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InAs/GaSb interfaces; the problem of boundary conditions

Smadar de-Leon, B Laikhtman and L D Shvartsman
Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel

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Abstract. We present here a derivation of phenomenological boundary conditions for envelope functions at the interface between an InAs layer and a GaSb layer. The overlap of the valence band of GaSb with the conduction band of InAs leads to a coupling between electrons with total angular momentum 1/2 and holes with total angular momentum 3/2. The method that we use to match these wave-functions is that of the minimizing of the total energy of the system including the surface energy. We consider the different spinor characters of the states explicitly, and derive the required boundary conditions, which are not dependent on any specific microscopic model. The proposed approach is general, and may be used to obtain boundary conditions for other complicated cases of interfaces.

1. Introduction

There is a challenge in the investigation of InAs/GaSb heterostructures. The strong motivation for exploring the system is its unique band alignment: the bottom of the conduction band in InAs lies below the top of the valence band in GaSb, so there is an overlap between the valence band in GaSb and the conduction band in InAs. From either side of the interface, there are allowed states that differ from each other in total angular momentum and in the sign of the effective mass. As a result, the ground state of the system is an electron gas in the InAs layer, coexisting with a hole gas in the GaSb layer (see figure 1). The coexistence of electrons and holes on different sides of the interface has been experimentally confirmed (see, e.g., reference [1]). This makes the system a natural candidate for investigation if one is trying to detect Bose–Einstein condensation of excitons [2–5]. This aspect of the system has been studied theoretically [6–8]. Experimentally, evidence has been obtained of an excitonic ground state for a specific InAs/GaSb structure [9].

The system also has considerable potential as regards device application. One feature making this apparent is the strongly non-linear behaviour of the current–voltage characteristics that was observed in measurements of vertical transport through GaSb–InAs–GaSb quantum wells. When the voltage reaches a certain value, a sharp drop in the current is measured [10–13].

The definition of boundary conditions for the interface between InAs and GaSb is one of the major keys to the understanding of this system. It is important for theoretical investigation of all of the aspects of the system that were described above. The coupling between the s-like conduction electrons and the p-like valence holes is a complicated problem. While the conduction band in InAs is quite simple, and a good approximation for it is given by a parabolic dispersion relation, the valence band in GaSb has a complicated structure, and is described by the Luttinger 4 × 4 Hamiltonian [14]. There are two bulk

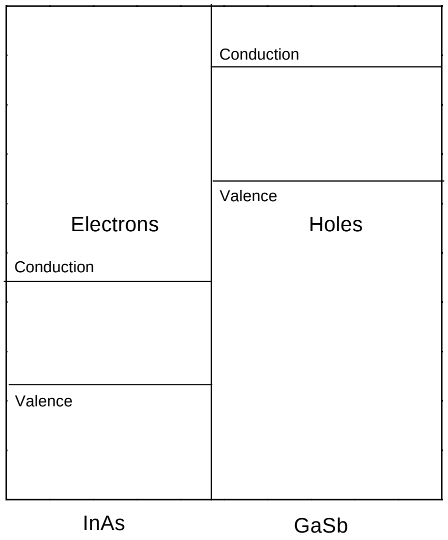

Figure 1. The InAs/GaSb band structure. We do not show band bending here.

valence sub-bands—those of the heavy and the light holes; both are anisotropic and doubly degenerate. We consider a thin layer of each material, which leads to size quantization, and while the quantization of the conduction electron in the InAs layer is simple, the quantization of the valence band leads to a number of non-trivial kinetic and optical phenomena caused by the hybridization between the heavy and the light holes, and anisotropy of the spectrum [15–19]. Finally, we need to couple the simple quantized electron sub-bands and the complicated quantized hole sub-bands.

Previous work that dealt with the boundary conditions for heterostructures usually consisted in some generalization of the continuity of the wave-functions, and the conservation of the quantum mechanical current normal to the interface [20–24, 26–32]. In most of the studies, the first condition was derived assuming the envelope function to be continuous at the interface [21–26, 28–30]. Harrison [20] generalized this assumption, by multiplying the envelope function and its normal derivative by different parameters, which depend on the energy and the transverse wave-vector. The second condition is usually obtained by assuming that the kinetic energy has a Hermitian form, and that the effective mass has a spatial dependence. Integration of the Schrödinger equation across the interface yields the boundary condition [21, 22, 26, 29–31]. However, for systems in which we need to match states with different symmetries and different effective masses, the assumption of continuity of the envelope function is no longer justified. It is also impossible to integrate the Schrödinger equation across the interface, because it is impossible to write down such an equation for the region between two materials with different symmetries and different numbers of wave-function components. This is the case for InAs/GaSb heterostructures due to the unique band alignment. Another example is that of GaAs/Al$_x$Ga$_{1-x}$As heterostructures, for which there is a mixing between Γ and X conduction band valleys.

In order to derive physical boundary conditions, we have to remember that the interface is not just a mathematical surface, dividing two materials with different Bloch functions. We can consider Bloch functions only at some distance from the interface, which has the scale of the lattice constant. Within this distance, the electric potential is created by the atoms of the two different materials, and the wave-functions are strongly distorted from their bulk forms.

However, the envelope functions, which describe the spatially dependent amplitude of the wave-function, do not vary within the atomic scale. So, within the framework of the envelope function, we can expect that the details of the microscopic structure of the interface will enter only as the coefficients in the boundary conditions. Nevertheless, the degeneracy of the valence band and the different symmetries of the Bloch functions on either side of the interface prevent us from using one of the simplifying assumptions of [20–24, 26–32]. First of all, there is no reason to assume *ab initio* that the envelope functions are continuous at the interface. Second, the condition that the normal current component must be continuous at the interface is not enough on its own to provide a number of boundary conditions for several wave-function components. The latter fact is especially important for the InAs/GaSb interface, for which the numbers of wave-function components on either side of the interface are different.

A number of model boundary conditions have been suggested in references [33–38]. In these papers, the valence band was simplified: it was taken to be non-degenerate and spherically symmetric, so the envelope functions of the two materials were considered as scalars. Such a simplification leads to the loss of some of the interesting spectral and transport phenomena of the system [15–19].

