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Boundary conditions for envelope functions in heterostructures

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In this paper a detailed derivation of the boundary conditions for envelope functions is carried out making use of the $\mathbf{k}\cdot\mathbf{p}$ method. The resulting conditions are different from those of Harrison by an extra term originating from a surface energy. This term removes the difference between expressions for the transmission coefficient obtained with the help of microscopical calculations and the envelope-function method. In the case of a simple band structure the resulting boundary conditions contain two independent parameters. It is shown that the general boundary conditions suggested by Ando and Mori contain a term which has to be neglected in the frame of the effective-mass method. The form of the boundary conditions for degenerate bands and for the case of different degrees of degeneracy in the interfacing materials is considered.

I. INTRODUCTION

The usefulness of the effective-mass method in the study of different properties of semiconductors has been well proven both theoretically and experimentally. Some important aspects of this method arise in its applications to heterostructures. When two semiconductor materials are in intimate contact and the bottom of the conduction band (or the valence band) of one of them is close to that of the other, one would expect that the effective-mass method can be used in the whole structure. However, the Bloch functions and effective masses in interfacing materials are usually different, and there may be a band offset. All this results in different amplitudes of the Bloch functions in the materials. Thus, a problem that is not encountered in uniform semiconductors comes about, determining the amplitudes. The amplitudes of the Bloch functions are usually called envelope functions, and the application of effective-mass theory to heterostructures is called the envelope-function approximation.

The effective-mass method easily leads to Schrödinger equations for the envelope functions in both materials. However, a question of boundary conditions for the envelope functions at the interface appears. Naive conditions, i.e., the continuity of the envelope function and its normal derivative at the interface, sometimes used for the conduction band at the GaAs/AlGaAs interface, apparently does not work in more complicated situations. These conditions cannot be applied directly for complex valence bands. They violate the conservation of the current normal to the interface (i.e., lead to a non-Hermitian quantum-mechanical problem) for materials with different effective masses. This problem is important, e.g., in the cases of electron transfer between minima of the conduction band located in different points of the Brillouin zone and at InAs/GaSb interfaces where the effective masses on different sides of the interface have different signs.

Harrison[1] suggested a generalization of the boundary conditions for a simple band. Instead of the assumption of the continuity of the envelope functions ψ, he used

$$\alpha_1\psi_1 = \alpha_2\psi_2 \,. \tag{1}$$

Then the conservation of the current normal to the interface led him to another condition,

$$\frac{1}{\alpha_1 m_1}\frac{\partial\psi_1}{\partial z} = \frac{1}{\alpha_2 m_2}\frac{\partial\psi_2}{\partial z} \,. \tag{2}$$

Here the subscripts 1 and 2 correspond to the different sides of the interface, m_1 and m_2 are the effective masses, α_1 and α_2 are real constants, and the z axis is normal to the interface. Many workers derived a simplified version of Eq. (2) with $\alpha_1 = \alpha_2$.[3–8] All these derivations assume that the envelope functions are continuous at the interface. The second condition is usually obtained by assuming that the kinetic energy has a Hermitian form with a coordinate dependent effective mass. Then, integration of the energy across the interface yields the boundary condition.[3,4,7] The same argument,[9] or equivalent to that, the continuity of the current across an interface,[10] was used to obtain the boundary condition for a degenerate band.

The application of the simplified conditions to the band-structure calculation of III-V and II-VI compounds heterostructures gave a reasonable agreement with experiments[11,12] so that they seemed to be more or less justified. However, when Stiles and Hamann[13] carried out numerical microscopic calculations of the transmission coefficient across a Si twin interface they found a contradiction with the result of the envelope-function approach. Grinberg and Luryi[14,15] compared the plane-wave transmission coefficient obtained with the help of Eqs. (1) and (2) with that obtained from the exact analytical solution for the Kronig-Penney model. They showed that the two methods give somewhat different expressions. The simple interpretation of this result is that the consideration of heterostructures in terms of envelope functions is too rude an approximation.[13,15] Such a conclusion, however, seems to be very strange in the region of energies and lengths where the phenomenological effective-mass approximation has been proven to be valid. That is, the only possible solution to the paradox shown by Stiles and Hamann[13] and Grinberg and Luryi[14,15] is that Eqs. (1) and (3) contain an unjustified simplification and cannot be used for description of all phenomena in heterostructures.

