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# Dirac equation approach to scattering from interface potential steps and existence of interface states

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*Abstract.* A relativistic-quantum approach to scattering by step-like potentials, characterising the interface between two periodic systems, is developed on the basis of Dirac equation and in terms of a transfer matrix method. The relevant  $R$ -matrices for the two possible types of interfaces are derived and the conditions for existence of bound states, localised at the interface, are obtained. The numerical analysis performed at the end enables us both to visualize the difference in the scattering behaviour of the two types of interfaces and to estimate the magnitude of the relativistic corrections.

## 1. Introduction

The quantum theory of scattering from steplike potentials, developed by Buslaev and Fomin [1] as early as 1962, remained for a long time mainly in the frames of pure mathematics [2, 3], despite the fact that two years earlier Aerts had already pointed to the role of the potential step as a scatterer in the  $S$ -matrix theory of localised surface and interface states [4]. To the best of our knowledge, until now there are only few papers devoted to the rigorous further development of this problem, especially as regards scattering by interface potential steps (see e.g. [5–11] and references therein).

The relativistic-quantum counter part of the problem, i.e. the Dirac equation approach to scattering of electrons from steplike potentials, is also of certain interest. What is more, it was Schrodinger who explicitly underlined that “Das beste, ja einzige Hilfsmittel” in the dynamics of an electron is Dirac equation [12].

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Hence, after Schrodinger, the Dirac equation approach in these cases is needed not only for evaluation of relativistic corrections which might be essential for heavy atoms; it is a must also in order to bring on firm ground the physical justification of calculations usually performed by using Schrodinger equation. Unfortunately, Schrodinger's assertion remained for a long time in hibernation, perhaps due to the fact that for many applied problems the relativistic-quantum corrections are relatively small, despite certain interesting results, e.g. [19–25].

As a matter of fact, there is a deep analogy in the study of scattering (especially from scalar potentials) based on the use of Schrodinger and Dirac operators [7, 13]. Nevertheless, the relativistic-quantum approach to scattering from steplike potentials in realistic physical models is still in its initial stage ([7, 14, 15], see also the review [22]).

It is our purpose in the present paper to work out one model clarifying the role of the steplike potential as a scatterer between two periodic structures. More specifically, the model we are here dealing with presents composite one-dimensional system of two diatomic crystals in contact, say of  $AB$  and  $BC$  atoms respectively, the last  $B$  atom of the one crystal being the first one in the other crystal (see Fig. 1). There is some real physics behind such a model, which might be considered as a heterojunction between, say a  $CdTe$  crystal and  $HgTe$  crystal (or  $PbTe-SnTe$ ). Thus, the model under consideration is the natural complement of the usual model

