Interface electronic states and boundary conditions for envelope functions

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The envelope-function method with generalized boundary conditions is applied to the description of localized and resonant interface states. A complete set of phenomenological conditions that restrict the form of connection rules for envelope functions is derived using the Hermiticity and symmetry requirements. Empirical coefficients in the connection rules play the role of material parameters that characterize an internal structure of every particular heterointerface. As an illustration we present the derivation of the most general connection rules for the one-band effective mass and four-band Kane models. The conditions for the existence of Tamm-like localized interface states are established. It is shown that a nontrivial form of the connection rules can also result in the formation of resonant states. The most transparent manifestation of such states is the resonant tunneling through a single-barrier heterostructure.

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I. INTRODUCTION

Over 50 years the effective-mass or envelope-function method is widely used to describe physical properties of various spatially inhomogeneous semiconductor systems. Originally the envelope-function approach was developed for external potentials that vary slowly on the atomic scale.[1] Nonetheless the application of this method to semiconductor nanostructures with microscopically abrupt heterointerfaces is commonly accepted and frequently gives unexpectedly good results.[2]

The central question to the effective-mass method in the context of heterostructure applications is how to connect envelopes at a heterointerface. The simplest and historically the first connection rules follow from the assumption that the effective Schrödinger equation for the envelope function $\psi(\mathbf{r})$

$$H\psi(\mathbf{r})=E\psi(\mathbf{r}) \tag{1}$$

is valid everywhere in space, and any abrupt variation of material parameters can be viewed as a limit of smooth function. This assumption allows one to obtain boundary conditions by integrating Eq. (1) over an infinitesimally small distance across the interface.[3] As a result we get the connection rules[4,2]

$$\psi(+0)=\psi(-0),$$

$$\hat{v}_z\psi(+0)=\hat{v}_z\psi(-0), \quad \hat{v}_z=\frac{\partial H}{\partial p_z}, \tag{2}$$

(p_z is the component of momentum perpendicular to the interface) which are commonly called the standard or BenDaniel-Duke boundary conditions. For the one-band effective-mass model the boundary conditions, Eq. (2), are reduced to the continuity of ψ and $(1/m)\partial_z\psi$, where m is the effective mass. Obviously, the standard connection rules cannot be universal, since they contain only bulk parameters of materials that constitute the heterojunction and thus completely neglect internal properties of the interface. In fact, they work quite well for GaAs/$Al_{1-x}Ga_xAs$ heteropair, but fail to describe properly more complicated situations.[5,6] The failure of the standard boundary conditions was also explicitly demonstrated for a number of particular microscopic models of heterostructures.[7–10]

A natural phenomenological way to take into account the above-mentioned results is to relax the assumption of applicability of Eq. (1) near an interface and to allow for the discontinuity of both, the envelops and their first derivatives. Due to the superposition principle, wave functions at opposite sides of the interface must be connected by a linear relation. Assuming locality of this relation, we arrive at the following connection rules:

$$\begin{pmatrix} \psi(+0) \\ \partial_z\psi(+0) \end{pmatrix}=\begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}\begin{pmatrix} \psi(-0) \\ \partial_z\psi(-0) \end{pmatrix}, \tag{3}$$

where $T_{ij}\equiv\hat{T}$ is the transfer matrix. Boundary conditions of the form Eq. (3) were introduced by Ando and Mori for the one-band effective-mass model.[5] Later they were also adopted to different miltiband models that describe Γ and X conduction bands,[11,12] degenerate heavy-hole and light-hole valence bands,[13] and conduction and valence bands within the spherical Kane approximation.[14]

The transfer-matrix approach unifies all possible boundary conditions that have been suggested in the literature (for particular examples see Refs. 7,15–19). In fact, the standard boundary conditions, Eq. (2), are described by the diagonal transfer matrix: $T_{11}=1$, $T_{12}=T_{21}=0$ and $T_{22}=m(-0)/m(+0)$; $\hat{T}$ matrix with $T_{11}=1$, $T_{12}=0$ and $T_{21}\neq 0$ corresponds to the introduction of a δ-function interface potential;[7,16–18] if only off-diagonal elements contribute to the transfer matrix we obtain ''inverted'' boundary conditions[19] (see also Ref. 5), which hold with a high accuracy for GaSb/InAs interface;[5] etc. In general, all components of the transfer matrix $\hat{T}$ can be nonzero. They reflect internal structure of the heterointerface and cannot be expressed in terms of only bulk parameters. For different par-

ticular cases components of $\hat{T}$ matrix were calculated using empirical tight-binding and/or pseudopotential approaches.[11–13,20]

The general connection rules, Eq. (3), can be rigorously justified within the generalized effective-mass theory.[21–25] This approach leads to a set of integral-differential equations for envelope functions that are defined using a single Bloch basis for the whole structure. The coefficients in these equations and, therefore, the envelopes, are smooth and continuous functions even for a system with microscopically abrupt interfaces. Near an interface the coefficients depend on microscopic details of the interface. Normally a perturbation, which is caused by the interface, is localized at the atomic scale. Hence, if we are interested in the behavior of envelop functions on the scale which is larger than the lattice constant, we can use extrapolated bulk envelopes instead of the exact envelop functions. Though the exact envelopes are smooth and continuous, the extrapolated functions obey general connection rules, Eq. (3), with parameters that depend on details of the interface.[26] The regular calculation of the transfer matrix using the generalized effective-mass theory[21–23,26] is an extremely tedious task. However this theory can be considered as a foundation for the phenomenological introduction of the transfer matrix.

In this paper we follow such a phenomenological approach and develop a general method for construction of the transfer matrix (Sec. II). Namely, we assume that the differential equation (or system of equations), Eq. (1), with piecewise smooth coefficients is not applicable at interface points [which are the points of discontinuity of the coefficients in Eq. (1)]. The Hamiltonian H in Eq. (1) is defined on a space of piecewise smooth and continuous functions with linear connection rules at the points of discontinuity. We show that the Hermiticity of the Hamiltonian on this space of functions imposes the first set of restrictions on the form of connection rules. A particular consequence of these restrictions is the conservation of the flow at the interface. Similar methodology, which can be found in quantum mechanics text books,[27] has been recently applied to the one-band effective-mass model with a general form of the kinetic-energy operator.[28] The second set of restrictions follows from the symmetry—the transfer matrix must be invariant with respect to transformations of the interface symmetry group. These two sets of restrictions strongly reduce the number of components in the transfer matrix. The rest of $\hat{T}$ matrix along with band offsets should be considered as empirical parameters, which are defined from experiment (see for example Ref. 30) and/or *ab initio* calculations. The method developed in Sec. II is closely related to the common method of invariants[29] that allows to construct effective $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians for bulk semiconductors using only Hermiticity and symmetry requirements.

