the matrix operator

$$\hat{j}_z = \begin{bmatrix} 2\gamma_0 p_z & \sqrt{\frac{2}{3}}P & \sqrt{\frac{1}{3}}P & 0 \\ \sqrt{\frac{2}{3}}P & -2\gamma_3 p_z & 0 & -\frac{\sqrt{3}}{2}\gamma_2(p_x + i\sigma_z p_y) \\ \sqrt{\frac{1}{3}}P & 0 & -2\gamma_3 p_z & 0 \\ 0 & -\frac{\sqrt{3}}{2}\gamma_2(p_x - i\sigma_z p_y) & 0 & -2(\gamma_2 + \gamma_3)p_z \end{bmatrix} \quad (44)$$

with the average value

$$\begin{aligned} \langle j_z \rangle = & P \left[\psi_0^* \left(\sqrt{\frac{2}{3}} \psi_1 + \sqrt{\frac{1}{3}} \psi_2 \right) + \text{c.c.} \right] \\ & - \frac{\sqrt{3}}{2} \gamma_2 [\psi_1^* (p_x + i \sigma_z p_y) \psi_3 + \text{c.c.}] \\ & - i \gamma_0 (\psi_0^* \psi_0' - \text{c.c.}) + i \gamma_3 (\psi_1^* \psi_1' + \psi_2^* \psi_2' - \text{c.c.}) \\ & + i (\gamma_2 + \gamma_3) (\psi_3^* \psi_3' - \text{c.c.}). \end{aligned} \quad (45)$$

Similar to the spinless model, current continuity analysis renders vanishing most of the nondiagonal blocks in Eq. (39). There is no mixing at the interface between the scalar and the vector wave-function components, and the submatrix \hat{S} vanishes identically. However, now the submatrix \hat{F} can have one nonzero nondiagonal matrix element, F_{21} . The existence of nondiagonal element in submatrix \hat{F} induces the existence of nonzero nondiagonal elements in submatrices \hat{G} (element G_{12}) and \hat{R} (elements R_{12} and R_{21}). Canonical relations between boundary condition matrix elements and bulk Hamiltonian parameters are given by

$$\begin{aligned} F_0 F_2 = \frac{P_B}{P_A}; \quad F_1 F_3 = \frac{\gamma_{2B}}{\gamma_{2A}}; \quad F_{21} = \sqrt{2}(F_2 - F_1); \\ G_{12} = \sqrt{2}(G_2 - G_1); \quad F_0 G_0 = \frac{\gamma_{0B}}{\gamma_{0A}}; \\ F_1 G_1 = F_2 G_2 = \frac{\gamma_{3B}}{\gamma_{3A}}; \quad F_3 G_3 = \frac{(\gamma_2 + \gamma_3)_B}{(\gamma_2 + \gamma_3)_A}; \\ F_1 R_{12} - F_2 R_{21} + F_{21} R_2 = 0. \end{aligned} \quad (46)$$

The matrix representation of the reflection operation in heterointerface plane ω_{xy} can be obtained as the product of inversion operator matrix $\hat{I} = \hat{B}_0 - \hat{B}_3$ and operator $\hat{\omega}_{z,\pi}$

$$\hat{\omega}_{xy} = \hat{\omega}_{z,\pi} \hat{I} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \otimes i \sigma_z. \quad (47)$$

Using this representation in reciprocity condition (28), we arrive at the same expression (31) for the elements of submatrix \hat{R} in eight-band Kane model.

For the Kane model with spin, the nondiagonal matrix element F_{21} plays the part of a third independent phenomenological parameter in the boundary conditions. Apparently, it is determined by spin-orbit interaction at the heterointerface. In what follows, we assume this interaction to be ‘relativistic’ small. Neglecting the parameter F_{21} , we can significantly simplify the boundary conditions. All submatrices become diagonal and, moreover, the relations

$$F_2 = F_1; \quad G_2 = G_1; \quad R_2 = R_1 \quad (48)$$

hold for diagonal matrix elements. It is interesting to note that only in this approximation and, additionally, if P_A

$= P_B$ and $\gamma_{2A} = \gamma_{2B}$, the component-by-component continuity of effective wave function becomes possible in the Kane model.