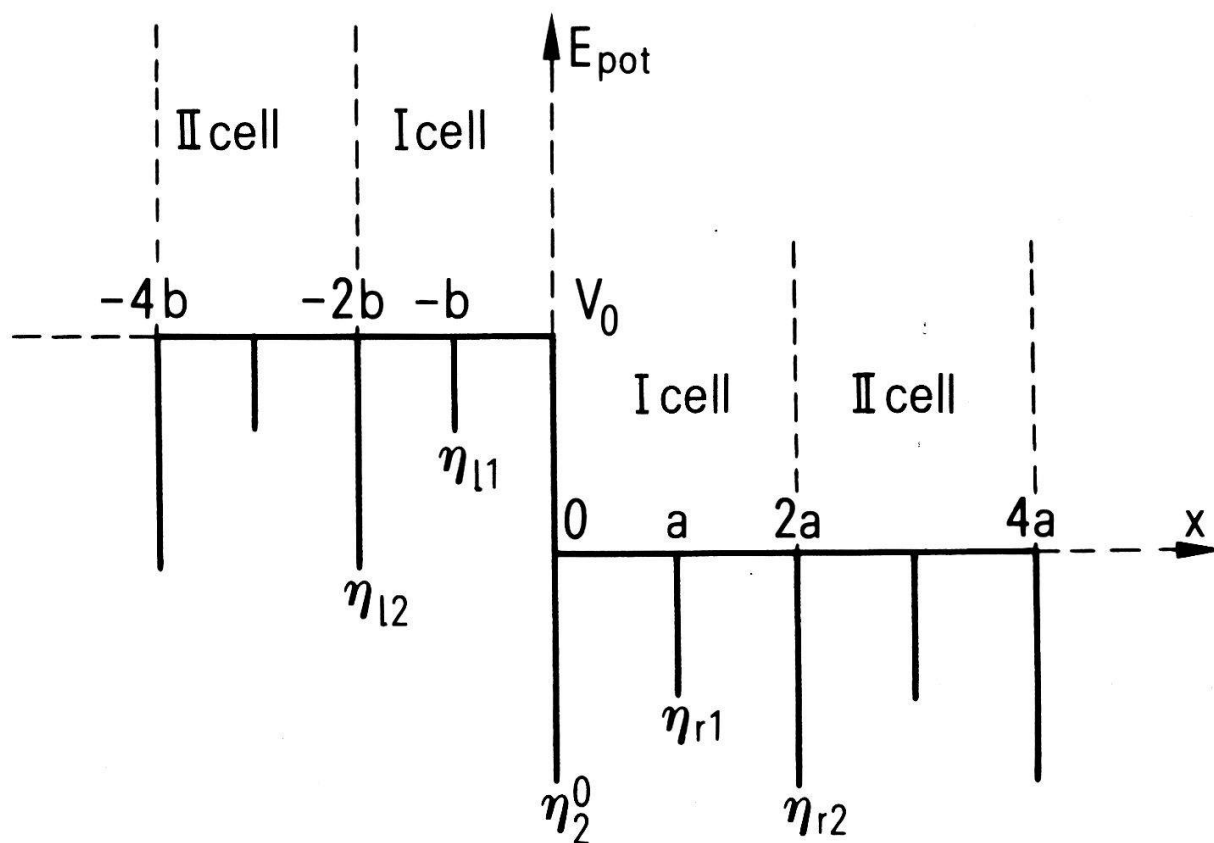


Figure 1

One-dimensional model of the second-type heterojunction between two diatomic semiconductors ( $\eta_{l2} = \eta_{r2}$ ).

of a heterojunction, where the interface potential step is placed somewhere between the end atoms of the two diatomic chains in contact [4, 14–16]. This enables us to compare the role of the interface as a scatterer in the two models.

In Section 2 we derive the  $R$ -matrices characterising the interface potential steps in the two different cases of interfaces. Let us only mention in passing that the  $R$ -matrix we are dealing with is in one-to-one correspondence with the relevant scattering matrices [17].

Being entirely in the framework of the one-electron theory, our treatment is based on the one-dimensional time-independent Dirac equation

$$i\hbar c\sigma_x \frac{d\psi(x)}{dx} - mc^2\sigma_z(x) = [E - V(x)]\psi(x) \quad (1)$$

with scalar-valued periodic potential  $V(x)$ . Here

$$\psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} \quad (2)$$

is the two component spinor wave function of the electron,  $\sigma_x$  and  $\sigma_z$  being the corresponding Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The noncovariant form of (1) in which Dirac has initially derived his equation is especially convenient for physical interpretations and discussions of the non-relativistic limits [18]. Let us remember that the reduction of the Dirac equation to a two component one here is due to the one-dimensional nature of the particular problem with scalar-valued periodic potential.

## 2. The interface as a scatterer

### 2.1. The model

Let us consider first the model of the  $AB-BC$  heterojunction between two semiinfinite diatomic crystals with attractive  $\delta$ -function potentials and lattice constants  $2a$  and  $2b$ , respectively. The interface barrier in this case (see Fig. 1) is combination of a potential step and a  $\delta$ -function, which results in an “asymmetric  $\delta$ -function” located at  $x = 0$ . The potential energy of the electron in the bulk of the two crystals in epitaxial contact is given by

$$E_{pot,r}(x) = -\eta_2^0\delta(x) - \eta_{r1} \sum_{n=1}^{\infty} \delta[x - (2n - 1)a] - \eta_{r2} \sum_{n=1}^{\infty} \delta(x - 2na), \quad x \geq 0 \quad (3)$$

$$E_{pot,l}(x) = -\eta_{l1} \sum_{n=0}^{\infty} \delta[x + (2n - 1)b] - \eta_{l2} \sum_{n=1}^{\infty} \delta(x + 2nb), \quad x < 0$$

where

$$\eta_{rj} = \frac{a\hbar^2}{m} U_{rj}(2a); \quad \eta_{lj} = \frac{b\hbar^2}{m} U_{lj}(2b) (j = 1, 2) \tag{4}$$

and, as a particular feature of second-type heterojunction, the relation  $\eta_{r2} = \eta_{l2} = \eta_2$  holds, which implies

$$aU_{r2}(2a) = bU_{l2}(2b). \tag{5}$$

Here, as usual, the  $\eta$ 's are measures for the strength of the corresponding  $\delta$ -function potentials; and we have denoted by  $\eta_2^0$  the potential strength  $\eta_2$  at  $x = 0$ . The potential energy  $E_{pot,l}$  is measured from the level  $V_0$  and we assume that  $V_0 < mc^2$ . The quantity  $U_{r1} + U_{r2}$  is proportional to the mean electron potential energy averaged over one unit cell in the right-hand crystal. Analogically,  $U_{l1} + U_{l2}$  has the same meaning for the left-hand crystal. The choice of the unit cells is defined in an unique way by the location of the interface (compare [16]).