The general connection rules, Eq. (3), allow to describe various physical consequences of nontrivial internal details of a heterointerface. It has been demonstrated in Ref. 30 that the use of general boundary conditions removes quantitative discrepancies between square well calculations and experiment.[31] There are also more transparent qualitative effects that come from the complex structure of boundary conditions. For example, in multiband models the off-diagonal element T_{21} (which is equivalent to an interface δ potential) is responsible for the interface heavy-light hole[18] and $\Gamma-X$ electron[12,32,33] mixing. In the present paper we concentrate on a description of interface localized and resonant states.

In 1932 Tamm[34] demonstrated the existence of electronic states localized at a surface of a semiconductor. It is quite natural to expect that similar localized states with energies inside the forbidden gap can occur at an abrupt heterojunction. Such a possibility was qualitatively considered by James[35] and later by Zhu and Kroemer.[16] In Ref. 36 the existence of interface donor states was postulated to explain anomalous transport properties of undoped InAs/AlSb quantum-well structures. However, general conditions for occurrence of interface states remained unclear for a long time. This problem was addressed in Ref. 37 and recently in Ref. 38 using the tight-binding approach. Since the effective-mass method is of extreme importance for heterostructure applications, it is desirable to have a description of interface states in terms of envelope functions.

It is known that envelope-function models with the standard boundary conditions possess interface states.[39,40] However the corresponding energy levels always lie in the region of band offsets outside the energy gap of a heterojunction.[39,40] An interesting exception is the formation of localized states at heterojunctions with band inversion.[39,41,42] These states have a topological nature and are related to the supersymmetry of an inverse contact.[41]

In Sec. III of our paper we show that different types of interface states, which have energies in the forbidden gap, can be described using generalized connection rules. We apply the boundary conditions derived in Sec. II to the one-band effective-mass model and to the four-band Kane model that describe Γ-point states in III-V semiconductors. We derive general conditions for the existence of interface states, and discuss the physical meaning of the off-diagonal components in the transfer matrix. In Sec. IV we study a scattering problem and demonstrate the existence of resonant states and resonant tunneling through a single barrier stricture, which are related to nonzero off-diagonal elements in the transfer matrix. In Sec. V we summarize our results.

II. GENERAL APPROACH AND BASIC EQUATIONS

To establish a general form of connection rules we consider the standard statement of a problem within the envelope-function approach that is to find eigen functions $\psi(\mathbf{r})$ and eigen values E of a Hamilton operator H. Let, as usual, the Hamiltonian H be a second-order matrix differential operator

$$H=H_0(\mathbf{r})-\tfrac{1}{2}M_{\alpha\beta}\partial_\alpha\partial_\beta+iL_\alpha\partial_\alpha, \tag{4}$$

where $H_0(\mathbf{r})$, $M_{\alpha\beta}$, and L_α are $m\times m$ Hermitian matrixes and $\alpha,\beta=x,y,z$. We assume that the growth direction of a structure coincides with z axis and the system is spatially homogeneous in x-y plane. In this case wave functions take the form $\psi(\mathbf{r})=e^{i\mathbf{k}_\perp\mathbf{r}}\psi(z)$ ($\mathbf{k}_\perp$ is the momentum perpendicu-

lar to z axis). The function $\psi(z)$ is a solution to the one-dimensional Schrödinger equation with the Hamiltonian

$$H_z = h(z) - \gamma\partial_z^2 + iP\partial_z, \tag{5}$$

where

$$h(z) = H_0(\mathbf{r}) - \tfrac{1}{2}M_{\alpha\beta}k_{\perp\alpha}k_{\perp\beta} + iL_\alpha k_{\perp\alpha},$$
$$\gamma = \tfrac{1}{2}M_{zz}, \tag{6}$$
$$P = L_z + iM_{\alpha z}k_{\perp\alpha}.$$

We consider a system that consists of N regions with different material parameters and introduce notations z_{n-1} and z_n for the left and the right boundaries of the nth region ($n=1,\ldots,N$). Assume that $h(z)$ is a piecewise smooth function of z, whereas γ and P are piecewise constant functions. In the nth region ($z_{n-1}<z<z_n$) matrices $h(z)$, γ and P, respectively, take the values $h_n(z)$, γ_n, and P_n, where $h_n(z)$ is a smooth and continuous function, and γ_n and P_n are constants.

Let $\mathcal{W}_T$ be the space of functions $\psi(z)$, which are piecewise smooth and square integrable on every interval $z_{n-1}<z<z_n$. Besides, at every point z_n values $\psi(z_n+0)$, $\partial_z\psi(z_n+0)$, and $\psi(z_n-0)$, $\partial_z\psi(z_n-0)$ are connected by linear relations

$$\begin{pmatrix} \psi(z_n+0) \\ \partial_z\psi(z_n+0) \end{pmatrix} = T_n \begin{pmatrix} \psi(z_n-0) \\ \partial_z\psi(z_n-0) \end{pmatrix}, \tag{7}$$

where T_n ($n=1,\ldots,N$) are $2m\times 2m$ matrixes.

The differential operator H_z, Eq. (5), is well defined on the space $\mathcal{W}_T$, but not necessarily Hermitian. The Hermiticity condition imposes a restriction on a possible form of the transfer matrices T_n.

By the definition the operator H_z is Hermitian on the space $\mathcal{W}_T$ if

$$I = \langle\varphi|H_z|\psi\rangle - \langle\psi|H_z|\varphi\rangle^* = 0, \tag{8}$$

where φ and ψ belong to $\mathcal{W}_T$. Matrix elements in Eq. (8) are defined as integrals over the whole structure with the points of discontinuity being excluded

$$\langle\varphi|H|\psi\rangle = \sum_{n=1}^{N}\int_{z_{n-1}}^{z_n}\varphi^+[h_n(z) - \gamma_n\partial_z^2 + iP_n\partial_z]\psi dz. \tag{9}$$

We assume for definiteness that $z_0=-\infty$, $z_N=\infty$, and $\psi(\pm\infty)=0$. It is convenient to introduce $2m$-component vectors

$$\Psi = \begin{pmatrix} \psi(z) \\ \partial_z\psi(z) \end{pmatrix}, \quad \Phi = \begin{pmatrix} \varphi(z) \\ \partial_z\varphi(z) \end{pmatrix}, \tag{10}$$

and a ''current'' operator J_n, which acts on these vectors,

$$J_n = \begin{bmatrix} P_n & -i\gamma_n \\ i\gamma_n & 0 \end{bmatrix}. \tag{11}$$