The most general boundary conditions consistent with the effective-mass approximation, where envelope functions satisfy differential equations of the second order, were suggested by Ando and Mori.[2] Those conditions were used for the calculation of the band structure of GaAs/AlGaAs and InAs/GaSb (Ref. 2) and for the description of the transition between Γ and X valleys in the GaAs/AlGaAs interface.[16]

In the next section it is argued that in the effective-mass approximation the conditions of Ando and Mori[2] can be replaced by Eq. (1) and a generalization of Eq. (2),

$$\frac{1}{\alpha_1 m_1}\frac{\partial\psi_1}{\partial z}+\beta_1\psi_1=\frac{1}{\alpha_2 m_2}\frac{\partial\psi_2}{\partial z}+\beta_2\psi_2\,, \tag{3}$$

where β_1 and β_2 are real constants. Equations (1) and (3) contain two independent parameters (each of the conditions of Ando and Mori[2] contains a wave-function derivative and so those conditions contain three independent parameters). The dimensionless parameter α_1/α_2 characterizes reflective properties of the interface at the band edge. The second parameter, $q=(m_1m_2)^{1/2}(\alpha_1\beta_2-\alpha_2\beta_1)$, has the dimension of an inverse length. If q^{-1} is much bigger than the length scale of ψ_1 and ψ_2 then the terms containing ψ_1 and ψ_2 in Eq. (3) can be neglected and it is reduced to Eq. (2). In the opposite case Eqs. (1) and (3) give $\psi_1=\psi_2=0$ which means that the interface is impenetrable. Another way to define the second parameter is to associate with the interface a surface energy density.[17]

It will be shown in Sec. IV that the application of Eq. (3) instead of Eq. (2) does not lead to the contradiction noticed by Stiles and Hamann[13] and Grinberg and Luryi.[14,15]

In microscopic derivations of boundary conditions for envelope functions an interface is sometimes assumed to be a mathematical surface dividing two materials with different Bloch functions.[6,8,18] It is important to note that models containing this assumption cannot be considered as a solid basis for phenomenological boundary conditions. In reality, bulk Bloch functions in both materials exist only at some distance from the interface which is larger or about the size of the unit cell, a_0. The electric potential created by 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. One also has to note the possibility of steps, dislocations, and impurities segregated to the interface during the growing of the structure. All these complications, however, are important only on the microscopic scale. Envelope functions do not vary on the length scale of a_0 and microscopic details of the interface can affect only the coefficients in boundary conditions for the envelope functions. On the other hand, the phenomenological boundary conditions for an envelope function have to be valid under the same conditions as the envelope-function approximation itself. That is, its form cannot depend on a specific microscopic model. This means that such conditions can be derived by making use of the $\mathbf{k}\cdot\mathbf{p}$ method.[11,12,18] The purpose of the present paper is to give such a derivation.

In the next section the detailed derivation of boundary conditions, Eqs. (1) and (3), is presented for the interface between materials with a simple band structure. In Sec. III modifications necessary for degenerate bands are shown. The case of different numbers of degenerate bands in the interfacing materials is also considered. The last section discusses the application of Eqs. (1) and (3) to electron transmission through an interface.

II. BOUNDARY CONDITIONS FOR A SIMPLE BAND STRUCTURE

In this section the boundary conditions for the envelope functions will be derived under the same assumptions which justify the effective-mass approximation in simple band semiconductors. Let us consider an interface between materials 1 and 2 such that material 1 occupies the region $z<0$ and material 2 occupies the region $z>0$. The interface is not actually the plane $z=0$ but occupies some region around this plane with width of about the size of the unit cell, a_0. The exact structure of this region is not important for the form of the boundary conditions.