### 2.2. R-matrix of the interface

As it was shown by Subramanian and Bhagwat [23] the effect of a  $\delta$ -potential on the solution of the Dirac equation (1) can be replaced by an equivalent boundary condition on the free electron wave function.

Let us denote by  $\psi(0_+)$  and  $\psi(0_-)$  the general (spinor) solution of (1) on both sides of the  $\delta$ -potential with strength  $\eta$ , situated at  $x = 0$ . Then the above boundary condition reads

$$\psi(0_+) = \begin{pmatrix} \cos \theta & i \sin \theta \\ i \sin \theta & \cos \theta \end{pmatrix} \psi(0_-) \tag{6}$$

where

$$\theta = 2 \tan^{-1}(\eta/2\hbar c). \tag{7}$$

Taking into account that the wave functions join continuously at a potential step, we arrive at the conclusion that the interface boundary condition for a second-type heterojunction reduces to (6) with  $\theta = \theta_2^0$  obtained from (7) for  $\eta = \eta_2^0$ . Of course equation (6) says that the wave function is indeed discontinuous across  $x = 0$  due to the fact that the interface is a combination of a potential step and a  $\delta$ -function potential.

It is easy to observe that close to both sides of the interface boundary there exist constant potential regions in which the general real-valued spinor solution of (1) can be put in the form

$$\psi_{ll}(x) = \begin{pmatrix} a_{ll} \cos \kappa_l x + b_{ll} \sin \kappa_l x \\ i\lambda_l a_{ll} \sin \kappa_l x - i\lambda_l b_{ll} \cos \kappa_l x \end{pmatrix} \tag{8}$$

for  $-b < x < 0$ , and

$$\psi_{r1}(x) = \begin{pmatrix} a_{r1} \cos \kappa_r x + b_{r1} \sin \kappa_r x \\ i\lambda_r a_{r1} \sin \kappa_r x - -i\lambda_r b_{r1} \cos \kappa_r x \end{pmatrix} \tag{9}$$

for  $0 < x < a$ , respectively. Here

$$\kappa_l = \frac{[(E - V_0)^2 - m^2c^4]^{1/2}}{\hbar c}; \quad \lambda_l = \frac{\hbar c \kappa_l}{E - V_0 + mc^2} = \frac{E - V_0 - mc^2}{\hbar c \kappa_l} \quad (10)$$

and

$$\kappa_r = \frac{(E^2 - m^2c^4)^{1/2}}{\hbar c}; \quad \lambda_r = \frac{\hbar c \kappa_r}{E + mc^2} = \frac{E - mc^2}{\hbar c \kappa_r} \quad (11)$$

where  $E$  is the relativistic total energy of the electron.

We define the relativistic  $R$ -matrix of the interface boundary for the second-type heterojunction, shown on Fig. 1, by

$$\begin{pmatrix} a_{r1} \\ b_{r1} \end{pmatrix} = R_{II} \begin{pmatrix} a_{l1} \\ b_{l1} \end{pmatrix} \quad (12)$$

where the amplitudes of the wave function spinors have to be specified on its own turn through the transfer matrices characterizing the bulk of the two crystals.

As it was already pointed out, the interface barrier in this case factorizes in a potential step and a symmetric  $\delta$ -function potential at  $x = 0$ . Hence,  $R_{II}$  naturally factorizes in

$$R_{II} = R_\delta R_{ps} \quad (13)$$

where (in real basis) the  $R$ -matrix of the potential step, given by (see [14])

$$R_{ps} = \begin{pmatrix} 1 & 0 \\ 0 & \lambda_l/\lambda_r \end{pmatrix} \quad (14)$$

coincides with the  $R$ -matrix  $R_I$  characterizing the interface of first-type heterojunctions; and  $R_\delta$  is obtained from the  $R$ -matrix reformulation of the Subramanian and Bhagwat boundary condition

$$R_\delta = \begin{pmatrix} \cos \theta & \lambda \sin \theta \\ -\frac{\sin \theta}{\lambda} & \cos \theta \end{pmatrix} \quad (15)$$

with  $\lambda \equiv \lambda_r$  and  $\theta \equiv \theta_2^0$  for the model under consideration. Thus

$$R_{II} = \begin{pmatrix} \cos \theta_2^0 & \lambda_l \sin \theta_2^0 \\ -\frac{\sin \theta_2^0}{\lambda_r} & \frac{\lambda_l}{\lambda_r} \cos \theta_2^0 \end{pmatrix} \quad (16)$$