In this paper we present the derivation of phenomenological boundary conditions for envelope functions, making use of the method of invariants [41]. These boundary conditions do not depend on a specific microscopic model, and have the same degree of validity as the envelope-function approximation itself. The microscopic nature of the interface enters only in the values of the phenomenological constants. The first step in this direction was made by one of us [39]; in that earlier work, a variational approach was used for the derivation of a particular boundary condition. Here we generalize this approach to obtain all of the boundary conditions for the case of spinor envelope functions with different angular momenta (and, consequently, with different number of components) on either side of the interface.

Such a generalization is absolutely necessary for the following reasons. First, the problem is general. It arises always when the materials to be matched have different symmetries of their electron spectra, e.g., electrons at the Ge/Si interface (L/X valleys), and the Γ/X transition at the interfaces between different III–V materials (see, e.g., [48]). Second, in the case of different ranks of matching spinors (in InAs–GaSb), even such an important result as the number of branches in the spectrum cannot be predicted *ab initio* without correct boundary conditions. The problem is non-trivial, because the formal combination of two generally accepted approximations, spinless electrons in InAs and fourfold-degenerate holes in GaSb, leads to an incorrect result. A phenomenological approach allows one to solve this class of problems. In the present paper we develop this approach for the particular and extremely important case of InAs–GaSb. It provides us with a way to consider the special features of this system, such as the anisotropy and non-parabolicity of the GaSb hole sub-bands, and the hybridization between the GaSb heavy and light holes and the InAs electrons.

The core of our approach is minimizing the total energy, including the surface energy. It is well known that for a uniform material the quantum mechanical variation principle leads to the Schrödinger equation [40]. We used this principle to derive the Schrödinger equations for the two materials, and the boundary conditions for the interface between them. This derivation can be applied to any interface between two media, and, in particular, for boundary conditions that match states with different symmetries and different numbers of components. In the next section we will describe the derivation of the boundary conditions from the principle of minimal energy. In the third section we clarify the meaning of the general conditions that we derived by implementing them in several important physical cases. We study properties of the interface between arbitrary materials, an interface between two identical materials, boundary conditions in the isotropic approximation, etc.

2. Derivation of the boundary conditions

In this section we derive the boundary conditions for envelope functions by minimizing the total energy including the surface energy. For this purpose, we first express the total energy in terms of electron and hole envelope functions. The assumptions that we use are the same assumptions as justify the envelope-function approximation in semiconductor heterostructures. First, we will define the framework that we use. As was mentioned above, the total angular momentum for the valence states is 3/2, so the hole wave-functions are four spinors. The total electron angular momentum is 1/2. Quite often, for simplicity, the electron states are treated as a single-component wave-function [23, 33, 35, 37, 38]. We want to match the electron states with the hole states, and considering holes as spinors and electrons as scalars we have to match fermions with bosons, which leads to decoupling. Because of this, the spinor character of the electrons cannot be neglected, and we represent electron states as 2-spinors:

$$\Psi_e = \begin{pmatrix} \Psi_{e,1/2} \\ \Psi_{e,-1/2} \end{pmatrix} \qquad \Psi_h = \begin{pmatrix} \Psi_{h,3/2} \\ \Psi_{h,1/2} \\ \Psi_{h,-1/2} \\ \Psi_{h,-3/2} \end{pmatrix}. \tag{2.1}$$

The geometry of the system is as follows: to the left, $-L_c < z < -a_c$, there is an InAs layer which is a quantum well for electrons; to the right, $a_v < z < L_v$, there is a GaSb layer which is a quantum well for holes. Between the two materials there is an interface region which we define to be some region around the plane $z = 0$: $-a_c < z < a_v$. We assume that the following condition is satisfied:

$$L_c, L_v \gg a_c, a_v > a_{0c}, a_{0v} \tag{2.2}$$

where a_{0c} and a_{0v} are the InAs and GaSb lattice constants respectively. This assumption makes the application of the envelope-function approximation valid for both materials.

The structure of the complete wave-function $\Psi(\boldsymbol{r})$ near the interface is very complicated because of the complicated electric potential in this region (figure 2). Bulk Bloch functions exist, in both materials, only at some distance from the interface, which is larger than or about the size of the unit cell. The electric potential created by the atoms in each material penetrates across the interface, and exact electron wave-functions near the interface can be substantially different from the bulk Bloch functions. Beyond the interface region, the wave-function in each material is proportional to the Bloch function. Using the envelope-function approximation, we can write down the wave-functions, away from the interface:

$$\Psi_{e,j}(\boldsymbol{r}) = \psi_{e,j}(\boldsymbol{r}) u_{e,j}(\boldsymbol{r}) \qquad -L_c < z < -a_c \tag{2.3a}$$

$$\Psi_{h,j}(\boldsymbol{r}) = \psi_{h,j}(\boldsymbol{r}) u_{h,j}(\boldsymbol{r}) \qquad a_v < z < L_v. \tag{2.3b}$$

Here $u_e(\boldsymbol{r})$, $u_h(\boldsymbol{r})$ are the Bloch functions, and $\psi_e(\boldsymbol{r})$, $\psi_h(\boldsymbol{r})$ are the envelope functions in the InAs, GaSb layers respectively. Again, the hole functions are 4-spinors, and the electrons functions are 2-spinors. (The jth component of the complete wave-function is the product of the jth components of the Bloch function, and the envelope function.)

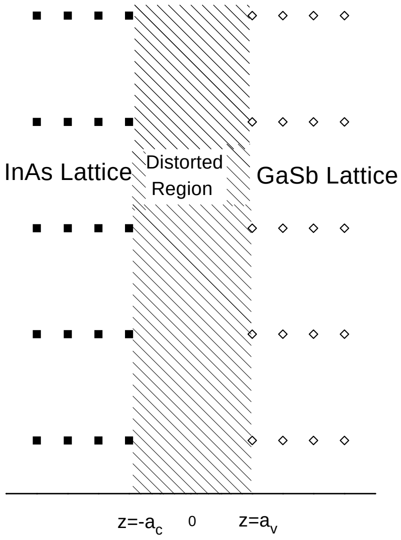

Figure 2. The InAs/GaSb heterostructure near the interface. At distances beyond a few lattice constants from the interface, the periodic potential is not affected by the interface. Near the interface, the potential is strongly distorted due to mutual penetration of the potentials of different lattices.

The envelope functions vary substantially only on the macroscopic scales L_c, L_v, and in the interface region their variation can be neglected. Thus, the wave-function in the interface region can be written as a linear combination:

$$\Psi(\boldsymbol{r}) = F_e(\boldsymbol{r})\psi_e(x, y, 0) + F_h(\boldsymbol{r})\psi_h(x, y, 0). \tag{2.4}$$

Here $F_e(\boldsymbol{r})$ is a 2-spinor, and $F_h(\boldsymbol{r})$ is a 4-spinor; these are distorted Bloch functions in the interface region.