Integration by parts in Eq. (8) leads to the following expression for the quantity I:

$$I = i\sum_{n=1}^{N}\Delta_n\{\Phi^+ J\Psi\}, \tag{12}$$

where $\Delta_n\{\Phi^+J\Psi\}$ is a jump of the quantity $\Phi^+J\Psi$ at the point $z=z_n$,

$$\Delta_n\{\Phi^+J\Psi\} = \Phi^+(z_n+0)J\Psi(z_n+0) - \Phi^+(z_n-0)J\Psi(z_n-0).$$

The Hermiticity condition $I=0$ is fulfilled if

$$\Delta_n\{\Phi^+J\Psi\} = 0$$

for every boundary and any pair of functions ψ and φ from $\mathcal{W}_T$. Using the definition of transfer matrixes, Eq. (7), we arrive at the Hermiticity condition of the following form:

$$J_n = T_n^+ J_{n+1} T_n, \tag{13}$$

which means the invariance of the ''current'' operator J under the transfer across a discontinuity point.

To simplify formulas, we consider bellow a system with a single boundary at $z=0$, which separates left ($n=1=L$) and right ($n=2=R$) regions. Hence the connection rules, Eq. (7), take the form

$$\Psi_R(0) = T\Psi_L(0), \tag{14}$$

where the transfer matrix T must satisfy the following Hermiticity condition:

$$J_r = T^+ J_l T. \tag{15}$$

Another set of restrictions follows from the fact that the T matrix in Eq. (14) should be invariant with respect to the symmetry group G of the interface plane

$$\hat{D}(g)T\hat{D}^{-1}(g) = T,$$

where $\hat{D}(g)$ is $2m\times 2m$ matrix that corresponds to an element g of the group G. Since $\psi(0)$ and $\partial_z\psi(0)$ have the same transformation properties with respect to operations of the interface symmetry group G, matrices $\hat{D}(g)$ take a block diagonal form

$$\hat{D}(g) = \begin{bmatrix} D(g) & 0 \\ 0 & D(g) \end{bmatrix}, \tag{16}$$

where $m\times m$ matrices $D(g)$ form a representation (reducible in general case) of the group G in the basis that corresponds to the bulk Hamiltonian Eq. (4). Hence the symmetry requirements can be written independently for every $m\times m$ block T_{ij} ($i,j=1,2$) of the full transfer matrix T,

$$D(g)T_{ij}D^{-1}(g) = T_{ij}. \tag{17}$$

Equations (15) and (17) provide a complete set of phenomenological requirements that restrict the form of the general connection rules Eq. (14). All transfer matrices in Eq. (14) that satisfy Eqs. (15) and (17) irrespective of their particular structure provide current conservation at a heterointerface. The structure of T matrix contains information about

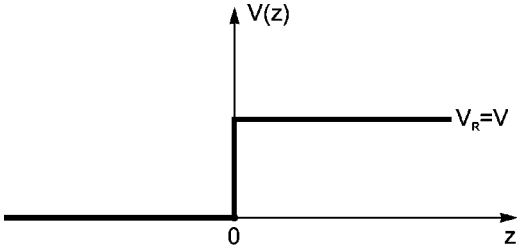

FIG. 1. One-band potential profile of the heterojunction (see text).

internal physical properties of the interface. In the following section we present a solution of these equations for the one-band effective-mass model and the four-band Kane model.

III. LOCALIZED TAMM-LIKE INTERFACE STATES WITHIN THE ENVELOPE-FUNCTION APPROACH

A. One-band effective-mass approximation

In this section we consider a single heterointerface located at the point $z=0$. The corresponding band diagram is shown in Fig. 1. The one-band effective mass Hamiltonian takes the form

$$H_n=-\frac{\nabla^2}{2m_n}+V_n, \tag{18}$$

where $n=L,R$ and $m_{L,R}$ and $V_{L,R}$ are effective masses and potentials in the left (L) and the right (R) bulk regions, respectively. The ''current'' operator, Eq. (11), for this model is $J_n=\sigma_y/2m_n$ (σ_y is the Pauli matrix). Hence the Hermiticity condition, Eq. (15), takes the form

$$\beta\sigma_y=T^+\sigma_y T, \quad \beta=\frac{m_R}{m_L}. \tag{19}$$

The general solution to this equation is

$$T=te^{i\chi}\sqrt{\beta}, \tag{20}$$

where χ is an arbitrary phase and t is a real 2×2 matrix with unit determinant

$$\det t=t_{11}t_{22}-t_{12}t_{21}=1. \tag{21}$$

Let us study the localized solutions that are allowed by the boundary condition, Eq. (14), with the transfer matrix Eq. (20). We assume for definiteness that $V_L=0$, and $V_R=V>0$ is a band offset (see Fig. 1). Wave functions of interface states take the following general form:

$$\psi_R=Ae^{i\mathbf{k}_\perp\mathbf{r}}e^{-\kappa_R z}, \quad z>0$$

$$\psi_L=Be^{i\mathbf{k}_\perp\mathbf{r}}e^{\kappa_L z}, \quad z<0. \tag{22}$$

The energy of the localized state is defined as

$$E=-\frac{\kappa_L^2}{2m_L}+\frac{\mathbf{k}_\perp^2}{2m_L},$$

where $\kappa_L^2/2m_L$ is the binding energy. Quantity κ_R in Eq. (22) is related to κ_L by the equation

$$\kappa_R=\sqrt{\beta\kappa_L^2+q^2}, \quad q^2=2m_RV+(1-\beta)\mathbf{k}_\perp^2. \tag{23}$$

Parameter q in Eq. (23) describes a degree of the heterointerface asymmetry, which is related both to the band offset and to the difference of effective masses.