From a formal point of view, the second-type interface is more general than those of the first type, since the case of a first-type heterojunction can be obtained as a particular case from it by putting  $\eta_2^0 = 0$ . This is especially transparent in the  $R$ -matrix approach used here, since the condition  $\eta_2^0 = 0$  immediately reduces  $R_{II}$  to  $R_I$ , as it is evident from (14) and (16).

### 3. Existence of interface states

#### 3.1. Energy equation for the interface states

As we have already mentioned, the amplitudes of the wave function spinors in (12) can be deduced by using the transfer matrices  $M_r$  and  $M_l$  of the two crystals and the requirement for the wave functions to remain finite when  $x \rightarrow \pm \infty$  (for details compare [26] with [14]). Thus

$$\begin{pmatrix} a_{r1} \\ b_{r1} \end{pmatrix} = A e^{2iak_r} \begin{pmatrix} 1 \\ \frac{e^{2iak_r} - (M_r)_{11}}{(M_r)_{12}} \end{pmatrix} \quad (17)$$

$$\begin{pmatrix} a_{l1} \\ b_{l1} \end{pmatrix} = C e^{2ibk_l} \begin{pmatrix} 1 \\ \frac{e^{2ibk_l} - (M_l)_{11}}{(M_l)_{12}} \end{pmatrix}$$

Substituting (16) and (17) in (12) we arrive at a homogeneous system of algebraic equations for the coefficients  $A$  and  $C$ . The condition for existence of nontrivial solutions of this system results in

$$\begin{aligned} \frac{1}{\lambda_r} \sin \theta_2^0 - \frac{\lambda_l}{\lambda_r} \cos \theta_2^0 \frac{e^{2ibk_l} - (M_l)_{11}}{(M_l)_{12}} \\ + \frac{e^{2iak_r} - (M_r)_{11}}{(M_r)_{12}} \left[ \cos \theta_2^0 + \lambda_l \sin \theta_2^0 \frac{e^{2ibk_l} - (M_l)_{11}}{(M_l)_{12}} \right] = 0. \end{aligned} \quad (18)$$

The equation which has to be satisfied by the energy of a bound state localized at the interface can be derived from (18) and the requirement that this state belongs to a common energy gap for the two crystals in contact, i.e. to the energy interval defined by the two simultaneous inequalities

$$|\text{Tr } M_l| > 2, \quad |\text{Tr } M_r| > 2. \quad (19)$$

Then

$$\begin{aligned} k_l &= \frac{n_l \pi}{2b} + i\gamma_l, & n_l &= 1, 2, \dots \\ k_r &= \frac{n_r \pi}{2a} + i\gamma_r, & n_r &= 1, 2, \dots \end{aligned} \quad (20)$$

where  $\gamma_l > 0$ ,  $\gamma_r > 0$  characterize the energy gaps, with  $n_l$  and  $n_r$  even (odd) for gaps opened at the centre (edge) of the Brillouin zone. More specifically, substituting (20) in (18) and taking into account the relevant Kronig–Penney relations

$$\cos 2bk_l = \frac{1}{2} \text{Tr } M_l, \quad \cos 2ak_r = \frac{1}{2} \text{Tr } M_r, \quad (21)$$

we obtain the equation for the energy of the interface states

$$\Gamma_l \cos \theta_2^0 + \sin \theta_2^0 = \Gamma_r (-\cos \theta_2^0 + \Gamma_l \sin \theta_2^0). \quad (22)$$

Here

$$\Gamma_l = -\lambda_l \frac{\frac{1}{2}[(M_l)_{22} - (M_l)_{11}] + (-1)^{n_l+1} \sinh 2b\gamma_l}{(M_l)_{12}} \quad (23)$$

and

$$\Gamma_r = \lambda_r \frac{\frac{1}{2}[(M_r)_{22} - (M_r)_{11}] + (-1)^{n_r+1} \sinh 2a\gamma_r}{(M_r)_{12}} \quad (24)$$

and the quantities  $\gamma_l$  and  $\gamma_r$  have to be eliminated from (22) through the Kronig–Penney relations for the relevant energy gaps. For the right-hand crystal this dispersion relation reads (compare [27])

$$(-1)^{n_r} \cosh 2a\gamma_2 = 2 \prod_{i=1}^2 \left[ \cos \theta_{ri} \cos a\kappa_r - \frac{1}{2} \left( \lambda_2 + \frac{1}{\lambda_r} \right) \sin \theta_{ri} \sin a\kappa_r \right] - \cos (\theta_{r1} - \theta_{r2}). \quad (25)$$

For the left-hand crystal the replacements  $a \rightarrow b$ ,  $r \rightarrow l$  and  $n_r \rightarrow n_l$  should be performed in (25).