The Schrödinger equation for the total wave-function, in all of the regions, can be obtained from the variational functional

$$\varepsilon = \int \left[-\frac{\hbar^2}{2m_0} |\boldsymbol{\nabla}\Psi|^2 + (U - E)|\Psi|^2 \right] \mathrm{d}^3 r \tag{2.5}$$

where $U(\boldsymbol{r})$ is the lattice potential and the integration is carried out over the whole system. We will show that the minimization of this functional can provide not just the Schrödinger equation for the envelope functions but also boundary conditions for them.

We can break the integration into a sum of the integrals for each region:

$$\varepsilon = \varepsilon_e + \varepsilon_h + \varepsilon_{surf} \tag{2.6a}$$

$$\varepsilon_e = \int_{-L_c<z<-a_c} \qquad \varepsilon_h = \int_{a_v<z<L_v} \qquad \varepsilon_{surf} = \int_{-a_c<z<a_v} . \tag{2.6b}$$

Here $\varepsilon_e, \varepsilon_h$ are the energies of the bulk InAs and GaSb respectively, and ε_{surf} is the surface energy.

The functionals $\varepsilon_e, \varepsilon_h$ can be calculated with the help of equation (2.3). Each of the integrals can be divided into a sum of the integrals over separate unit cells. Inside every unit cell, the envelope functions and their derivatives are considered to be constants. The Bloch functions are normalized with respect to the volume of the unit cell. For the electron functional, the result is the replacement of the electron free mass with the electron effective mass in InAs. For the holes, the calculation is more complicated, since we need to consider also the spin–orbit coupling. The calculation of the valence band effective Hamiltonian was performed by Luttinger and Kohn [14]. We will use here their results, expressed in terms of the system invariants [41]:

$$\varepsilon_e = \int_{-\infty}^{\infty} \int_{z=-L_c}^{z=0} \frac{\hbar^2}{2m_e} \nabla\psi_e^\dagger \nabla\psi_e - E\psi_e^\dagger\psi_e \, \mathrm{d}^2r \, \mathrm{d}z \tag{2.7a}$$

$$\begin{aligned}\varepsilon_h = \int_{-\infty}^{\infty} \int_{z=0}^{z=L_v} & -\frac{\hbar^2}{2m_0} \left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right) \nabla\psi_h^\dagger \nabla\psi_h - \gamma_3 \nabla_\alpha\psi_h^\dagger \left(J_\alpha J_\beta + J_\beta J_\alpha\right) \nabla_\beta\psi_h \right] \\ & - \frac{\hbar^2}{m_0}(\gamma_3 - \gamma_2) \left[\left(J_x \frac{\partial\psi_h}{\partial x}\right)^\dagger \left(J_x \frac{\partial\psi_h}{\partial x}\right) + \left(J_y \frac{\partial\psi_h}{\partial y}\right)^\dagger \left(J_y \frac{\partial\psi_h}{\partial y}\right) \right. \\ & \left. + \left(J_z \frac{\partial\psi_h}{\partial z}\right)^\dagger \left(J_z \frac{\partial\psi_h}{\partial z}\right) \right] + (\Delta - E)\psi_h^\dagger\psi_h \, \mathrm{d}^2r \, \mathrm{d}z \end{aligned} \tag{2.7b}$$

where $\boldsymbol{J}$ is the total angular momentum vector, for the hole states. In the second term of equation (2.7*b*) we use the summation rule. γ_1, γ_2, and γ_3 are the Luttinger parameters for GaSb. $\Delta \approx 150$ meV is the energy difference between the bottom of the conduction band in the InAs layer and the top of the valence band in the GaSb layer.

The functional ε_{surf} is calculated with the help of equation (2.4), in the same way as was described for the functionals $\varepsilon_e, \varepsilon_h$. The exact calculation is very complicated, due to the complicated structure of the potential and the exact wave-function. But the result is a Hermitian form of ψ_e and ψ_h:

$$\varepsilon_{surf} = \int_{-\infty}^{\infty} \psi_h^\dagger \mathcal{A}_h \psi_h + \psi_e^\dagger \mathcal{A}_e \psi_e + \psi_h^\dagger \mathcal{B} \psi_e + \psi_e^\dagger \mathcal{B}^\dagger \psi_h \big|_{z=0} \, \mathrm{d}^2r. \tag{2.8}$$

Here $\mathcal{A}_e$ is a 2×2 matrix, and represents the interface energy of the electron states. $\mathcal{A}_h$ is a 4×4 matrix, which represents the interface energy of the hole states. $\mathcal{B}$ is a 4×2 matrix, and represents the energy that is related to tunnelling between the two wells. The units of the matrix elements are [E L]—energy multiplied by length. The characteristic values of the energy and length are respectively the width of the band and the lattice constant. The matrices have to obey the symmetry of the problem. In particular, they have to be symmetric with respect to rotations of $\pi/2$ about the z-direction. The rotation generation operator is J_z. So the symmetry condition can be written as

$$\exp\left(\mathrm{i}\frac{\pi}{2} J_z\left(\frac{3}{2}\right)\right)\mathcal{A}_h = \mathcal{A}_h \exp\left(\mathrm{i}\frac{\pi}{2} J_z\left(\frac{3}{2}\right)\right) \tag{2.9a}$$

$$\exp\left(\mathrm{i}\frac{\pi}{2} J_z\left(\frac{1}{2}\right)\right)\mathcal{A}_e = \mathcal{A}_e \exp\left(\mathrm{i}\frac{\pi}{2} J_z\left(\frac{1}{2}\right)\right) \tag{2.9b}$$

$$\exp\left(\mathrm{i}\frac{\pi}{2} J_z\left(\frac{3}{2}\right)\right)\mathcal{B} = \mathcal{B} \exp\left(\mathrm{i}\frac{\pi}{2} J_z\left(\frac{1}{2}\right)\right). \tag{2.9c}$$

Here $J_z(S)$ is the matrix of the angular momentum z-projection. If the total angular momentum $S = 3/2$, it is a 4×4 matrix, and if $S = 1/2$, it is the Pauli matrix σ_z. We work in the representation where $J_z(S)$ is diagonal. $\exp[(\mathrm{i}\pi/2)J_z(S)]$ is the operator for rotation by $\pi/2$. Comparing each matrix element from either side of each equation, we see that in order to satisfy the equations both $\mathcal{A}_e$ and $\mathcal{A}_h$ have to be diagonal. The only non-vanishing matrix elements of $\mathcal{B}$ are $\mathcal{B}_{21}$ and $\mathcal{B}_{32}$. These limitations reduce the number of parameters in the problem. (More precisely, the symmetry of the interface is lower, and does not have a fourfold axis. However, the corresponding anisotropy is small and we neglect it [43].)