Substitution of Eq. (22) into the boundary conditions leads to the following dispersion equation for κ_L:

$$\sqrt{\beta\kappa_L^2+q^2}=-\frac{t_{21}+t_{22}\kappa_L}{t_{11}+t_{12}\kappa_L}. \tag{24}$$

It is natural to assume that the diagonal elements of the matrix t are positive ($t_{11}>0, t_{22}>0$). In this case, Eq. (24) has real solutions only if t_{21} and/or t_{12} are negative. There are two types of solutions. Solutions of the first type correspond to the case $t_{21}<0$, $t_{12}\geqslant0$. The existence condition takes the form

$$-\frac{t_{21}}{t_{11}}>q. \tag{25}$$

These states occur near the lowest band edge and move down into the energy gap with an increase in $|t_{21}|$. Equation (25) shows that the existence of such solutions is restricted by the value of the asymmetry parameter q, Eq. (23). It was mentioned in the Introduction that a nonzero element t_{21} can be modeled by an interface δ potential. Negative t_{21} corresponds to an attractive interface potential. Hence Eq. (25) is analogous to the well-known condition for the existence of bound states in a potential well with asymmetric barriers.[43] If $m_L\neq m_R$ ($\beta\neq1$) the asymmetry parameter q depends on two-dimensional (2D) momentum $k_\perp$ [see Eq. (23)]. Therefore Eq. (25) defines a line in $\mathbf{k}_\perp$ space, which separates localized 2D interface states and delocalized 3D continuum states. Analogous 2D-3D transformations were recently studied in asymmetric quantum wells.[44]

Solutions of the second type are related to negative values of the second off-diagonal element t_{12}. They exist at arbitrary $t_{12}<0$ and $t_{21}\geqslant0$. At small negative t_{12} the energy levels, which correspond to these states, lie deep in the forbidden gap and approach the band edge with an increase in $|t_{12}|$. The solutions of the second type can be naturally viewed as states that originate from a lower (for example, valence) band and move up with an increase in an effective interface potential. In Sec. III C we shall return to this point and discuss a possible interpretation of the element t_{12} in terms of a local perturbation of remote bands.

Obviously, the solutions of both types can coexist if both off-diagonal elements are negative.

B. Interface states in the four-band Kane model

To study interface states in multiband systems and to illustrate the importance of the symmetry requirements Eq. (17), we consider the four-band Kane model, which describes Γ-point states in III-V zinc blend semiconductors without spin-orbit splitting. We focus our attention on the conditions of formation of interface states. These conditions can be obtained with $\mathbf{k}_\perp$ being taken zero, which is assumed

below. Specifically we consider a single (001) heterojunction and find the interface states that originate from Δ-line states ($\mathbf{k}_\perp = 0$).

It is convenient to introduce the following basis:

$$\{\chi_j\} = \{|S\rangle, |Z\rangle, |X_+\rangle, |X_-\rangle\}, \tag{26}$$

where $|X_\pm\rangle = \frac{1}{\sqrt{2}}(|X\rangle \pm |Y\rangle)$. In this basis the Δ-line Hamiltonian takes a block diagonal form[29]

$$H_n = \begin{bmatrix} H^n_{sz} & 0 \\ 0 & H^n_\pm \end{bmatrix}, \tag{27}$$

where H^n_{sz} and $H^n_\pm$ are 2×2 matrices that correspond to $|S\rangle$, $|Z\rangle$, and $|X_+\rangle$, $|X_-\rangle$ pairs of states, respectively, ($n = L, R$)

$$H^n_{sz} = \begin{bmatrix} E_{cn} - \dfrac{\partial_z^2}{2m_n} & P_n \partial_z \\ -P_n \partial_z & E_{vn} - \dfrac{\partial_z^2}{2m'_n} \end{bmatrix},$$

$$H^n_\pm = \left(E_{vn} + \frac{\partial_z^2}{2m_{vn}} \right) I. \tag{28}$$

In Eq. (28) E_{cn} and E_{vn} are the energies of conduction and valence band edges, respectively, and I is the 2×2 unit matrix.

First we establish the general form of boundary conditions for this system. The transfer matrix

$$T = \begin{bmatrix} \hat{T}_{11} & \hat{T}_{12} \\ \hat{T}_{21} & \hat{T}_{22} \end{bmatrix}, \tag{29}$$

which enters the connection rules, Eq. (14), consists of four 4×4 blocks. Every block $\hat{T}_{ij}$ ($i,j = 1,2$) must satisfy the symmetry conditions Eq. (17). The symmetry group of (001) plane for zinc blend structure is the group C_{2v} (Ref. 18) which has four elements: the unit element E, a second-order axis C_2, and two mutually perpendicular reflection planes σ_1 and σ_2. This group has four classes and thus four irreducible representations. Each function from the set $\{\chi_j\}$, Eq. (26), is the basis function for one of the irreducible representations. Namely, functions $|S\rangle$ and $|Z\rangle$ correspond to the same representation A_1, whereas functions $|X_+\rangle$ and $|X_-\rangle$ are related to the representations B_1 and B_2, respectively. Thus matrices $D(g)$—which enter the symmetry conditions, Eq. (17)—have a diagonal form in the basis Eq. (26)

$$\begin{aligned} D(E) &= \mathrm{diag}(1,1,1,1), \\ D(C_2) &= \mathrm{diag}(1,1,-1,-1), \\ D(\sigma_1) &= \mathrm{diag}(1,1,1,-1), \\ D(\sigma_2) &= \mathrm{diag}(1,1,-1,1), \end{aligned} \tag{30}$$

where $\mathrm{diag}(\cdots)$ stands for the set of diagonal elements. Straightforward calculations show that the general solution to Eq. (17) with $D(g)$ Eq. (30) takes the form

$$\hat{T}_{ij} = \begin{bmatrix} \hat{T}^{ij}_{sz} & 0 & 0 \\ 0 & T^{ij}_+ & 0 \\ 0 & 0 & T^{ij}_- \end{bmatrix}, \tag{31}$$

where $\hat{T}^{ij}_{sz}$ is an arbitrary 2×2 matrix and $T^{ij}_\pm$ are arbitrary numbers. Consequently, pairs of states ($|S\rangle, |Z\rangle$) and ($|X_+\rangle, |X_-\rangle$) as well as the states $|X_+\rangle$ and $|X_-\rangle$ are decoupled due to the symmetry requirements. It is worth mentioning that the solution, Eq. (31), to Eq. (17) for C_{3v} interface symmetry group is absolutely general and is valid for arbitrary 4×4 Hamiltonian in the basis Eq. (26). For a particular case of the Δ-line Kane Hamiltonian Eq. (27), we get three independent problems. Two of them correspond to the solution of two independent one-band Schrödinger equations with general boundary conditions (see Sec. III A) for decoupled $|X_+\rangle$ and $|X_-\rangle$ valence bands. It is worth mentioning that if $T^{ij}_+ \neq T^{ij}_-$, which is allowed by the symmetry, the connection rules, Eqs. (14), (29), (31), lead to a heavy-light hole mixing. In fact, the connection rules

$$\begin{aligned} \partial_z \psi_{XR}(0) &= \partial_z \psi_{XL}(0) + T_{l-h} \psi_Y(0), \\ \psi_{X,YL}(0) &= \psi_{X,YR}(0), \end{aligned} \tag{32}$$

which are used[18] to describe the heavy-light hole mixing at the normal hole incidence, represent a particular case of the T matrix Eqs. (29), and (31), with $T^{jj}_\pm = 1$, $T^{12}_\pm = 0$ and $T^{21}_+ = -T^{21}_- = T_{l-h}$.