The energy  $E$  of the bound state enters in (22) through the quantities  $\lambda$  and  $\kappa$  defined by (10) and (11), and the transfer matrices.

The matrix elements of the diatomic crystal transfer matrices  $M_l$  and  $M_r$  (in the same real basis used here) can be taken from [16, 17], so that

$$(M_l)_{22} - (M_l)_{11} = \left( \frac{1}{\lambda_l} - \lambda_l \right) \sin \theta_2 \left[ \left( \frac{1}{\lambda_l} + \lambda_l \right) \sin \theta_{l1} \sin^2 b\kappa_l - \cos \theta_{l1} \sin 2b\kappa_l \right] \quad (26)$$

$$(M_l)_{12} = \left[ \begin{aligned} & -\cos (\theta_{l1} + \theta_2) \sin 2b\kappa_l - \lambda_l \sin (\theta_{l1} + \theta_2) \cos 2b\kappa_l \\ & - \frac{1}{2}(1 - \lambda_l^2) \sin \theta_{l1} \sin \theta_2 \sin 2b\kappa_l - \left( \lambda_l - \frac{1}{\lambda_l} \right) \sin \theta_{l1} \cos \theta_2 \sin^2 b\kappa_l \end{aligned} \right] \quad (27)$$

$$(M_r)_{22} - (M_r)_{11} = \left( \frac{1}{\lambda_r} - \lambda_r \right) \sin \theta_2 \left[ \left( \frac{1}{\lambda_r} + \lambda_r \right) \sin \theta_{r1} \sin^2 a\kappa_r - \cos \theta_{r1} \sin 2a\kappa_r \right] \quad (28)$$

$$(M_r)_{12} = \left[ \begin{aligned} & \cos (\theta_{r1} + \theta_2) \sin 2a\kappa_r + \lambda_r \sin (\theta_{r1} + \theta_2) \cos 2a\kappa_r \\ & + \frac{1}{2}(1 - \lambda_r^2) \sin \theta_{r1} \sin \theta_2 \sin 2a\kappa_r + \left( \lambda_r - \frac{1}{\lambda_r} \right) \sin \theta_{r1} \cos \theta_2 \sin^2 a\kappa_r. \end{aligned} \right] \quad (29)$$



In order to obtain the final form of the condition for existence of interface states we have to complete the energy equation with all the consequences following from the positivity of both  $\gamma_l$  and  $\gamma_r$ . Aerts was the first to perform such an analysis for the simplest case of a heterojunction between two monatomic crystals [4]. Thus, he arrived at the conclusion that interface states may exist if and only if their energy satisfy a relevant energy equation and the common energy gap is the common part of the first energy gap of the one crystal and the second gap of the other. It is easy to observe, that this result about the common gap still holds by the relativistic generalization of this simplest model of first-type heterojunction. In fact, it immediately follows from the conditions for the energy of interface states in this case (see [14])

$$\lambda_r \frac{(-1)^{n_r} \sinh 2a\gamma_r}{(M_r)_{12}} = \lambda_l \frac{(-1)^{n_l} \sinh 2b\gamma_l}{(M_l)_{12}}$$

by taking into account that the relevant matrix elements  $(M_r)_{12}$  and  $(M_l)_{12}$  have opposite signs.

As regards the analogical considerations for second-type heterojunctions, a preliminary treatment is given by us in [28] for the case of nonrelativistic quantum mechanics. Even in this relatively simpler case some numerical analysis was needed. The expressions derived here for the relativistic generalization of this model are much more complicated. What is more, the exhaustive treatment of the second-type heterojunctions naturally incorporates also its comparison with the first-type heterojunction between the same diatomic crystals. This problem was not approached at all in [28]. Hence, our aim in the following section is (i) to perform the relevant numerical analysis of the condition for existence of interface states (22); (ii) to develop the comparison of this condition with its counterpart for interface states in first-type heterojunctions; (iii) to estimate the magnitude of the relativistic corrections in the energy of the interface states.