There are two assumptions which make the application of the effective-mass approximation possible in both materials. The first is that all macroscopic length scales (distances between different interfaces, the length scales of external fields and all length scales related to the envelope functions due to external fields) are much larger than the microscopic length scale, a_0. It is convenient to introduce a specific notation, L, for the minimum macroscopic length scale. Then the first condition for the effective-mass approximation in the bulk is $a_0\ll L$. The second assumption is that all macroscopic energy scales (the difference between the considered energy and band edges, the band offset of the interfacing materials and all energies related to external fields) are much smaller than the widths of the conduction and the valence band and the gap between them. In the bulk this assumption is usually equivalent to the first one because the estimates for microscopic and macroscopic energies are respectively $\hbar^2/ma_0^2$ and $\hbar^2/mL^2$. In heterostructures this assumption has a new meaning because the band offset has nothing to do with external fields or the geometry of a structure. To abbreviate notations it is convenient to introduce an additional limitation on L in such a way that $\hbar^2/mL^2$ would be of the order or bigger than the band offset. Then both conditions can be expressed in terms of only one inequality, $a_0\ll L$.

This inequality allows one to separate a region $\mathcal{B}$ with the boundaries $z=z_1<0$ and $z=z_2>0$ which satisfy the condition $a_0\ll z_2,|z_1|\ll L$. It is important to note that the exact values of z_1 and z_2 do not matter.

A. The first boundary condition

Let us consider the matching of electron wave functions in the region $\mathcal{B}$ at an energy close to the band edges of both materials. The structure of an exact wave function, $\Psi(\mathbf{r})$, near the interface is very complicated because of the mismatch between the band structure and the Bloch functions in the interfacing materials. In general, evanescent waves and a distortion of the Bloch wave functions arising from the mismatch penetrate only a distance of about a_0 in each material. If the energy appears to be in the energy gap of one of the materials, the envelope function inside this material is also evanescent. But because of the small energy difference between the energy and the band edge this envelope function falls down on the distance of about L and such a decrease can be neglected in the region $\mathcal{B}$. This means that, in each material away from the region of the width of a_0 around the interface, $\Psi(\mathbf{r})$ has to be proportional to the Bloch function. On the distance less than L around the interface the difference between the Bloch function for the considered energy and that at the band edge, $u_n^{(j)}(\mathbf{r})$, is of the order of a_0/L or less (here n is the number of the considered band which for simplicity of notations is taken to be the same for both materials and $j = 1, 2$ labels the material). That is for $|z| \gg a_0$

$$\Psi(\mathbf{r}) = C_1 u_n^{(1)}(\mathbf{r}),\ z < 0,\quad \Psi(\mathbf{r}) = C_2 u_n^{(2)}(\mathbf{r}),\ z > 0 \tag{4}$$

with an accuracy of a_0/L.

The physical meaning of the constants C_1 and C_2 can be seen from the consideration of the transmission and reflection of a plane wave from the interface. In general, for a plane wave incident normally from the first material

$$\Psi_{k_1}(\mathbf{r}) = e^{ik_1 z} u^{(1)}_{n,k_1}(\mathbf{r}) + R_1(k_1) e^{-ik_1 z} u^{(1)}_{n,-k_1}(\mathbf{r}),\ z < 0,\quad \Psi_{k_1}(\mathbf{r}) = T_1(k_1) e^{ik_2 z} u^{(2)}_{n,k_2}(\mathbf{r}), z > 0, \tag{5a}$$