Next, we consider the problem of approximate boundary conditions for the most important limiting situations. First of all, we suppose the remote band effects to be small, $\gamma_0, \gamma_3 \ll 1/m_l$, as is usually the case for all materials of interest. One spurious ‘light’ state Ψ_{13} and, correspondingly, two matching conditions for the effective wave function derivatives should be truncated in accordance with the small parameter $\sqrt{\gamma_0 \gamma_3} E_g / P^2$, as was described in previous section. In the basis of coupled momenta first two vector components of the spurious state Ψ_{13} are linearly dependent (see the Appendix), therefore, in the boundary condition set we should keep the matching condition only for the linear combination $(\psi_1' - \sqrt{2} \psi_2')$, where the components of the spurious solution Ψ_{13} are absent. Taking into account Eq. (48), we arrive at a simple truncated boundary condition system:

$$\begin{aligned} \Psi_A = \hat{F} \Psi_B; \\ (\psi_1 - \sqrt{2} \psi_2)'_A = G_1 (\psi_1 - \sqrt{2} \psi_2)'_B + R_1 (\psi_1 - \sqrt{2} \psi_2)_B; \end{aligned} \quad (49)$$

$$\psi'_{3A} = G_3 \psi'_{3B} + R_3 \psi_{3B}.$$

For narrow band-gap semiconductors, the limit of large spin-orbit splitting of the valence band is often used. If $\Delta \gg E_g, E$, then from Eqs. (A14) and (A16) it follows that the third line of each boundary condition submatrices (39) can be omitted. Two solutions of the dispersion Eq. (A17) become spurious in this limit and should be rejected in the effective wave-function expansion. One of these eigenfunction relates to the ‘remote’ spin-orbit split-off band, the other has the matrix structure similar to Eq. (32). As a result, for the so-called six-band Kane model we obtain the following truncated system of boundary conditions in the coupled angular momentum basis:

$$\Psi = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_3 \end{pmatrix};$$

$$\begin{aligned} \psi_{0A} = F_0 \psi_{0B}; \quad \psi_{1A} = F_1 \psi_{1B}; \quad \psi_{3A} = F_3 \psi_{3B}; \\ \psi'_{3A} = G_3 \psi'_{3B} + R_3 \psi_{3B}. \end{aligned} \quad (50)$$

The total effective wave function in this model is represented by a superposition of smooth wave packets of one ‘light’ and one ‘heavy’ states with sufficiently small wave vectors $\Psi = \Psi_l + \Psi_h$.

Finally, we obtain the approximate boundary conditions for Luttinger’s model, describing the valence-band states in the energy region $|E| \ll E_g, \Delta$. In this limit the dispersion relation (A17) for ‘light’ eigenstates has only one solution with the dispersion

$$E_l \simeq -(\gamma_3 + 2P^2/3E_g)k^2. \quad (51)$$

Multicomponent eigenfunctions of the Luttinger model in the coupled momenta basis do not contain the first and the third rows. For ‘light’ solutions, these components are small in

TABLE I. Material and boundary condition parameters for GaAs-based heterointerfaces.

	GaAs	AlAs	Al _{0.2} Ga _{0.8} As		GaAs/AlAs	GaAs/Al _{0.2} Ga _{0.8} As
m_c/m_0	0.0665	0.150	0.083	F_0F_1	1.10	1.02
γ_1^L	6.85	3.45	5.64	F_1F_3	2.53	1.29
γ_2^L	2.10	0.68	1.57	F_0G_0	-7.92	0.60
γ_3^L	2.90	1.29	2.32	F_1G_1	0.63	9.67
E_g, eV	1.519	3.130	1.746	F_3G_3	3.12	1.20
E_P, eV	25.7	21.1	24.8	R_0/ρ_0	2.82	0.77
Δ, eV	0.341	0.275	0.328	R_1/ρ_1	0.79	3.11
				R_3/ρ_3	1.77	1.10

accordance with small parameters E/E_g and E/Δ , respectively, and the dispersionless partial boundary conditions for the four-component Luttinger effective wave function are given by

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_3 \end{pmatrix};$$

$$\psi_{1A} = F_1 \psi_{1B}; \quad \psi_{3A} = F_3 \psi_{3B};$$

$$\psi'_{1A} = G_1 \psi'_{1B} + R_1 \psi_{1B}; \quad \psi'_{3A} = G_3 \psi'_{3B} + R_3 \psi_{3B}. \quad (52)$$