Now we will vary the energy ε with respect to $\psi_h^\dagger$, and with respect to $\psi_e^\dagger$. The variation vanishes near the point of minimum energy, so the condition that we apply here is

$$0 = \delta\varepsilon = \delta\varepsilon_e + \delta\varepsilon_h + \delta\varepsilon_{surf}. \tag{2.10}$$

After integration by parts with respect to z, we have contributions to the surface functional from the integrated terms of the functionals ε_e, ε_h. The contributions come from the terms which include partial derivatives, with respect to z. These integrated terms have non-vanishing value at the boundary, $z = 0$. For example, the contribution from the variation with respect to $\psi_e^\dagger$ is

$$\int_{-\infty}^{\infty}\int_{z=-L_c}^{z=0} \frac{\partial\,\delta\psi_e^\dagger}{\partial z}\frac{\partial\psi_e}{\partial z}\,\mathrm{d}^2r\,\mathrm{d}z = \int_{-\infty}^{\infty} \delta\psi_e^\dagger\,\frac{\partial\psi_e}{\partial z}\bigg|_{z=0}\mathrm{d}^2r - \int_{-\infty}^{\infty}\int_{z=-L_c}^{z=0} \delta\psi_e^\dagger\,\frac{\partial^2\psi_e}{\partial z^2}\,\mathrm{d}z\,\mathrm{d}^2r. \tag{2.11}$$

The integrated part depends only on the value of $\delta\psi_e$ at the interface, and has to be added to the functional ε_{surf}.

The finite result of the variation with respect to $\psi_e^\dagger$, $\psi_h^\dagger$ is

$$0 = \int_{-\infty}^{\infty}\int_{z=-L_c}^{z=0} \delta\psi_e^\dagger\left(-\frac{\hbar^2}{2m_e}\nabla^2\psi_e - E\psi_e\right)\mathrm{d}^2r\,\mathrm{d}z \tag{2.12a}$$

$$\begin{aligned}0 = \int_{-\infty}^{\infty}\int_{z=0}^{z=L_v} \delta\psi_h^\dagger\Bigg(\frac{\hbar^2}{2m_0}\bigg[\Big(\gamma_1 + \frac{5}{2}\gamma_2\Big)\nabla^2\psi_h - 2\gamma_3(\boldsymbol{J}\cdot\boldsymbol{\nabla})^2\psi_h \\ + 2(\gamma_3 - \gamma_2)\left(\frac{\partial^2}{\partial x^2}J_x^2 + \frac{\partial^2}{\partial y^2}J_y^2 + \frac{\partial^2}{\partial z^2}J_z^2\right)\psi_h\bigg] + (\Delta - E)\psi_h\Bigg)\,\mathrm{d}^2r\,\mathrm{d}z\end{aligned} \tag{2.12b}$$

$$0 = \int_{-\infty}^{\infty} \delta\psi_e^\dagger\left(\frac{\hbar^2}{2m_e}\frac{\partial\psi_e}{\partial z} + \mathcal{A}_e\psi_e + \mathcal{B}^\dagger\psi_h\right)\mathrm{d}^2r\bigg|_{z=0} \tag{2.12c}$$

$$\begin{aligned}0 = \int_{-\infty}^{\infty} \delta\psi_h^\dagger\Bigg(\frac{\hbar^2}{2m_0}\bigg[\Big(\gamma_1 + \frac{5}{2}\gamma_2 - 2\gamma_2 J_z^2\Big)\frac{\partial\psi_h}{\partial z} - \gamma_3(J_zJ_x + J_xJ_z)\frac{\partial\psi_h}{\partial x} \\ - \gamma_3(J_zJ_y + J_yJ_z)\frac{\partial\psi_h}{\partial y}\bigg] + (\mathcal{A}_h\psi_h + \mathcal{B}\psi_e)\Bigg)\,\mathrm{d}^2r\bigg|_{z=0}.\end{aligned} \tag{2.12d}$$

The first equation yields the Schrödinger equation for the electrons, where we replace the free-electron mass with its effective mass in InAs. The second equation yields the Schrödinger equation for the holes, where the Hamiltonian is the Luttinger Hamiltonian [14]. From the last two equations, we obtain the following boundary conditions for the interface between the two layers:

$$\mathcal{A}_e\psi_e + \mathcal{B}^\dagger\psi_h = -\frac{\hbar^2}{2m_e}\frac{\partial\psi_e}{\partial z} \tag{2.13a}$$

$$\mathcal{B}\psi_e + \mathcal{A}_h\psi_h = -\frac{\hbar^2}{2m_0}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2 - 2\gamma_2 J_z^2\right)\frac{\partial\psi_h}{\partial z} - \gamma_3(J_z\boldsymbol{J}_\parallel + \boldsymbol{J}_\parallel J_z)\cdot\boldsymbol{\nabla}_\parallel\psi_h\right]. \tag{2.13b}$$

Here we use the following notation for the in-plane vectors: $\boldsymbol{J}_\parallel = (J_x, J_y)$, $\boldsymbol{\nabla}_\parallel = (\partial/\partial x, \partial/\partial y)$. The hole function is on the right-hand side of the interface and the electron function is on the left. We used the representation from [42] for the angular momentum matrices, and the explicit form of the boundary conditions is as follows:

$$\mathcal{A}_{e,11}\psi_{e,1/2} + \mathcal{B}_{21}^\star\psi_{h,1/2} = -\frac{\hbar^2}{2m_e}\frac{\partial\psi_{e,1/2}}{\partial z} \tag{2.14a}$$

$$\mathcal{A}_{e,22}\psi_{e,-1/2} + \mathcal{B}^{\star}_{32}\psi_{h,-1/2} = -\frac{\hbar^2}{2m_e}\frac{\partial\psi_{e,-1/2}}{\partial z} \tag{2.14b}$$