and for a plane wave incident normally from the second material

$$\Psi_{-k_2}(\mathbf{r}) = e^{-ik_2 z} u^{(2)}_{n,-k_2}(\mathbf{r}) + R_2(-k_2) e^{ik_2 z} u^{(2)}_{n,k_2}(\mathbf{r}),\ z > 0,\quad \Psi_{-k_2}(\mathbf{r}) = T_2(-k_2) e^{-ik_1 z} u^{(1)}_{n,-k_1}(\mathbf{r}), z < 0 \tag{5b}$$

outside the region of the width of a_0 near the interface. Here k_1 and k_2 are wave vectors in the first and second materials and the periodic parts of the Bloch functions, $u^{(j)}_{n,k_j}(\mathbf{r})$, depend on these vectors. When k_1 and k_2 go to 0 a plane wave in the region $\mathcal{B}$ differs from any other function satisfying the condition $a_0/L \ll 1$ only by a constant factor, so that

$$\frac{C_1}{C_2} = \frac{1 + R_1(0)}{T_1(0)} = \frac{T_2(0)}{1 + R_2(0)}\ . \tag{6}$$

In the region $\mathcal{B}$, $\Psi(\mathbf{r})$ differs from $\Psi^*(\mathbf{r})$ by a phase which is constant with accuracy of a_0/L. That is, the ratio C_1/C_2 can be chosen to be real. Now, according to the definition of envelope functions, $C_1 = \psi_1(0)$ and $C_2 = \psi_2(0)$ so that Eqs. (4) and (6) are equivalent to Harrison's condition, Eq. (1).

It is worth making two remarks concerning the above arguments. The relation between $R_1(0), T_1(0)$ and $R_2(0), T_2(0)$ reflects the fact that to the first order in a_0/L the band-edge energies of the materials are equal and at that energy there is only one solution to the Schrödinger equation which is a constant. Corrections to Eq. (1) which are obtained from the boundary conditions of Ando and Mori[2] and contain $\frac{\partial \psi_l}{\partial z}$ are of the order of a_0/L and have to be neglected in the effective-mass approximation.

B. The second boundary condition

The second boundary condition concerns a matching of normal derivatives of the envelope functions and needs to take into account terms of the order of a_0/L. With such an accuracy, the expansion of an electron wave function near the edge of the nth band outside the region $\mathcal{B}$ has the form

$$\Psi = \psi_1 u_n^{(1)} - \frac{i\hbar}{m_0} \sum_{j \neq n} \frac{p_{jn}^{\mu(1)}}{\epsilon_n^{(1)} - \epsilon_j^{(1)}} \frac{\partial \psi_1}{\partial r_\mu} u_j^{(1)}\ ,\ z < z_1\ , \tag{7a}$$

$$\Psi = \psi_2 u_n^{(2)} - \frac{i\hbar}{m_0} \sum_{j \neq n} \frac{p_{jn}^{\mu(2)}}{\epsilon_n^{(2)} - \epsilon_j^{(2)}} \frac{\partial \psi_2}{\partial r_\mu} u_j^{(2)}\ ,\ z > z_2\ . \tag{7b}$$

Here m_0 is the free electron mass, $\epsilon_j^{(l)}$ and $u_j^{(l)}$ are the energy and Bloch function of the jth band at the center of the Brillouin zone in the lth material, and $p_{jn}^{\mu(l)}$ is the matrix element of the μth component of the momentum between functions $u_j^{(l)}$ and $u_n^{(l)}$. Inside the region $\mathcal{B}$ terms of the order of a_0/L can be neglected and

$$\Psi = u\ , \tag{8}$$

where $u(\mathbf{r})$ is the function with asymptotes $\psi_1(0) u_n^{(1)}(\mathbf{r})$ at $z < 0$, $a_0 \ll |z| \ll L$ and $\psi_2(0) u_n^{(2)}(\mathbf{r})$ at $z > 0$, $a_0 \ll z \ll L$.