To describe localized states that correspond to the subspace $\{|S\rangle, |Z\rangle\}$ we have to solve the two-band Schrödinger equation with the Hamiltonian H_{sz} Eq. (28). The boundary conditions to this equation are defined via the transfer matrix $\hat{T}_{sz}$, which has no symmetry restrictions since both $|S\rangle$ and $|Z\rangle$ correspond to the same representation A_1 of the interface group C_{2v}.

To simplify further calculations we neglect the second-derivative terms in H_{sz}. This reduces the problem to the solution of two coupled first-order differential equations

$$\begin{bmatrix} E_{cn} - E & P_n \partial_z \\ -P_n \partial_z & E_{vn} - E \end{bmatrix} \psi_n(z) = 0. \tag{33}$$

Since the highest spatial derivative in Eq. (33) is of the first order we should not include the derivatives of wave functions in the boundary condition. Therefore, the transfer matrix $\hat{T}_{sz}$ has only one nonzero 2×2 block $T^{11}_{sz} \equiv T_{sz}$, which is restricted only by the Hermiticity condition. The "current" operator for the problem Eq. (33) takes the form $J_j = P_j \sigma_y$. Hence the Hermiticity condition, Eq. (15), formally coincides with Eq. (19)

$$\gamma \sigma_y = T^+_{sz} \sigma_y T_{sz}, \quad \gamma = \frac{P_L}{P_R}. \tag{34}$$

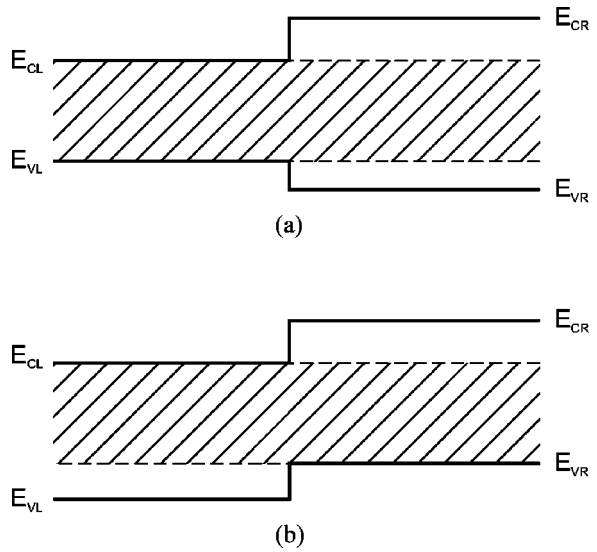

FIG. 2. (a) Band digram for a heterojunction of the I type; (b) Band digram for a heterojunction of the II type

The solution to Eq. (34) is an arbitrary real 2×2 matrix with fixed determinant and with an arbitrary phase (see Sec. III A)

$$T_{sz}=te^{i\chi}\sqrt{\gamma}, \quad \det t=1. \tag{35}$$

Considering a localized interface solution

$$\psi_R(z)=A\begin{pmatrix}u_R\\ v_R\end{pmatrix}e^{-\kappa_R z}, \quad \psi_L(z)=B\begin{pmatrix}u_L\\ v_L\end{pmatrix}e^{\kappa_L z}, \tag{36}$$

we get the following dispersion equation:

$$F_R(E)=\frac{t_{12}-t_{11}F_L(E)}{t_{22}-t_{21}F_L(E)}, \tag{37}$$

where

$$F_n(E)=\sqrt{\frac{E-E_{vn}}{E_{cn}-E}}. \tag{38}$$

The localized solution of the form Eq. (36) exists if the energy E lies in the forbidden gap of the heterojunction

$$\max\{E_{vL},E_{vR}\}<E<\min\{E_{cL},E_{cR}\},$$

which is shown by shaded region in Fig. 2. It is convenient to introduce a new variable

$$x(E)=F_L(E)=\sqrt{\frac{E-E_{vL}}{E_{cL}-E}} \tag{39}$$

and rewrite the dispersion equation, Eq. (37), in the form

$$F_R(x)=\frac{t_{12}-t_{11}x}{t_{22}-t_{21}x}, \tag{40}$$

where the function $F_R(x)$ is defined as follows:

$$F_R(x)=\sqrt{\frac{E_{vL}-E_{vR}+x^2(E_{cL}-E_{vR})}{E_{cR}-E_{vL}+x^2(E_{cR}-E_{cL})}}. \tag{41}$$

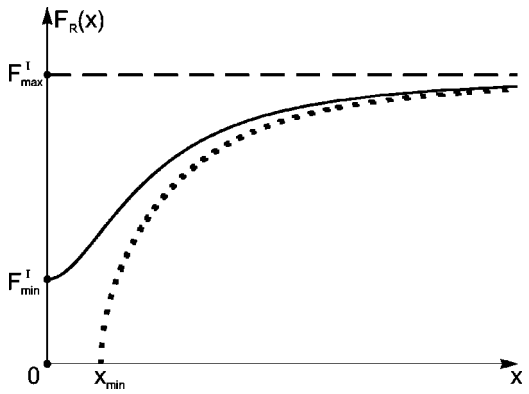

FIG. 3. Dependence F_R vs x [see Eq. (40) in the text]. Solid (dotted) line shows $F_R(x)$ for the heterojunction of the I (II) type.

We analyze the solutions of Eq. (40) under the natural assumption $t_{11}>0$ and $t_{22}>0$. We also assume that $E_{cR}>E_{cL}$, i.e., the conduction-band offset $V=E_{cR}-E_{cL}$ is positive (see Fig 2). Therefore, a heterointerface of the I type [Fig. 1(a)] corresponds to the condition

$$E_{vR}<E_{vL}, \tag{42}$$

whereas the inverse inequality

$$E_{vR}>E_{vL} \tag{43}$$

holds if the heterostructure belongs to the II type [see Fig. 2(b)].