$$\mathcal{A}_{h,11}\psi_{h,3/2} = -\frac{\hbar^2}{2m_0}\left[(\gamma_1 - 2\gamma_2)\frac{\partial\psi_{h,3/2}}{\partial z} - \sqrt{3}\gamma_3\left(\frac{\partial\psi_{h,1/2}}{\partial x} - \mathrm{i}\frac{\partial\psi_{h,1/2}}{\partial y}\right)\right] \tag{2.14c}$$

$$\mathcal{A}_{h,22}\psi_{h,1/2} + \mathcal{B}_{21}\psi_{e,1/2} = -\frac{\hbar^2}{2m_0}\left[(\gamma_1 + 2\gamma_2)\frac{\partial\psi_{h,1/2}}{\partial z} - \sqrt{3}\gamma_3\left(\frac{\partial\psi_{h,3/2}}{\partial x} + \mathrm{i}\frac{\partial\psi_{h,3/2}}{\partial y}\right)\right] \tag{2.14d}$$

$$\begin{aligned}\mathcal{A}_{h,33}\psi_{h,-1/2} &+ \mathcal{B}_{32}\psi_{e,-1/2} \\ &= -\frac{\hbar^2}{2m_0}\left[(\gamma_1 + 2\gamma_2)\frac{\partial\psi_{h,-1/2}}{\partial z} + \sqrt{3}\gamma_3\left(\frac{\partial\psi_{h,-3/2}}{\partial x} - \mathrm{i}\frac{\partial\psi_{h,-3/2}}{\partial y}\right)\right]\end{aligned} \tag{2.14e}$$

$$\mathcal{A}_{h,44}\psi_{h,-3/2} = -\frac{\hbar^2}{2m_0}\left[(\gamma_1 - 2\gamma_2)\frac{\partial\psi_{h,-3/2}}{\partial z} + \sqrt{3}\gamma_3\left(\frac{\partial\psi_{h,-1/2}}{\partial x} + \mathrm{i}\frac{\partial\psi_{h,-1/2}}{\partial y}\right)\right]. \tag{2.14f}$$

From this we see that there is a direct coupling between the electron and the light-hole components of the hole functions (components with total angular momentum projections on the z-direction equal to $\pm 1/2$), while the coupling to the heavy-hole components (components with total angular momentum projections on the z-direction equal to $\pm 3/2$) is through the derivatives of the hole function.

We can reduce the number of parameters in this problem by assuming that the system is invariant under a change in the sign of the total angular momentum. According to this assumption, states that have the same z-component of the total angular momentum, but with different signs, have the same energy. In particular, they have the same surface energy. This yields the following equations:

$$\mathcal{A}_{e,11} = \mathcal{A}_{e,22} \qquad \mathcal{A}_{h,11} = \mathcal{A}_{h,44} \qquad \mathcal{A}_{h,22} = \mathcal{A}_{h,33} \qquad \mathcal{B}_{21} = \mathcal{B}_{32}. \tag{2.15}$$

Here the numbers given as subscripts label the matrix elements. This and the assumption that the matrix elements have real values reduce the number of parameters in this problem to 4.

3. Discussion

The main result of this paper is the boundary condition equations (2.13) and (2.14) for the InAs/GaSb interface. Generally speaking, boundary conditions of this kind can be used for interfaces between any materials. The specifics of the material determine the structure of the matrices $\mathcal{A}$ and $\mathcal{B}$ and also the effective-mass tensor in the rhs of equation (2.13). The values of the matrix elements depend on the microscopic structure of the interface (see section 2) and this is the only effect of the microscopic structure. For instance, experimentally the InAs/GaSb interface can be formed of InSb or of GaAs. For these two cases one can expect different values of the matrix elements. In this section, we clarify the boundary conditions by applying them to a number of important physical situations. First, we consider an interface between arbitrary materials and show that the boundary conditions of the type (2.13) lead to known results if the interface is impenetrable. In the case of an interface between two identical materials with simple band structure, our conditions are equivalent to the presence of a potential barrier. Then we produce simplified boundary conditions for the isotropic approximation.

Finally, we consider some approximations for InAs/GaSb interfaces by means of which equation (2.13) can be simplified. In many practically important cases, hole sub-bands are split so strongly that only one of them (the heavy-hole sub-band) is occupied. For that reason it is desirable to have boundary conditions that include only this band. We derive these boundary conditions from the general case.

3.1. Interfaces between arbitrary materials

Generally speaking, almost any interface between different materials is impenetrable. Indeed, as was mentioned above, the units of the interface matrix elements $\mathcal{A}_e$, $\mathcal{A}_h$, and $\mathcal{B}$ are [E L]—energy multiplied by length. The length scale of the interface region is around the lattice constant, so a good estimate for the interface matrix elements is $\hbar^2/2\sqrt{m_e m_h}a_0$, where m_e, m_h are the effective masses of electrons and holes respectively. Since the length scale of the interface is of the order of the lattice constant and much smaller than the widths of the quantum wells (equation (2.2)), the order of magnitude of the interface matrix elements is much larger than the order of the rhs of the boundary condition equations (2.13):

$$\mathcal{A} \sim \mathcal{B} \sim \frac{\hbar^2}{2\sqrt{m_e m_h a_{0c} a_{0v}}} \gg \frac{\hbar^2}{m_h L_v}, \frac{\hbar^2}{m_e L_c}. \tag{3.1}$$

In the leading approximation, the rhs of equation (2.13) can be neglected. Then equation (2.13) is reduced to a system of homogeneous equations for wave-functions at the interface. In general, the determinant of this system is non-zero, and as a result the wave-functions at the interface equal zero. This boundary condition corresponds to an impenetrable barrier, i.e., two separate infinite quantum wells for electrons and holes.

So, in general, the penetration across an interface is an effect of the order of a_0/L. The penetration can be much larger if the determinant of the system is anomalously small. The value of the determinant depends on the parameters of the materials (symmetry, lattice geometry, Bloch functions). The determinant can be expected to be small if there is some similarity of the materials on either side of the interface. This is the case for a large number of practically important cases in which the materials are specifically chosen to be alike, such as different III–V materials (the Bloch functions of the same bands in these materials are similar), for which the penetration across an interface between Γ points of different materials is typically strong. One of the most important examples is the (001) GaAs/AlAs interface, for which the surface energy can be discarded, and the boundary conditions are the continuity of the wave-functions and that of $(1/m)(\partial\psi/\partial z)$. For the Γ/X matching, the same interface is nearly impenetrable [34, 48], and boundary conditions of the type of equation (2.13) are more appropriate [28]. One should keep in mind that, even if the penetration of wave-functions across the barrier is as small as a_0/L, it can still lead to substantial effects, e.g., a significant shift of the energy levels.