The Schrödinger equation for Ψ can be obtained from a variation functional

$$\mathcal{E} = \int \left(\frac{\hbar^2}{2m_0} |\nabla \Psi|^2 + (U - E) |\Psi|^2 \right) d^3 r\ , \tag{9}$$

where $U(\mathbf{r})$ is the lattice potential. For simplicity no external field is included in $\mathcal{E}$. The integral in Eq. (9) can be broken into the sum of three integrals over the regions outside and inside $\mathcal{B}$,

$$\mathcal{E} = \mathcal{E}_1 + \mathcal{E}_b + \mathcal{E}_2 \ , \ \mathcal{E}_1 = \int_{z<z_1} \ ,$$
$$\mathcal{E}_2 = \int_{z>z_2} \ , \ \mathcal{E}_b = \int_{z_1<z<z_2} \ . \tag{10}$$

Functionals $\mathcal{E}_1$ and $\mathcal{E}_2$ can be calculated with the help of Eqs. (7a) and (7b). The energy E is assumed to be close to $\epsilon_n^{(1)}$ and $\epsilon_n^{(2)}$ so that the difference between them is of the second order in a_0/L. That means that the omission of terms of the order of a_0/L leads to zero result. A nonzero result appears only in the second order in the integrands, i.e., one has to keep the second terms in Eqs. (7a) and (7b) and all the derivatives of $\psi_l(\mathbf{r})$ arising from the first terms, which means that the calculations are made with the accuracy of the second order in a_0/L. Each of the integrals can be broken into the sum of the integrals over separate unit cells. Inside every cell the envelope functions and their derivatives have to be considered to be constants. Bloch functions are suitable to be normalized on the volume of the unit cell. The result is

$$\mathcal{E}_1 = \int_{z<z_1} \left[\frac{\hbar^2}{2m_1} |\nabla\psi_1|^2 + (\epsilon_n^{(1)} - E)|\psi_1|^2 \right] d^3r \ , \tag{11a}$$

$$\mathcal{E}_2 = \int_{z>z_2} \left[\frac{\hbar^2}{2m_2} |\nabla\psi_2|^2 + (\epsilon_n^{(2)} - E)|\psi_2|^2 \right] d^3r \ , \tag{11b}$$

where

$$\frac{1}{m_l} = \frac{1}{m_0} + \frac{2}{3m_0^2} \sum_{j\neq n} \frac{p_{nj}^{\mu(l)} p_{jn}^{\mu(l)}}{\epsilon_n^{(l)} - \epsilon_j^{(l)}} \tag{12}$$

is the effective mass (for simplicity only an isotropic mass considered). The variable of integration in Eqs. (11a) and (11b) scales as L so that $\mathcal{E}_1$ and $\mathcal{E}_2$ are of the first order in a_0/L.

The functional $\mathcal{E}_b$ is calculated with the help of Eq. (8). Inside the region $\mathcal{B}$ it is impossible to carry out detailed calculations because of the complicated structure of $u(\mathbf{r})$. However, one can notice that the value of $\mathcal{E}_b$ has to be a linear combination of $|\psi_1(0)|^2$ and $|\psi_2(0)|^2$ since these quantities determine the values of $u(\mathbf{r})$ at the boundaries of the region $\mathcal{B}$. $|\psi_1(0)|^2$ and $|\psi_2(0)|^2$ are not independent because of the first boundary condition and it is possible to write down the result in a symmetric form,

$$\mathcal{E}_b = \frac{\hbar^2}{2}[\alpha_1\beta_1|\psi_1(0)|^2 - \alpha_2\beta_2|\psi_2(0)|^2] \ . \tag{13}$$

$\mathcal{E}_b$ can be considered as the energy of the interface.