First we consider heterointerfaces of the I type. In this case the region of the energy gap [shaded region in Fig. 2(a)]

$$E_{vL}<E<E_{cL}$$

maps to the region

$$0<x<\infty$$

of the variable x. When x goes from 0 to ∞, the function $F_R(x)$ in the right-hand side of Eq. (40) monotonically increases from

$$F^I_{\min}=\sqrt{(E_{vL}-E_{vR})/(E_{cR}-E_{vL})} \tag{44}$$

at $x=0$ (which corresponds to $E=E_{vL}$) to the value

$$F^I_{\max}=\sqrt{(E_{cL}-E_{vR})/(E_{cR}-E_{cL})} \tag{45}$$

at $x=\infty$ ($E=E_{cL}$). The function $F_R(x)$ for a heterojunction of the I type is shown by solid line in Fig. 3. The behavior of the right-hand side in Eq. (40) depends on the signs of the off-diagonal elements t_{12} and t_{21}. The dispersion equation, Eq. (40), has real solutions if at least one of the off-diagonal elements is positive. If t_{12} and t_{21} have opposite signs there exists only one solution to Eq. (40).

Let us analyze different cases separately.

(i) $t_{12}>0$, $t_{21}\leqslant 0$. In this case the right-hand side in Eq. (40) is a decreasing function of x. A solution exists if

$$\frac{t_{12}}{t_{22}}>\sqrt{\frac{E_{vL}-E_{vR}}{E_{cR}-E_{vL}}}=F^I_{\min}. \tag{46}$$

This solution can be identified with an acceptor interface state that originates from the valence band and moves up from the edge of the valence band E_{vL} to the edge of the conduction band E_{cL} with an increase in t_{12}.

(ii) $t_{21}>0$, $t_{12}\leqslant 0$. A solution to Eq. (40) exists under the following condition

$$\frac{t_{21}}{t_{11}}>\sqrt{\frac{E_{cR}-E_{cL}}{E_{cL}-E_{vR}}}=(F^{I}_{\max})^{-1}. \tag{47}$$

This is a donor interface state originated from the conduction band. With an increase in t_{21} the energy level, which corresponds to this state, moves through the energy gap from E_{cL} to E_{vL}.

If the heterointerface belongs to the II type, then E_{vR} forms a lower bound of the energy gap [shaded region in Fig. 2(b)]. Hence the energy gap

$$E_{vR}<E<E_{cL}$$

maps to the region

$$x_{\min}\equiv\sqrt{(E_{vR}-E_{vL})/(E_{cL}-E_{vR})}<x<\infty$$

in the x axis.

The function $F_R(x)$ in Eq. (40) increases from zero at $x=x_{\min}$ $(E=E_{vR})$ to the value $F^{\mathrm{II}}_{\max}=F^{\mathrm{I}}_{\max}$ Eq. (45) at $x=\infty$ $(E=E_{cL})$. This function is shown by the dotted line in Fig. 3. Consequently, only the condition for the existence of the acceptor state is changed. For the heterointerface of the II type, the existence condition, Eq. (46), is replaced by the inequality

$$\frac{t_{12}}{t_{11}}>\sqrt{\frac{E_{vR}-E_{vL}}{E_{cL}-E_{vR}}}=x_{\min}. \tag{48}$$

The condition for the existence of the donor state, Eq. (47), remains unchanged.

Acceptor and donor interface states coexist if $t_{12}t_{21}<t_{11}t_{22}$ $(t_{12}>0,t_{21}>0)$ and the conditions (46) [Eq. (48) for the II-type structure] and (47) are fulfilled simultaneously.

C. Physical meaning of the off-diagonal elements in the transfer matrix

In this section we discuss a possible interpretation of the elements T_{12} and T_{21} in the transfer matrix for the one-band effective mass model.

It is well known[20,17] that the element T_{21} can be interpreted as an interface δ-function potential. Indeed, a nonzero T_{21} introduces a jump of the first derivative, which is proportional to the value of the wave function, exactly as an interface δ potential does. The physical meaning of the second element T_{12} is less clear (see, for example, discussions in Refs. 20,17, and 26). In Sec. III A we have shown that there exist localized states that are related to nonzero T_{12}. These states behave as ''acceptor'' states that originate from remote lower bands. Therefore, it is natural to expect that the element T_{12} is related to a local perturbation of these remote bands though they are not explicitly included in the bulk one-band Hamiltonian. To confirm this interpretation we consider a one-band model as the limit of the two-band model with the following Hamiltonian:

$$H=\begin{bmatrix} E_c(z) & P\partial_z \\ -P\partial_z & E_v(z)\end{bmatrix}+\begin{bmatrix} g_c & 0 \\ 0 & g_v\end{bmatrix}\delta(z), \tag{49}$$

where $E_{c(v)}(z)$ describes the profile of the conduction (valence) band. The first term in Eq. (49) corresponds to bulk regions, whereas the second term models a local perturbation caused by the interface.

The boundary conditions for the two-component envelope function can be obtained by the integration of the Schrödinger equation

$$H\begin{pmatrix}\psi\\ \varphi\end{pmatrix}=E\begin{pmatrix}\psi\\ \varphi\end{pmatrix} \tag{50}$$

over a small segment $[-a,a]$ and taking the limit $a\to 0$. The result of the integration takes the form

$$\psi_R(0)-\psi_L(0)=\frac{g_v}{P}\lim_{a\to 0}\int_{-a}^{a}\delta(z)\varphi(z)dz,$$

$$\varphi_R(0)-\varphi_L(0)=-\frac{g_c}{P}\lim_{a\to 0}\int_{-a}^{a}\delta(z)\psi(z)dz.$$

Using the identity

$$\int_{-a}^{a}\delta(z)\,\theta(z)dz=\frac{1}{2}$$

[$\theta(z)$ is the Heaviside function] we arrive at the connection rules

$$\begin{pmatrix}\psi_R\\ \varphi_R\end{pmatrix}=\begin{pmatrix}t_{11} & t_{12}\\ t_{21} & t_{22}\end{pmatrix}\begin{pmatrix}\psi_L\\ \varphi_L\end{pmatrix}, \tag{51}$$

where

$$t_{11}=t_{22}=\frac{1-g_cg_v/4P^2}{1+g_cg_v/4P^2}, \tag{52}$$

$$t_{12}=\frac{g_v/P}{1+g_cg_v/4P^2},\quad t_{21}=-\frac{g_c/P}{1+g_cg_v/4P^2}. \tag{53}$$

Equations (51)–(53) show that both off-diagonal elements for two-band model are reproduced by the simple interface term [Eq. (49)], though the transfer matrix in Eq. (51) is still not of the most general form [compare to Eq. (35)]. We can also clarify the physical meaning of the interface solutions for the two-band model which has been considered in Sec. III B. According to the results of Sec. III B the interface solution of acceptor type exists if t_{12} is positive. Positive t_{12} corresponds to positive g_v [see Eq. (53)] and, consequently, to a local perturbation of the valence band, which is attractive for holes. Analogously, the solution of the donor type is related to a positive value of t_{21}, which corresponds to negative g_c and a local perturbation of the conduction band, attractive for electrons.