Parameters $\gamma_{3A,B}$ should be renormalized according to Eq. (51) to include the contribution of the basis S states, which now become ‘‘remote’’ states. In the isotropic model it is much more convenient to use the matching parameters expressed in terms of the quasiparticle effective masses, m_l and m_h ,

$$F_1G_1 = \frac{m_{lA}}{m_{lB}}; \quad F_3G_3 = \frac{m_{hA}}{m_{hB}}; \quad F_1F_3 = \frac{(1/m_l - 1/m_h)_A}{(1/m_l - 1/m_h)_B}. \quad (53)$$

Similar boundary conditions hold in Luttinger’s model with anisotropic quasiparticle spectrum, if the heterointerface is orthogonal to one three-fold or four-fold axis and one surface of symmetry of the bulk energy spectrum. For example, consider the $\{001\}$ boundary of a diamond-like semiconductor. The Luttinger Hamiltonian can be written in the traditional manner¹ using matrices $\hat{\mathbf{J}}$ of angular momentum 3/2, which now play the part of a quasispin:

$$\hat{H}_L = \frac{1}{2m_0} \left[\left(\gamma_1^L + \frac{5}{2} \gamma_2^L \right) \mathbf{p}^2 \hat{B}_4 - 2 \gamma_2^L (p_x^2 \hat{J}_x^2 + \dots) \right. \\ \left. - 2 \gamma_3^L (p_x p_y \hat{J}_x \hat{J}_y + \dots) \right]; \quad (54)$$

$$[\hat{H}_L, (\hat{\mathbf{L}} + \hat{\mathbf{J}})]_- = 0; \quad \hbar \hat{\mathbf{L}} = \hat{B}_4 (\mathbf{r} \times \mathbf{p}).$$

$$\hat{J}_x = \begin{bmatrix} \sigma_x & -\frac{\sqrt{3}}{2} \sigma_z \\ -\frac{\sqrt{3}}{2} \sigma_z & 0 \end{bmatrix}; \quad \hat{J}_y = \begin{bmatrix} \sigma_y & -i \frac{\sqrt{3}}{2} \\ i \frac{\sqrt{3}}{2} & 0 \end{bmatrix};$$

$$\hat{J}_z = \begin{bmatrix} \frac{1}{2} \sigma_z & 0 \\ 0 & \frac{3}{2} \sigma_z \end{bmatrix}.$$

Here we use the canonical basis $\{u_1^v; u_3^v\}$, diagonalizing quasispin component \hat{J}_z . In this basis, successively applying symmetry operations $\omega_{z, \pi/2}$ and ω_{xz} ,²⁶ we again arrive at the boundary conditions (52) with parameters

$$F_1G_1 = \frac{(\gamma_1^L + 2\gamma_2^L)_B}{(\gamma_1^L + 2\gamma_2^L)_A}; \quad F_3G_3 = \frac{(\gamma_1^L - 2\gamma_2^L)_B}{(\gamma_1^L - 2\gamma_2^L)_A};$$

$$F_1F_3 = \frac{\gamma_{3B}^L}{\gamma_{3A}^L}, \quad (55)$$

which in the spherical approximation $\gamma_2^L \approx \gamma_3^L$ results in Eq. (53). In this approximation, the Luttinger Hamiltonian reduces to the form

$$\hat{H}_L = \frac{1}{2m_0} \left[\left(\gamma_1^L + \frac{5}{2} \bar{\gamma}^L \right) \mathbf{p}^2 \hat{B}_4 - 2 \bar{\gamma}^L (\mathbf{p} \hat{\mathbf{J}})^2 \right], \quad (56)$$

and we can easily relate the phenomenological parameters used in our form of Kane’s Hamiltonian (37) to the original Luttinger parameters γ_1^L and $\bar{\gamma}^L = \frac{1}{2}(\gamma_2^L + \gamma_3^L)$:

$$\gamma_2 = -\frac{1}{m_0} 2 \bar{\gamma}^L; \quad \gamma_3 = \frac{1}{m_0} \left(\frac{1}{2} \gamma_1^L + \bar{\gamma}^L - \frac{E_P}{3E_g} \right);$$

$$E_P = 2m_0 P^2. \quad (57)$$

Parameter γ_0 can be evaluated through the experimentally determined conduction-band mass m_c using relation (A17)

$$\gamma_0 = \frac{1}{2m_0} \left[\left(\frac{m_c}{m_0} \right)^{-1} - \frac{E_P \left(E_g + \frac{2}{3} \Delta \right)}{E_g (E_g + \Delta)} \right]. \quad (58)$$

In Table I we show the results of exemplary calculation of the main relations between the boundary condition parameters (46) for Γ -envelopes at GaAs/AlAs and GaAs/Al_{0.2}Ga_{0.8}As heterointerfaces. Material parameters used in the calculation are taken from tables of Landolt-Bornstein.²⁷ It is interesting to note the strong dependence of the matching parameters for wave-function derivative G_i on the Luttinger parameters of constitutive semi-

conductors. The basic phenomenological parameters of the boundary conditions, for example F_0 and ρ_i , should be obtained by a more detailed microscopic analysis of the boundary condition problem, which is beyond the scope of the present article.