The Schrödinger equations for the envelope functions can be obtained by the variation of $\mathcal{E}$ with respect to $\psi_1^*(\mathbf{r})$ and $\psi_2^*(\mathbf{r})$. The variation $\delta\mathcal{E}$ contains also an integrated term

$$\delta\psi_1^*(0)\frac{\hbar^2}{2}\left[\frac{1}{m_1}\left.\frac{\partial\psi_1}{\partial z}\right|_{z=0} + \alpha_1\beta_1\psi_1(0)\right]$$
$$-\delta\psi_2^*(0)\frac{\hbar^2}{2}\left[\frac{1}{m_2}\left.\frac{\partial\psi_2}{\partial z}\right|_{z=0} + \alpha_2\beta_2\psi_2(0)\right] \ . \tag{14}$$

In this term the difference between z_1, z_2 and 0 is neglected. The variations $\delta\psi_1^*(0)$ and $\delta\psi_2^*(0)$ are not independent due to the first boundary condition, Eq. (1). Thus the requirement of the variation Eq. (14) to be zero results in the second boundary condition, Eq. (3). The $\mathbf{k}\cdot\mathbf{p}$ method does not show a definite sign for the surface energy and the parameter q can, in general, have either sign.

Equation (3) contains terms with derivatives of the envelope functions which are of the order of a_0/L compared to the terms containing the envelope functions themselves. This difference appears because the terms with derivatives originated from $\mathcal{E}_1$ and $\mathcal{E}_2$ where the integrands are of the second order in a_0/L while the terms containing the envelope functions came from the surface energy, $\mathcal{E}_b$, where corrections of the order of a_0/L were neglected. Usually the terms with derivatives can be neglected in Eq. (3) and then the interface is impenetrable. This means that those interfaces which allow electrons to tunnel through have a surface energy which is anomalously small for some microscopical reasons. One has to remember that the last remark is relevant only to the interfaces between materials with small band offsets, so that the effective-mass method can be used in both of them.

III. BOUNDARY CONDITIONS IN THE CASE OF DEGENERATE BANDS

The generalization of boundary conditions for the case of degenerate bands is straightforward when the interfacing materials have the same number of degenerate bands, N. The resulting equations have the same structure as Eqs. (1) and (3) although they now connect N envelope functions of each material, $\psi_1^{(j)}$ and $\psi_2^{(j)}$, and contain square matrices instead of scalar coefficients. That is, the condition analogous to Eq. (1) is

$$\psi_1^{(j_1)} = A_{j_1 j_2}\psi_2^{(j_2)} \ . \tag{15}$$

The functionals $\mathcal{E}_1$ and $\mathcal{E}_2$ are easily constructed if the Hamiltonians for the envelope functions are known. The boundary energy can be written as

$$\mathcal{E}_b = B_{jj'}\psi_2^{(j)*}(0)\psi_2^{(j')}(0) \ , \tag{16}$$

where $B_{jj'}$ is a Hermitian matrix. Then the second condition is

$$D^{zx}_{1,jj_1}\frac{\partial\psi_1^{(j_1)}}{\partial x}+D^{zy}_{1,jj_1}\frac{\partial\psi_1^{(j_1)}}{\partial y}+D^{zz}_{1,jj_1}\frac{\partial\psi_1^{(j_1)}}{\partial z}=D^{zx}_{2,jj_2}\frac{\partial\psi_2^{(j_2)}}{\partial x}+D^{zy}_{2,jj_2}\frac{\partial\psi_2^{(j_2)}}{\partial y}+D^{zz}_{2,jj_2}\frac{\partial\psi_2^{(j_2)}}{\partial z}+B_{jj_2}\psi_2^{(j_2)}\ . \qquad (17)$$

If the term resulting from the surface energy in Eq. (17) can be neglected this equation becomes identical with the boundary condition suggested by Altarelli.[10] The advantage of the derivation presented in this paper is that the boundary conditions for envelope functions satisfying all conservation laws arise naturally along with the equations for them. Another advantage is that the same scheme easily takes into account the surface energy, which cannot be obtained from the continuity of the current.