Let us derive the one-band model, which is related to the two-band Hamiltonian Eq. (49). If the energy E in Eq. (50) is close to the edge of the conduction band

$$|E-E_c(z)|/\Delta(z)\ll 1$$

($2\Delta=E_c-E_v$ is the energy gap), we can express the lower component of the spinor in Eq. (50) in terms of the upper component

$$\varphi(z)\approx -\frac{P}{2\Delta(z)}\partial_z\psi(z). \tag{54}$$

The upper component $\psi(z)$ plays the role of the wave function, which in the bulk regions satisfies the one-band Schrödinger equation

$$-\partial_z\frac{1}{2m}\partial_z\psi(z)=[E-E_c(z)]\psi(z), \tag{55}$$

where $m(z)=\Delta(z)/P^2$ is the effective mass. Equation (55) should be supplemented by boundary conditions that are obtained by the substitution, Eq. (54), to the connection rules [Eq. (51)]. The final boundary conditions for the one-band model take the form

$$\begin{pmatrix}\psi_R\\ \partial_z\psi_R\end{pmatrix}=\begin{pmatrix}T_{11} & T_{12}\\ T_{21} & T_{22}\end{pmatrix}\begin{pmatrix}\psi_L\\ \partial_z\psi_L\end{pmatrix}, \tag{56}$$

with the following elements of the transfer matrix:

$$T_{11}=\frac{m_L}{m_R}T_{22}=\frac{1-g_cg_v/4P^2}{1+g_cg_v/4P^2}, \tag{57}$$

$$T_{12}=-\frac{g_v/2\Delta_L}{1+g_cg_v/4P^2},\quad T_{21}=\frac{2m_Rg_c}{1+g_cg_v/4P^2}. \tag{58}$$

Thus, the off-diagonal element T_{12}, Eq. (57), is proportional to the strength g_v of the local perturbation of the remote valence band. A potential, which is attractive for holes, corresponds to positive g_v and thus negative T_{12}. This explains the results of Sec. III A and confirms our interpretation of the interface state related to the element T_{12}.

IV. RESONANT TUNNELING THROUGH A SINGLE BARRIER WITH COMPLEX INTERFACES

As we have seen in Sec. III, a nontrivial internal structure of a single heterointerface, which is described by the generalized boundary conditions, allows for the existence of localized interface states. In this section we show that the interference effects in a system with more than one interface can result in the formation of resonant interface state. The most transparent manifestation of these states is the resonant tunneling through a single-barrier structure. We shall demonstrate this effect for the one-band effective-mass model.

Let us consider a single-barrier heterostructure with a rectangular potential barrier of the height V and the width L. The standard scattering solution to the Schrödinger equation is defined by the following asymptotic form of the wave function:

$$\psi(z)=\begin{cases}e^{ikz}+r_ke^{-ikz}, & z\to-\infty\\ t_ke^{ikz}, & z\to+\infty,\end{cases} \tag{59}$$

where the wave vector k is related to the energy of the incident wave $E=k^2/2m$. Using the general connection rules, Eq. (14), and performing straightforward calculations we arrive at the following expression for the transparency coefficient $D_k=|t_k|^2$:

$$D_k=4k^2\kappa^2\{[(\kappa^2T_{11}^2+k^2T_{22}^2+T_{21}^2+k^2\kappa^2T_{12}^2)\sinh\kappa L +2\kappa(T_{11}T_{21}+k^2T_{22}T_{12})\cosh\kappa L]^2+4k^2\kappa^2\}^{-1}, \tag{60}$$

where

$$\kappa=\sqrt{2mV-k^2}.$$

The transparency D_k, Eq. (60), has an explicit resonant structure and turns into unity at the condition

$$\tanh\kappa L=-\frac{2\kappa(T_{11}T_{21}+k^2T_{22}T_{12})}{\kappa^2T_{11}^2+k^2T_{22}^2+T_{21}^2+k^2\kappa^2T_{12}^2}. \tag{61}$$

If $L\to\infty$, Eq. (61) has no solutions. However, the resonance occurs if the width of the barrier L becomes smaller than some critical value L_c and if at least one of the off-diagonal elements is negative.

To reveal the physical nature of the resonance condition, Eq. (61), we consider the simplest nontrivial transfer matrix with only one nonzero off-diagonal element. Namely, we assume that $T_{11}=T_{22}=1$, $T_{12}=0$, and $T_{21}\neq 0$. This transfer matrix corresponds to the δ-function interface potential of the strength $g=2mT_{21}$. Since the resonant solution exists only for negative T_{21}, we also assume that $T_{21}<0$. Under the above assumptions the resonance condition, Eq. (61), reduces to the equation

$$\tanh\kappa L=\frac{2\kappa|T_{21}|}{2mV+T_{21}^2}. \tag{62}$$

Introducing the following dimensionless variables:

$$x=\frac{\kappa}{\sqrt{2mV}}=\sqrt{1-\frac{E}{V}}, \tag{63}$$

$$\tau=2\frac{|T_{21}|/\sqrt{2mV}}{1+(|T_{21}|/\sqrt{2mV})^2}, \tag{64}$$

$$l=L\sqrt{2mV}, \tag{65}$$

we transform Eq. (62) to the form

$$\tanh xl=\tau x. \tag{66}$$

Parameter τ in the right hand side in Eq. (66) cannot exceed unity ($\tau\leqslant 1$). In fact, the function $\tau(|T_{21}|/\sqrt{2mV})$ [Eq. (64)] (see Fig. 4) reaches its maximum value $\tau_{\max}=1$ at

$$|T_{21}|/\sqrt{2mV}=1. \tag{67}$$

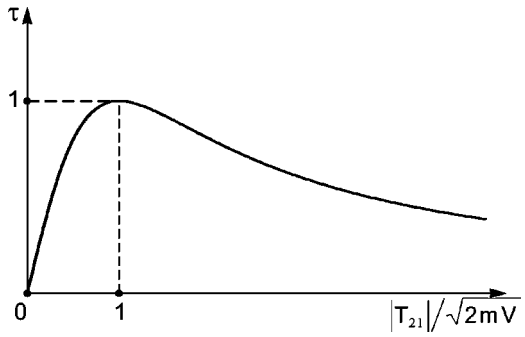

FIG. 4. Functional dependence of τ on $|T_{21}|/\sqrt{2mV}$ [Eq. (64)].