IV. CONCLUSIONS

The virtue of the phenomenological description of an abrupt heterointerface lies in the simplicity of the resulting boundary condition matrix. At an abrupt heterointerface, the multiband effective wave function should satisfy the boundary conditions of the most general form (1). In this paper, we have analyzed the structure of boundary conditions in eight-band Kane model and shown that in the canonical basis the boundary condition matrix assume a rather simple form. Only two independent phenomenological parameters are needed to characterize the matching conditions at the abrupt heterointerface in the case when bulk energy spectrum of quasiparticles is isotropic and spin-orbit interaction at the interface is small. In the spirit of the effective-mass theory, these parameters are determined by the microstructure of the interface and do not depend explicitly on the energy of the charge-carrier state. This provides the easiest way to treat the nonparabolicity effects in direct band-gap semiconductor heterostructures. Simple canonical relations have been established between the boundary condition matrix elements and parameters of the Kane's Hamiltonian in constitutive semiconductors. It follows that in general situation, when Hamiltonian parameters in both semiconductors are different, the assumption of effective wave-function component-by-component continuity is unapplicable. The relations between major boundary condition parameters has been evaluated for two exemplary GaAs-based heterointerfaces to demonstrate strong dependence of the matching conditions on the effective Hamiltonian parameters.

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APPENDIX

In this Appendix we consider the matrix structure of spin-including eight-band Kane Hamiltonian (37) and corresponding eigenfunctions. First of all, to avoid confusion, we note that all hatted matrices used in the model, for example $\hat{\mathbf{s}}$ and $\hat{\mathbf{J}}$, have trivial matrix structure only in the basis of direct product

$$\{u_n^\nu\} = \{S, X, Y, Z\} \otimes \{\alpha, \beta\} = \begin{Bmatrix} S\alpha & X\alpha & Y\alpha & Z\alpha \\ S\beta & X\beta & Y\beta & Z\beta \end{Bmatrix}; \quad (\text{A1})$$

$$n = 0, 1, 2, 3; \nu = \pm 1.$$

In this basis we have

$$\hat{s}_i = (\hat{B}_0 + \hat{B}_3) \otimes s_i; \quad \hat{J}_i = (0 \cdot B_0 + J_i \cdot B_3) \otimes B_2, \quad (\text{A2})$$

and the relation

$$(\hat{\mathbf{J}}\mathbf{s}) = \sum_i J_i \otimes s_i \quad (\text{A3})$$

holds true. When the basis is changed, the matrices \hat{J}_i and \hat{s}_i , as well as matrices \hat{A}_i , suffer a unitary transformation and cannot be decomposed into the direct product of the orbital and spin parts. For example, the unitary matrix

$$w = \begin{bmatrix} \frac{1}{\sqrt{6}} \begin{pmatrix} i\sigma_y \\ -i\sigma_x \\ 2 \end{pmatrix} & \frac{1}{\sqrt{3}} \begin{pmatrix} -i\sigma_y \\ i\sigma_x \\ 1 \end{pmatrix} & \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i\sigma_z \\ 0 \end{pmatrix} \end{bmatrix} \quad (\text{A4})$$

describes the transition from basis (A1) to the coupled angular momenta basis (38) used in the text. Only the nontrivial part of the matrix, corresponding to the vector subspace transformation, is shown here. All the vector columns, like $\bar{\mathbf{v}}$, $\bar{\mathbf{k}}$, $\bar{\mathbf{q}}$, which we use in the eight-band Kane model, are to be transformed also and become six-component columns with complex spin structure. For instance, the vector column $\bar{\mathbf{k}}$ is represented in the coupled momenta basis as

$$\bar{\mathbf{k}} = w^{-1} \begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix} = \begin{pmatrix} 2(k_z + iq_z)/\sqrt{6} \\ (k_z - 2iq_z)/\sqrt{3} \\ (k_x - i\sigma_z k_y)/\sqrt{2} \end{pmatrix};$$