For some specific choice of the materials, the determinant may appear to be zero. That means that there are linear relations between the left-hand sides of equations (2.13). If equations (2.13) contain n scalar equations and there are $r < n$ relations between their left-hand sides, then these equations are consistent only if there are r similar relations between their right-hand sides. These latter r relations provide r boundary conditions. Now, among all n scalar equations (2.13), there are only $n - r$ linearly independent equations, and they provide the rest of the boundary conditions. The simplest example of such a situation is for a barrier between two identical materials, which is considered in the next subsection.

The general approach used in this article is applicable to the interface of almost any pair of semiconductors, including electron/hole interfaces, and interfaces between different valleys (e.g., Γ/X, Γ/L, and L/X). To obtain a boundary condition in each particular case, it is necessary to write down a variational functional (2.5) to break it into bulk and surface terms (see equation (2.6)) and to find an invariant expression for the surface energy (analogous to equation (2.8)).

3.2. Interfaces between identical materials with simple band structure

In this section, as an illustration of the application of equation (2.13) and how to check it, we consider the simplest situation: boundary conditions matching wave-functions of the same band at the interface between two identical materials with simple band structure. In this case the wave-functions on both sides of the interface are scalars, and the effective-mass tensors are equal. For a scalar wave-function, equation (2.13) takes the form

$$\mathcal{A}\psi_R + \mathcal{B}^*\psi_L = \frac{\hbar^2}{2m}\frac{\partial\psi_R}{\partial z} \tag{3.2a}$$

$$\mathcal{B}\psi_R + \mathcal{A}\psi_L = -\frac{\hbar^2}{2m}\frac{\partial\psi_L}{\partial z} \tag{3.2b}$$

where $\mathcal{A}$ and $\mathcal{B}$ are scalar parameters (there is only one parameter $\mathcal{A}$, because of the symmetry of the barrier). An interface with these matching conditions is equivalent to a potential barrier whose height V is much larger than the energy and the width ϵ, where

$$\mathcal{A} = \frac{q\cosh(q\epsilon)}{\sinh(q\epsilon)} \tag{3.3a}$$

$$\mathcal{B} = -\frac{q}{\sinh(q\epsilon)}. \tag{3.3b}$$

Here $q = \sqrt{2m_1V}/\hbar$ and m_1 is the effective mass in the barrier region. If $q\epsilon \ll 1$, then $\mathcal{A} = -\mathcal{B} = 1/\epsilon$. In this extreme case, equations (3.2) are consistent only if the normal derivatives are continuous, and the boundary conditions become

$$\psi_R - \psi_L = \epsilon\frac{\hbar^2}{2m}\frac{\partial\psi_R}{\partial z} \tag{3.4a}$$

$$\frac{\partial\psi_R}{\partial z} = \frac{\partial\psi_L}{\partial z}. \tag{3.4b}$$

If the width of the barrier goes to zero, then these conditions are reduced to the continuity of the wave-functions and that of their normal derivatives.

3.3. The isotropic approximation

It is interesting to note that equation (2.13) is invariant with respect to any rotation around the z-axis. In other words, the symmetry of the boundary condition equation (2.13) is higher than the symmetry of the Hamiltonian equation (2.7b).

To simplify the calculations, an isotropic approximation is sometimes used for the hole spectrum [44]. It is defined by replacing both γ_2 and γ_3 with

$$\gamma = \frac{2\gamma_2 + 3\gamma_3}{5}. \tag{3.5}$$

Then the boundary condition equation (2.13b) becomes

$$\mathcal{A}_h\psi_h + \mathcal{B}\psi_e = -\frac{\hbar^2}{2m_0}\left[\left(\gamma_1 + \frac{5}{2}\gamma\right)(\boldsymbol{n}\cdot\boldsymbol{\nabla}) - \gamma\left[(\boldsymbol{n}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{\nabla}) + (\boldsymbol{\nabla}\cdot\boldsymbol{J})(\boldsymbol{J}\cdot\boldsymbol{n})\right]\right]\psi_h \tag{3.6}$$

where $\boldsymbol{n}$ is the unit vector normal to the interface. This result includes all of the physical invariants of the problem, up to second order in $\boldsymbol{J}$, and is exactly what we would expect from symmetry considerations.

3.4. Reduction to scalar wave-functions for the electrons and for the holes

There is a practically important problem of treating the InAs/GaSb interface in the case in which only the ground hole sub-band is of importance. It is logical for such a case to have simplified boundary conditions, which couple a scalar electron function with the scalar function of the ground hole sub-band. In this section we derive such a condition.

We consider two thin layers, one of InAs and one of GaSb, sandwiched between two high potential barriers. The envelope functions vanish at the interfaces with the potential barrier. The InAs layer is a quantum well for electrons, and the GaSb is a quantum well for holes. When the wells are narrow, the second heavy-hole and the first light-hole sub-bands are well above the first heavy-hole sub-band, and the light-hole components of the hole wave-function of the first heavy-hole sub-band are small compared with the heavy-hole components. A natural approach to this problem is to simplify the description, eliminating small components from the problem, and to reduce it to the matching of the electron and heavy-hole components of the hole wave-function. To carry out such a programme, it is necessary to separate the problem for the light-hole components, calculate them, and substitute the result in the equations for the heavy-hole components. For this separation, it is convenient to introduce the notation

$$\psi_e = \begin{pmatrix} \psi_{e,1/2} \\ \psi_{e,-1/2} \end{pmatrix} \qquad \psi^{(1/2)} = \begin{pmatrix} \psi_{h,1/2} \\ \psi_{h,-1/2} \end{pmatrix} \qquad \psi^{(3/2)} = \begin{pmatrix} \psi_{h,3/2} \\ \psi_{h,-3/2} \end{pmatrix}. \tag{3.7}$$

So the hole envelope function takes the form

$$\psi_h = \begin{pmatrix} \psi^{(1/2)} \\ \psi^{(3/2)} \end{pmatrix}. \tag{3.8}$$