### 3.2. Numerical analysis

For the numerical analysis it seem useful to rewrite the condition for existence of interface states (22) in the form

$$W_l^R = -BW_r^R + \frac{2B}{K_r} \Gamma_r \Gamma_l \sin \theta_2^0, \tag{30}$$

where

$$W_i^R = 2 \frac{\Gamma_i \cos \theta_2^0 + \frac{1}{2} \sin \theta_2^0}{K_i}, \quad i = r, l \tag{31}$$

and

$$B = b/a; \quad K_r = \frac{\hbar}{amc}, \quad K_l = \frac{\hbar}{bmc} = \frac{K_r}{B}.$$

In the non-relativistic (NR) limit eq. (30) becomes

$$W_l = -BW_r. \tag{30a}$$

which coincides with the relevant condition already derived for the *NR* case in [28], and

$$W_i(X_i, A_{i1}, A_{i2}) = (-1)^{n_i} \left( X_i - \frac{A_{i2}}{2} \tan X_i \right) \times \left[ \frac{A_{i1} A_{i2} - 2X_i(A_{i1} + A_{i2}) \cotan X_i - 4X_i^2}{\prod_{j=1}^2 (2X_i - A_{ij} \tan X_i)} \right]^{1/2} \quad (32)$$

is the *NR* limit of  $W_i^R$ . The dimensionless variables  $X_i$  are defined by

$$X_r = a\kappa_r^0, \quad X_l = b\kappa_l^0,$$

$\kappa_i^0$  being the *NR* limits of  $\kappa_i$  from equations (10) and (11). The dimensionless parameters  $A_{ij}$  are introduced by

$$A_{rj} = a^2 U_{rj}(a), \quad A_{lj} = b^2 U_{lj}(b), \quad j = 1, 2. \quad (33)$$

For what follows it is easy to observe that equation (5) leads to

$$A_{l2} = BA_{r2}.$$

Let us point out that the first-type interface may be obtained as a particular case from the second-type interface by putting  $\theta_2^0 = 0$ , as it follows immediately from equations (16) and (14). Then equation (22) reduces to

$$\Gamma_l = -\Gamma_r, \quad (34)$$

which is just the condition for existence of interface states in first-type heterojunctions we have already derived in [16]. In the *NR* limit

$$\Gamma_i \rightarrow \frac{K_i}{2} \left( W_i - \frac{A_{i2}}{2} \right), \quad i = r, l,$$

$W_i$  being given by (32).

Obviously, the behaviour of the function  $W_i^R$  plays a crucial role in the numerical analysis of the condition for existence of interface states and its physical interpretation. Of course, for any given heterojunction,  $W_i^R$  may be presented as a function of the dimensionless variable  $X_i^R$  and the dimensionless parameters  $A_{i1}$  and  $A_{i2}$ , where

$$X_r^R = a\kappa_r, \quad X_l^R = b\kappa_l.$$

In Fig. 2 the function  $W_i^R(X_i^R)$  is plotted against its argument  $X_i^R$  for given  $A_{i1}$  and  $A_{i2}$ . The shape of this curve practically coincides with the relevant *NR* relation between  $W_i$  and  $X_i$ . In agreement with equation (30a) it is also seen that in second type heterojunctions there are not interface states in a common gap defined as the common part of two even energy gaps.

The magnitude of the relativistic corrections in the energy of the interface states is smaller than  $10^{-3}$  eV.