$$q_z = \frac{1}{2}(\sigma_x k_y - \sigma_y k_x). \quad (\text{A5})$$

The matrix structure of the spin split-off operator \hat{H}_{so} in Eq. (37) has been chosen to keep the energy zero at the top of the valence band, assuming that the highest energy level corresponds to the four-fold degenerate valence basis state. Indeed, the eigenvalues λ of the operator $(\mathbf{J}\boldsymbol{\sigma})$ can be easily obtained from the well-known relation for Pauli matrices, $(\mathbf{a}\boldsymbol{\sigma})(\mathbf{b}\boldsymbol{\sigma}) = (\mathbf{a}\cdot\mathbf{b}) + i[\mathbf{a}\times\mathbf{b}]\boldsymbol{\sigma}$, if we put $\mathbf{a} = \mathbf{b} = \mathbf{J}$:

$$(\mathbf{J}\boldsymbol{\sigma})^2 = \mathbf{J}^2 - (\mathbf{J}\boldsymbol{\sigma}) = 2 - (\mathbf{J}\boldsymbol{\sigma}); \quad \lambda^2 = 2 - \lambda. \quad (\text{A6})$$

The eigenvalues λ , which are $\lambda_{1/2} = -2$ and $\lambda_{3/2} = +1$, are twofold degenerate. Moreover, since all the spin matrices, J_i and σ_i , are traceless, there should be an additional two-fold degeneracy of the second eigenvalue $\lambda_{3/2}$. According to the form of the spin split-off operator, the energy of this four-fold degenerate state is precisely zero, while the energy of the two-fold degenerate state is equal $-\Delta$. In the basis of coupled angular momenta operator \hat{H}_{so} becomes diagonal with only nonzero matrix elements

$$(H_{so})_{33}^{(1)} = (H_{so})_{33}^{(-1)} = -\Delta. \quad (\text{A7})$$

Now, let us consider the structure of the last term of the eight-band Hamiltonian (37). In the absence of external fields the total angular momentum of the quasiparticle must be conserved. By analogy with Eq. (13), it thus follows that matrix operators of quasispin $\hat{\mathbf{S}}$ and quasihelicity $\hat{\mu} = (\mathbf{m}\hat{\mathbf{S}})$ should exist. Quasispin operator can be defined as

$$\hat{\mathbf{S}} = \hat{\mathbf{s}} + \hat{\mathbf{J}}; \quad [\hat{H}, (\hat{\mathbf{S}} + \hat{\mathbf{L}})]_- = 0. \quad (\text{A8})$$

In basis of coupled momenta this operator has the matrix representation

$$(\mathbf{m}\hat{\Sigma}) = \begin{bmatrix} \frac{1}{2}(\mathbf{m}\sigma) & 0 & 0 & 0 \\ 0 & (\mathbf{m}_{\parallel}\sigma_{\parallel}) + \frac{1}{2}m_z\sigma_z & 0 & -\frac{i\sqrt{3}}{2}\sigma_y(\mathbf{m}_{\parallel}\sigma_{\parallel}) \\ 0 & 0 & \frac{1}{2}(m_z\sigma_z - (\mathbf{m}_{\parallel}\sigma_{\parallel})) & 0 \\ 0 & \frac{i\sqrt{3}}{2}(\mathbf{m}_{\parallel}\sigma_{\parallel})\sigma_y & 0 & \frac{3}{2}m_z\sigma_z \end{bmatrix}. \quad (\text{A9})$$

Since quasihelicity of a free quasiparticle is a good quantum number, the scalar invariant $(\mathbf{p}\hat{\Sigma})^2$ should enter the eight-band Kane Hamiltonian instead of the matrix form $(\mathbf{p}\hat{\mathbf{J}})^2$, which has been used in spinless model. In Eq. (37) we use the operator

$$\hat{\Lambda}_h = \frac{1}{2} \left[(\mathbf{m}\hat{\Sigma})^2 - \frac{1}{4} \right] = \frac{1}{2} (\mathbf{m}\hat{\mathbf{J}}) [\mathbf{m}(\hat{\mathbf{J}} + 2\hat{\mathbf{s}})], \quad (\text{A10})$$

which in vector subspace of basis (38) is represented by the matrix

$$\Lambda_h = \frac{1}{2} \begin{bmatrix} \frac{3}{2}(1-m_z^2) & 0 & -\frac{i\sqrt{3}}{2}(\mathbf{m}\sigma + m_z\sigma_z)\sigma_y(\mathbf{m}_{\parallel}\sigma_{\parallel}) \\ 0 & 0 & 0 \\ \frac{i\sqrt{3}}{2}(\mathbf{m}_{\parallel}\sigma_{\parallel})\sigma_y(\mathbf{m}\sigma + m_z\sigma_z) & 0 & \frac{1}{2}(1+3m_z^2) \end{bmatrix}. \quad (\text{A11})$$