The projections of the boundary conditions (equation (2.13)) onto the subspaces ±1/2 and ±3/2 gives

$$\mathcal{A}_e\psi_e + \mathcal{B}^\dagger\psi^{(1/2)} = -\frac{\hbar^2}{2m_e}\frac{\partial\psi_e}{\partial z} \tag{3.9a}$$

$$\mathcal{A}_{1/2}\psi^{(1/2)} + \mathcal{B}\psi_e = -\frac{\hbar^2}{2m_0}\left[(\gamma_1+2\gamma_2)\frac{\partial\psi^{(1/2)}}{\partial z} - \sqrt{3}\gamma_3\left(\sigma_z\frac{\partial}{\partial x} + \mathrm{i}\frac{\partial}{\partial y}\right)\psi^{(3/2)}\right] \tag{3.9b}$$

$$\mathcal{A}_{3/2}\psi^{(3/2)} = -\frac{\hbar^2}{2m_0}\left[(\gamma_1-2\gamma_2)\frac{\partial\psi^{(3/2)}}{\partial z} - \sqrt{3}\gamma_3\left(\sigma_z\frac{\partial}{\partial x} - \mathrm{i}\frac{\partial}{\partial y}\right)\psi^{(1/2)}\right]. \tag{3.9c}$$

Here σ_z is the Pauli 2×2 spin matrix. Assuming that the boundary conditions do not depend on the sign of the spin z-projection, $\mathcal{A}_e$, $\mathcal{A}_{1/2}$, $\mathcal{A}_{3/2}$, and $\mathcal{B}$ can be considered as numbers.

We consider a weak coupling between the electrons and the holes, i.e., the case where the rhs in equations (3.9) is of a higher order of magnitude than the lhs. In the first approximation, the rhs is neglected, and the boundary conditions for the interface between the layers, $z = 0$, are reduced to

$$\psi_e^{(0)} = 0 \qquad \psi_h^{(0)} = 0. \tag{3.10}$$

In this case the electron and hole wells are decoupled, and the eigenvalues in the electron and hole wells can be different:

$$H_e\psi_e^{(0)} = E_e\psi_e^{(0)} \tag{3.11a}$$

$$H_h\psi_h^{(0)} = E_h\psi_h^{(0)}. \tag{3.11b}$$

Here H_h, H_e are the effective Hamiltonians for the holes and for the electrons respectively.

We consider the coupling as a small perturbation to the decoupled problem. We can expand the envelope functions of the coupled problem in the solutions of the decoupled problem:

$$\psi_e = u_e \psi_e^{(0)} + \delta\psi_e \tag{3.12a}$$

$$\psi_h = u_h \psi_h^{(0)} + \delta\psi_h \tag{3.12b}$$

where the correction to the first approximation is orthogonal to it. u_e and u_h satisfy the relations

$$u_e = \int_{-L_c}^{0} \psi_e^{\dagger(0)} \psi_e \, \mathrm{d}z \qquad u_h = \int_{0}^{L_v} \psi_h^{\dagger(0)} \psi_h \, \mathrm{d}z. \tag{3.13}$$

These relations can be used to find u_e and u_h. For this purpose it is necessary to multiply the effective Schrödinger equation for the electron and the hole by the decoupled solutions $\psi_e^{\dagger(0)}$ and $\psi_h^{\dagger(0)}$ respectively, and to integrate with respect to z over the relevant well region. Then

$$\int_{-L_c}^{0} \psi_e^{\dagger(0)} (H_e - E) \psi_e \, \mathrm{d}z = 0 \tag{3.14a}$$

$$\int_{0}^{L_v} \psi_h^{\dagger(0)} (H_h - E) \psi_h \, \mathrm{d}z = 0. \tag{3.14b}$$

The Hamiltonians are Hermitian, so we can operate, using the terms that do not consist of derivatives with respect to z, on the unperturbed wave-functions, and use the definition of the amplitudes (equation (3.13)) to simplify the calculation. The terms which consist of derivatives with respect to z are integrated twice by parts. The integrated terms have non-vanishing contributions only from the interface between the layers. The results are

$$\int_{-L_c}^{0} \psi_e^{\dagger(0)} H_e \psi_e \, \mathrm{d}z = E_e u_e - \frac{\hbar^2}{2m_e} \left[\frac{\mathrm{d}\psi_e^{\dagger(0)}}{\mathrm{d}z} \psi_e \right]_{z=0} \tag{3.15a}$$

$$\int_{0}^{L_v} \psi_h^{\dagger(0)} H_h \psi_h \, \mathrm{d}z = E_h u_h - \frac{\hbar^2}{2m_0} \left[\frac{\mathrm{d}\psi_h^{\dagger(0)}}{\mathrm{d}z} \begin{pmatrix} \gamma_1 + 2\gamma_2 & 0 & 0 & 0 \\ 0 & \gamma_1 + 2\gamma_2 & 0 & 0 \\ 0 & 0 & \gamma_1 - 2\gamma_2 & 0 \\ 0 & 0 & 0 & \gamma_1 - 2\gamma_2 \end{pmatrix} \psi_h \right]_{z=0} . \tag{3.15b}$$

Now we can use the boundary condition equations (3.9) to replace the coupled envelope functions with the matching derivatives at the interface between the layers, $z = 0$. As was mentioned above, the right-hand sides of equations (3.9) are of a higher order of the perturbation theory than the left-hand sides. So in the right-hand sides of equations (3.9), we can replace the perturbed wave-functions with the unperturbed ones, with the help of equations (3.12), neglecting the contributions from the higher levels. We substitute the expressions for the coupled envelope functions in equations (3.15), and equation (3.14) now has the form

$$\begin{pmatrix} E_e & w \\ w^\dagger & E_h \end{pmatrix} \begin{pmatrix} u_e \\ u_h \end{pmatrix} = E \begin{pmatrix} u_e \\ u_h \end{pmatrix} \tag{3.16}$$

where

$$w = -\frac{\hbar^2}{2m_e}\frac{\hbar^2}{2m_0}\frac{(\gamma_1+2\gamma_2)\mathcal{B}^\dagger}{\mathcal{A}_e\mathcal{A}_{1/2}-|\mathcal{B}|^2}\left[\frac{\partial\psi_e^{\dagger(0)}}{\partial z}\frac{\partial\psi^{(1/2)(0)}}{\partial z}\right]_{z=0}. \tag{3.17}$$