There is, however, a complication if the number of degenerate bands in one of the interfacing materials, N_1, is different from that in the other, N_2, as, e.g., in the case of the InAs/GaSb interface when both light and heavy holes in GaSb have to be taken into account. Now two types of the first boundary condition, Eq. (15) and

$$A'_{j_2j_1}\psi_1^{(j_1)}=\psi_2^{(j_2)}\ , \qquad (15')$$

are not equivalent because the number of equations in them is different. From a pure mathematical point of view both problems are correct. Really, the total number of envelope functions is N_1+N_2. If the first condition, Eq. (15), contains N_1 equations they leave N_2 independent functions. So the variation of the corresponding functional $\mathcal{E}$ with respect to independent ψ^* gives N_2 equations for the second condition and the necessary total number of equations in the boundary conditions, N_1+N_2. Nevertheless, the possibility of two different boundary conditions seems to be unsatisfactory because they really correspond to different quantum-mechanical problems. The situation is aggravated by the fact that other types of boundary conditions are also conceivable.

The right form of the boundary condition can be found from a consideration of whole wave functions near the interface. Within the region $\mathcal{B}$, where the envelope functions can be considered as constants, there are N_0 linear independent solutions of the Schrödinger equations. For $a_0 \ll |z| \ll L$ they have asymptotes

$$\Psi^{(\nu)}(\mathbf{r})=\sum_{j=1}^{N_1}C_{1j}^{(\nu)}u_j^{(1)}(\mathbf{r})\ ,\quad z<0, \qquad (18a)$$

$$\Psi^{(\nu)}(\mathbf{r})=\sum_{j=2}^{N_2}C_{2j}^{(\nu)}u_j^{(2)}(\mathbf{r})\ ,\quad z<0, \qquad (18b)$$

$1\le\nu\le N_0$. Let $N_1<N_2$. The full system of solutions, $\Psi^{(\nu)}(\mathbf{r})$, has to contain all possible states with a given energy in both materials. This means that the ranks of the matrices $C_{1j}^{(\nu)}$ and $C_{2j}^{(\nu)}$ equal N_1 and N_2 respectively. That is, $N_0\ge N_2$. It is possible to choose the functions $\Psi^{(\nu)}$ in such a way that the right-hand sides of Eqs. (18b) are zeros for $\nu>N_2$. If $N_0>N_2$ then the right-hand sides of Eqs. (18a) with $\nu>N_2$ can contain N_1' linear independent combinations of the Bloch functions $u_j^{(1)}(\mathbf{r})$ $(0\le N_1'\le N_1)$. If $N_0>N_2+N_1'\equiv N_b$ it is possible to choose the functions $\Psi^{(\nu)}$ with $\nu>N_2$ in such a way that all these linear independent combinations are contained in the right-hand sides of Eqs. (18a) with $N_2<\nu\le N_b$ while the right-hand sides of Eqs. (18a) with $\nu>N_b$ are zeros. This choice has selected functions $\Psi^{(\nu)}$ with $\nu>N_b$ which have zero asymptotes both at $z<0$ and $z>0$. These functions describe surface states and have nothing to do with the envelope functions.[19] The algorithm of the choice shows that any linear combination of functions $\Psi^{(\nu)}$ with $\nu\le N_b$ has a nonzero asymptote at least on one side of the interface. These functions describe transmission and reflection of bulk states. Their number satisfies the inequality $N_2\le N_b\le N_1+N_2$.

The matrix elements $C_{1j}^{(\nu)}$ and $C_{2j}^{(\nu)}$ in the N_b Eqs. (18a) and (18b) are the values of the envelope functions at the interface. The first N_2 equations for them can be obtained by a linear transformation of the first N_2 functions $\Psi^{(\nu)}$ which diagonalizes the right-hand side of Eqs. (18b) and subsequent projection of these equations onto the solutions to the Schrödinger equation with asymptotes at $z>0$ equal to corresponding Bloch functions $u_j^{(2)}(\mathbf{r})$. If $N_b=N_2$ the derivation is completed. If $N_b>N_2$ then a similar procedure can be carried out with the other N_1' functions $\Psi^{(\nu)}$. The right-hand side of Eqs. (18a) $(N_2<\nu\le N_b)$ can be diagonalized with respect to any N_1' of the Bloch functions $u_j^{(1)}(\mathbf{r})$ and then the equations have to be projected onto the solutions to the Schrödinger equation with asymptotes at $z<0$ equal to corresponding Bloch functions. The resulting boundary condition has the form