According to the definition (A10), operator $\hat{\Lambda}_h$ affects the wave functions with quasihelicity $\hat{\mu} = \pm \frac{1}{2}$ like a zero operator, therefore, it can be considered as a projection operator onto the subspace of two-fold degenerate ‘‘heavy’’ states,²⁸ which are characterized now by the quasihelicity $\hat{\mu} = \pm \frac{3}{2}$ and have the dispersion

$$E_h(k) = \frac{1}{2} \text{Sp}(\hat{\Lambda}_h \hat{H}) = -(\gamma_2 + \gamma_3)k^2; \text{Sp}\hat{\Lambda}_h = 2. \quad (\text{A12})$$

In basis (A1) spin matrices \mathbf{s} are diagonal in index n and vector column $\bar{\mathbf{V}}_h$ of a free ‘‘heavy’’ quasiparticle state has an especially simple form

$$\bar{\mathbf{V}}_h = \bar{\mathbf{V}} - (\mathbf{m}\mathbf{V})\bar{\mathbf{m}} + 2i(\mathbf{m}\mathbf{s})[\bar{\mathbf{m}} \times \bar{\mathbf{V}}]. \quad (\text{A13})$$

Using Eq. (A4) we obtain the corresponding representation in the basis of coupled momenta

$$\bar{\mathbf{V}}_h = \begin{pmatrix} \sqrt{3}k_{\parallel} \\ 0 \\ 4\frac{q_z\sigma_y}{k_{\parallel}}(p_z - iq_z) \end{pmatrix} U_h. \quad (\text{A14})$$

Here $k_{\parallel} = \sqrt{k_x^2 + k_y^2}$, and U_h is normalizing factor. For ‘‘light’’ quasiparticle eigenstates, substituting Eq. (42) into

Schrödinger equation with Hamiltonian (37) and making use of $\hat{\Lambda}_h \Psi_l = 0$, we easily obtain the coefficients $a(E)$ and $b(E)$

$$a = \frac{\bar{E} + \frac{2}{3}\Delta}{\bar{E}(\bar{E} + \Delta)}; \quad b = \frac{\frac{2}{3}\Delta}{\bar{E}(\bar{E} + \Delta)}; \quad \bar{E} = E + \gamma_3 k^2, \quad (\text{A15})$$

the matrix representation of the vector column $\bar{\mathbf{V}}_l$ in the coupled momenta basis

$$\bar{\mathbf{V}}_l = \begin{bmatrix} \frac{1}{\bar{E}} & 0 & 0 \\ 0 & \frac{1}{\bar{E} + \Delta} & 0 \\ 0 & 0 & \frac{1}{\bar{E}} \end{bmatrix} P\bar{\mathbf{k}}U_l, \quad (\text{A16})$$

and the dispersion relation for corresponding ‘‘light’’ bands

$$(E_g + \gamma_0 k^2 - E) + P^2 k^2 \frac{\bar{E} + \frac{2}{3}\Delta}{\bar{E}(\bar{E} + \Delta)} = 0, \quad (\text{A17})$$

which is third order in k^2 . As a result, in eight-band Kane model we have three different types of “light” eigenstates. Usually, $\gamma_0, \gamma_3 \ll P^2/E_g$, and only two of these states, Ψ_{11} and Ψ_{12} , are physically relevant. They can be attributed to conduction–light-hole and spin-orbit split-off bands, respectively. The third k^2 solution of Eq. (A17), $k_3^2 \approx -P^2/\gamma_0\gamma_3$, leads to spurious “light” eigenstate, Ψ_{13} . Using Eqs. (A5)

and (A16), we find the matrix structure of this column

$$\Psi_{13} = \begin{pmatrix} 1 \\ i \sqrt{\frac{\gamma_0}{3\gamma_3}} \begin{pmatrix} \sqrt{2} \\ 1 \end{pmatrix} \\ 0 \end{pmatrix} U_{13}(z). \quad (\text{A18})$$

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