Note, that Eq. (67) defines the critical value of $|T_{21}|$, which is required for the existence of the localized state at the single heterointerface. Indeed, Eq. (25) shows that the interface bound state exists if $|T_{21}|/\sqrt{2mV}>1$. Since the behavior of solutions to Eq. (66) is governed by the parameter τ, the existence of the under-the-barrier resonances is independent of the presence or absence of bound states in the separate single interface. We shall see, however, that these resonances are closely related to the bound states, which exist in the combined double-interface structure.

Under-the-barrier resonances correspond to the solutions to Eq. (66) in the region $0<x<1$ $(0<E<V)$. Graphical solution of Eq. (66) is illustrated in Fig. 5, where the functions τx and $\tanh xl$ are plotted by dashed and solid lines, respectively. The required solution exists if parameter l, which is proportional to the width of the barrier, satisfies the inequalities

$$\tau<l<l_c, \tag{68}$$

where l_c is the solution to the equation $\tanh l_c=\tau$

$$l_c=\frac{1}{2}\ln\frac{1+\tau}{1-\tau}. \tag{69}$$

Figure 5 shows that with a decrease in l we first meet the resonance condition at $l=l_c$. The solution $x=1$ corresponds to the resonant transparency $D_k=1$ at zero energy $E=0$. With the further decrease in l the resonance energy moves up, reaches the the top of the barrier $E=V$ $(x=0)$ at $l=\tau$, and enters the over-the-barrier continuum.

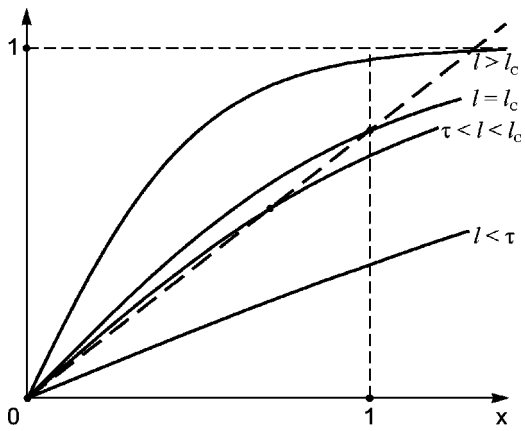

FIG. 5. Graphical solution of the equation $\tanh xl=\tau x$ [Eq. (66)], which defines the behavior of the under-the-barrier resonance.

The asymptotic form of the scattering solution, Eq. (59), at $k=-iq$, $t_{iq}=\pm 1$ and $r_{iq}=0$ exactly coincides with the asymptotic form of a localized solution. Hence the condition for the resonant transparency at zero energy $|t_{k=0}|=1$ is, in fact, the condition for appearance/disappearance of a localized state (symmetric or antisymmetric). Thus, the resonant state is nothing but the localized state (obviously antisymmetric) pushed out of the band gap.

Now we are able to describe the evolution of both resonant and localized states with the change of the barrier width L at fixed V and $|T_{21}|$. We consider separately two different cases.

(i) $|T_{21}|/\sqrt{2mV}>1$. At $L\to\infty$ there exist two degenerate localized states that are related to the well-separated heterointerfaces. With a decrease in L the degeneracy is lifted and, at $L=L_c=l_c/\sqrt{2mV}$, the upper state is pushed out of the band gap to form the resonance. With a further decrease in L the resonance moves up and crosses the top of the barrier at $L=\tau\sqrt{2mV}$. At $L<\tau\sqrt{2mV}$ we have no resonance, but only the localized state.

(ii) $|T_{21}|/\sqrt{2mV}<1$. At $L>L_c$ there exists neither localized nor resonant state. The critical value $L=L_c$ corresponds to the creation of the resonance-bound state pair. When L becomes smaller than L_c the resonance moves up and reaches the top of the barrier at $L=\tau\sqrt{2mV}$, whereas the localized state moves down into the energy gap.

Thus in either case the resonant transparency is always accompanied by the bound state. The resonance and the localized state can be qualitatively interpreted as antibonding and bonding orbitals, respectively.

It is interesting to note that in the simple case of zero element T_{12} the resonant transparency of the single-barrier structure has a clear counterpart in the classical electrodynamics. The corresponding system is a metallic slab, which is covered on either side by dielectric layers. The metallic region with $\varepsilon(\omega)<0$ models the barrier, whereas the dielectric coating corresponds to the attractive interface potential. The resonant transparency of electromagnetic waves through such a system has been described theoretically[45,46] and observed experimentally in Ref. 46. If both off-diagonal elements are nonzero, the resononant tunneling through a single-barrier heterostructure apparently has no optical analog.

V. CONCLUSION

It it commonly accepted that the effects of a microscopic structure of a heterointerface can be incorporated into the envelope-function method by the use of generalized connection rules. Such connection rules are normally formulated in terms of the interface transfer matrix. In this paper we presented the general method that allows to construct the transfer matrix for an arbitrary system. We showed that the Hermiticity of the Hamiltonian and the symmetry of the interface plane impose the restrictions on the form of the transfer matrix. These restrictions can be formulated as a set of equations for components of the transfer matrix. Solution

of these equations defines the general form of the boundary conditions for a given interface. To illustrate this approach we considered the one-band and four-band envelope-function models and established the conditions for the existence of Tamm-like localized interface states. We have also demonstrated that in a system with more than one heterointerface there exists a possibility for new physical effects, such as the resonant tunneling through a single potential barrier.

In this paper we did not discuss the application of our general results to particular heterostructures, which often requires a consideration of multiband Hamiltonians with the spin-orbit interaction and in-plane dispersion being taken into account and deserves a separate publication.[47] It is, however, more important that such an application also requires a knowledge of phenomenological parameters that enter into the generalized boundary conditions. Identification of these parameters using the results of experiments or *ab initio* calculations is by far not a simple task. We believe, however, that the physical effects that have been described in our paper and which originate solely from the nontrivial structure of the boundary conditions, could be helpful in resolving this problem.

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