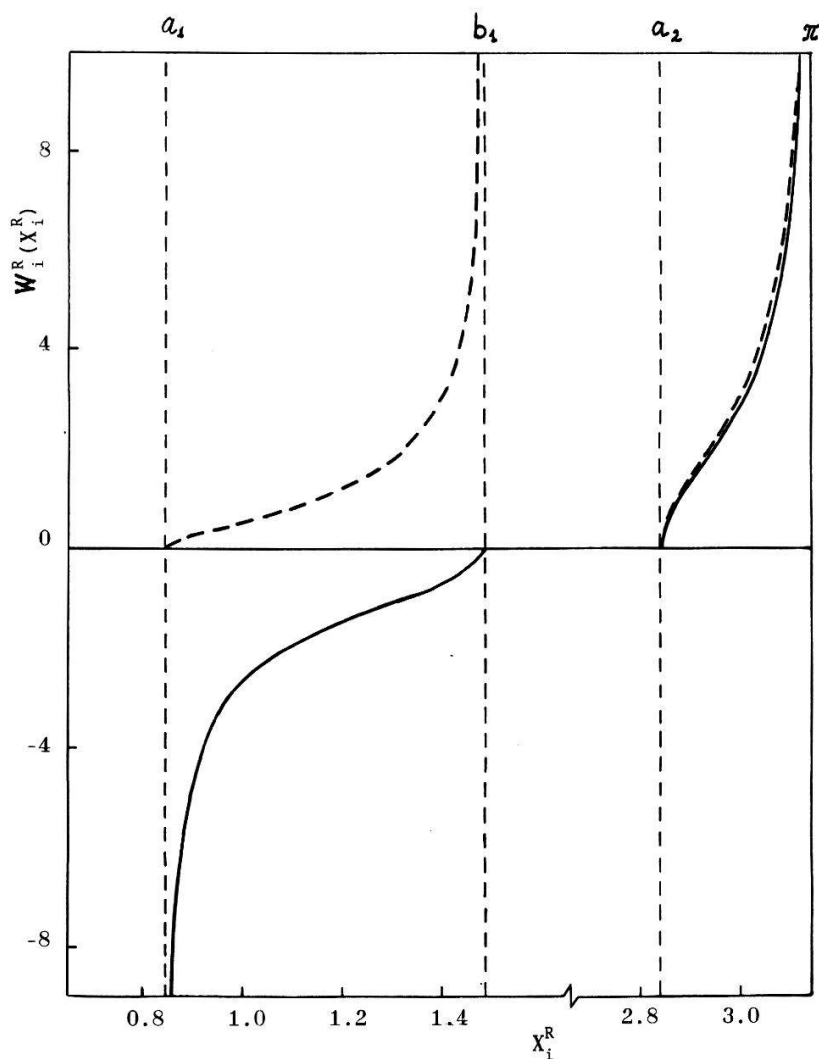


Figure 2  
 $W_i^R$  as function of  $X_i^R$ . The full-line (dashed-line) curves are calculated for  $A_{i1} = 1.50$  and  $A_{i2} = 0.25$  (for  $A_{i1} = 0.25$  and  $A_{i2} = 1.50$ );  $a_1$  and  $b_1$  correspond to the bottom and top of the first energy gap,  $a_2$  and  $\pi$  being the relevant edges for the second gap.

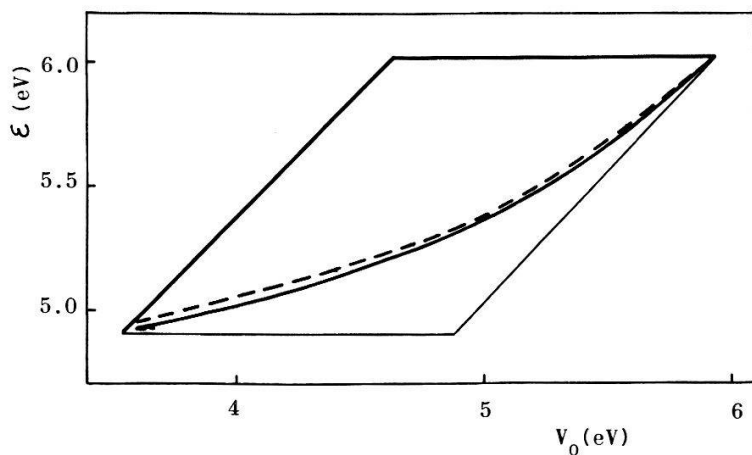


Figure 3  
 Energy  $\epsilon$  of the interface state versus the interface potential step  $V_0$  for a variety of heterojunctions with  $B = 1$ ;  $A_{r1} = 0.2$ ;  $A_{r2} = 1.5$ ;  $A_{l1} = 1.9$ ;  $A_{l2} = 1.5$ . The common gap is formed from the second gap of the right-hand crystal and the first gap of the left-hand crystal. Thick straight lines: bottom of the common gap. Full-line curves corresponds to second-type interface states. Dashed-line curve corresponds to first-type interface states.

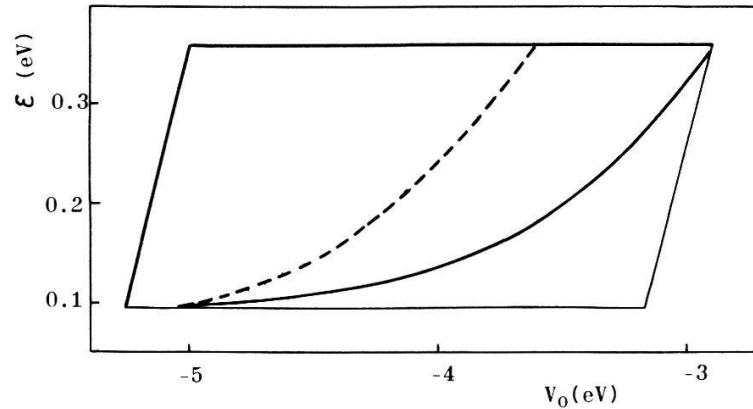


Figure 4

The same as Fig. 3 for  $B = 1.0625$ ;  $A_{r1} = 1.9$ ;  $A_{r2} = 1.6$ ;  $A_{l1} = 1.8$ ;  $A_{l2} = 1.7$  and common gap formed from the first gap of the right-hand crystal and the second gap of the left-hand crystal.