$$A_{jj_1}^{(1)}\psi_1^{(j_1)}=A_{jj_2}^{(2)}\psi_2^{(j_2)}\ ,\quad 1\le j\le N_b\ , \qquad (19)$$

where the matrices $A_{jj_1}^{(1)}$ and $A_{jj_2}^{(2)}$ have dimensions $N_b\times N_1$ and $N_b\times N_2$, respectively. The value of N_b as well as the values of the matrix elements $A_{jj_1}^{(1)}$ and $A_{jj_2}^{(2)}$ depend on specific materials and the microscopic structure of the interface.

Equation (19) holds for the case of $N_1=N_2=N$ and seems to contradict Eq. (15′) if $N_b>N$. However, in some of the Eqs. (17) the terms containing B_{jj_2} which result from the interface energy can be so great that all terms with derivatives, which are of the first order in a_0/L, can be neglected. The resulting equations together with Eq. (15′) are equivalent to Eq. (19).

The last argument hints that it may be possible to derive all the boundary conditions from a single variational principle.

One can also notice that in the case of an interface between materials with a degenerate band structure there may exist plane waves that are totally reflected from the interface even if a transmission is not forbidden by conservation laws. The total reflection is described by those functions $\Psi^{(\nu)}$ which have zero asymptote in one of the materials. They definitely exist for $N_1 \neq N_2$ and for $N_1 = N_2 = N$ if $N_b > N$.

IV. DISCUSSION

The simplest problem where it is necessary to use interface boundary conditions is the transmission and reflection of an electron beam incident normal to an interface. If the transmission and reflection coefficients are defined according to

$$\begin{aligned} \psi_{k_1}(z) &= e^{ik_1 z} + R(k_1) e^{-ik_1 z}\,, \quad && z > 0\,, \\ \psi_{k_1}(z) &= T(k_1) e^{ik_2 z}\,, && z < 0\,, \end{aligned} \tag{20}$$

then Eqs. (1) and (3) give

$$|T(k_1)|^2 = \frac{4m_1 m_2 k_1 k_2}{\left(\frac{\alpha_2}{\alpha_1} m_2 k_1 + \frac{\alpha_1}{\alpha_2} m_1 k_2\right)^2 + m_1 m_2 q^2}\,. \tag{21}$$

Equation (21) differs from the transmission coefficient resulting from Harrison's boundary conditions in the denominator term which contains the parameter q characterizing the interface energy. Equation (21) is identical with the result of Grinberg and Luryi[14] for the Kronig-Penney model. For zero band offset the transmission coefficient goes to zero with the energy of the incident beam while Harrison's boundary conditions, where $q = 0$, give for $|T(0)|^2$ a finite value. Zero value for $|T(0)|^2$ was obtained by Stiles and Hamann.[13]

The appearance of the parameter q detected in Refs. 13–15 sheds some doubts on the results of all band-structure calculations made with the help of simpler boundary conditions. Naturally, an additional parameter makes a comparison with experiments more difficult. The comparison is complicated also by the fact that the main band-structure calculation results relate to details of the energy spectrum while typically experimentalists measure either energy differences between very specific points in **k** space or kinetic phenomena. The importance of the parameter q for the transmission coefficient shows that it can be crucial for the calculation of the current across an interface. However, for a finite band offset the energy dependence of the transmission coefficient does not change dramatically with the introduction of q. Thus, a careful consideration is necessary in the comparison of experimental results with theoretical calculations.

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