In equation (3.16), we neglected the contribution of the coupling to the diagonal terms. This is justified by the smallness of these corrections in comparison with the decoupled spectra E_e and E_h. We would like to express the light-hole component in terms of the heavy-hole component. We can use the effective Schrödinger equation for this. In the case where $kL_v \ll 1$, the equation can be reduced to

$$\frac{\mathrm{d}^2\psi^{(1/2)(0)}}{\mathrm{d}z^2} + \lambda^2\psi^{(1/2)(0)} = \frac{2\sqrt{3}\gamma_3}{\gamma_1+2\gamma_2}(\mathrm{i}\sigma_z k_x - k_y)\frac{\mathrm{d}\psi^{(3/2)(0)}}{\mathrm{d}z} \tag{3.18}$$

where

$$\lambda^2 = \frac{(\gamma_1-2\gamma_2)\pi^2}{(\gamma_1+2\gamma_2)L_v^2}. \tag{3.19}$$

We assume that $\lambda L_v \ll 1$, and consider $\psi^{(3/2)(0)}$, $\psi_e^{(0)}$ as solutions for infinite quantum wells. The z-dependent parts of these envelope functions will be

$$\zeta_{3/2}^{(0)}(z) = \sqrt{\frac{2}{L_v}}\sin\frac{\pi z}{L_v} \qquad \zeta_e^{(0)}(z) = \sqrt{\frac{2}{L_c}}\sin\frac{\pi z}{L_c}. \tag{3.20}$$

Now we can solve equation (3.18) with the help of equation (3.20). The substitution of the electron function, and of $\psi^{(1/2)(0)}$ expressed in terms of $\psi^{(3/2)(0)}$, in equation (3.17) gives

$$w = \frac{\hbar^2}{2m_e}\frac{\hbar^2}{2m_0}\frac{\mathcal{B}^\dagger\sqrt{\gamma_1^2-4\gamma_2^2}}{\mathcal{A}_e\mathcal{A}_{1/2}-|\mathcal{B}|^2}\frac{\sqrt{3}\gamma_3}{\gamma_2}(\mathrm{i}\sigma_z k_x - k_y)\frac{1}{\sqrt{L_cL_v}}\frac{\pi}{L_c}\frac{\cos(\lambda L_v/2)}{\sin(\lambda L_v/2)}\cos\lambda L_v. \tag{3.21}$$

It is instructive to compare the results of this calculation with the approximate boundary condition for scalar electron and hole envelope functions:

$$\psi_v = \frac{a_2}{2}\sqrt{\frac{m_{h\perp}}{m_e}}\left(\frac{\partial}{\partial x}+\mathrm{i}\frac{\partial}{\partial y}\right)\frac{\partial\psi_c}{\partial z} \qquad \psi_c = -\frac{a_2}{2}\sqrt{\frac{m_e}{m_{h\perp}}}\left(\frac{\partial}{\partial x}-\mathrm{i}\frac{\partial}{\partial y}\right)\frac{\partial\psi_v}{\partial z} \tag{3.22}$$

where

$$\frac{1}{m_{h\perp}} = \frac{\gamma_1-2\gamma_2}{m_0}. \tag{3.23}$$

ψ_c is the electron envelope function, and ψ_v is the hole envelope function which corresponds to the heavy-hole component. From these boundary conditions, one can derive an equation similar to equation (3.16), where now

$$w = \frac{\hbar^2}{2\sqrt{m_{h\perp}m_e}}\frac{\pi^2 a_2}{(L_cL_v)^{3/2}}(\mathrm{i}k_x - k_y). \tag{3.24}$$

If $\lambda L_v \ll 1$, then comparison gives

$$a_2 = \frac{\hbar^2}{\sqrt{m_0m_e}}\frac{\mathcal{B}^\dagger\sqrt{\gamma_1+2\gamma_2}}{\mathcal{A}_e\mathcal{A}_{1/2}-|\mathcal{B}|^2}\frac{\sqrt{3}\gamma_3}{\gamma_2}\frac{L_v}{\pi^2}. \tag{3.25}$$

As was mentioned in the previous section, the units of the interface matrix elements are energy multiplied by length, and the scales are the atomic scales, so a good approximation will be $\mathcal{A} \sim \mathcal{B} \sim (\hbar^2/m_{lh}a_0)$, where $m_{lh} = m_0/(\gamma_1+2\gamma_2)$ is the effective mass of the light hole. With the help of this approximation, we obtain $a_2 \sim a_0 L$. We used these simplified results for deriving an analytic model for the calculations of the spectrum of the system, including the self-consistent potential [45].

We compare these results with the results of the effective bond–orbital technique [46], that are in agreement with the Ando and Mori conditions [33, 38]

$$\psi_v = -\frac{a}{2}\sqrt{\frac{m_h}{m_e}}\frac{\partial \psi_c}{\partial z} \tag{3.26a}$$

$$\psi_c = -\frac{a}{2}\sqrt{\frac{m_e}{m_h}}\frac{\partial \psi_v}{\partial z} \tag{3.26b}$$

where a is the scale of the lattice constant. We see that the major difference between the results is the dependence of our boundary conditions on the in-plane vector $k_\parallel$. We assumed the wells to be narrow, so the overlap is only between the first electron sub-band and the first heavy-hole sub-band. At the centre of the band, where $k_\parallel$ is small, the light-hole components of the hole function are small in comparison with the heavy-hole components. However, the coupling is only between the light holes and the electrons, which have the same projection of the total angular momentum on the z-direction. Hence the coupling should depend on the in-plane vector, and therefore the boundary conditions should contain derivatives with respect to the in-plane coordinates. In this sense, our simplified results (equation (3.16)) resemble Fasolino and Altarelli's results [47]; they calculated the energy spectrum for InAs/GaSb superlattices in the presence of a magnetic field. The off-diagonal terms in their effective Hamiltonian depend on the in-plane vector $k_\parallel$.

4. Conclusions

Boundary conditions at the InAs/GaSb interface are derived. The conditions take into account the complex band structure of the holes, the symmetry, and the different spin structures of the wave-functions on either side of the interface. The general boundary conditions match simple parabolic 2-spinor InAs electrons, and highly anisotropic, non-parabolic, degenerate 4-spinor GaSb holes. In the case in which only the ground hole sub-band is important, simplified boundary conditions are obtained from the general ones. For the derivation of the conditions, we used a variational approach that can be applied also for other heterostructures. Various kinds of popular simplified boundary condition are obtained as different extreme cases of the general conditions. We used these boundary conditions to calculate the energy spectrum of the carriers in InAs/GaSb quantum wells, without losing the important features of the hole spectrum. The results reveal that very interesting phenomena are exhibited by the spectra of the system, and these will be presented in a future publication [19].

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