However, from a physical point of view, what is more interesting is the comparative study of the appearance of interface states at first-type and second-type interfaces for a given pair of diatomic crystals forming a heterojunction.

Details are seen in Figs. 3–5, each of which presents the dependence of the energy of the interface states on the interface potential step for a variety of heterojunctions characterised by given dimensionless parameters  $A_{ij}$ . In these three figures the thick line (i.e. the left and upper straight lines) correspond to the top of the common energy gap, and the thin straight lines correspond to its bottom. By

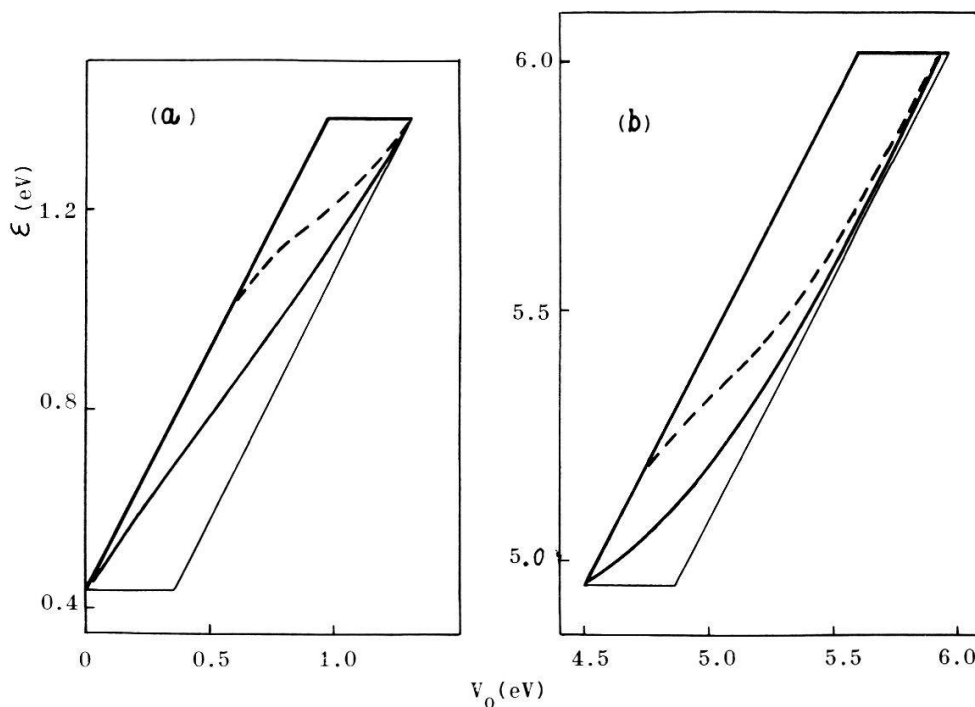


Figure 5

The same as Fig. 3 for  $B = 1$ ;  $A_{r1} = 0.2$ ;  $A_{r2} = 1.5$ ;  $A_{l1} = 1.9$ ;  $A_{l2} = 1.5$ .

- (a) common gap formed from first gaps
- (b) common gap formed from the second gap of the right-hand crystal and the first gap of the left-hand crystal.

this way each point of the curves visualizes the position of the interface state in the common energy gap of a particular heterojunction.

There are certain cases in which the position of the interface states in the common energy gap is almost the same for first type and second-type heterojunctions of given pairs of crystals. This is e.g. the case (shown in Fig. 3) for heterojunctions, characterized with  $B = b/a = 1$ ,  $A_{r1} = 1.5$ ;  $A_{r2} = 0.25$ ;  $A_{l1} = 1.9$ ;  $A_{l2} = 0.25$  and a common gap defined as the common part of the first energy gap of the left-hand crystal and the second gap of the right-hand one.

In other heterojunctions there is a considerable difference in the energy of the interface states for first-type and second-type interfaces, and the magnitude of this difference depends on the interface potential step (see e.g. Fig. 4). In all heterojunctions the interface states at second-type interfaces have energies below the energy of the relevant first-type interface states.

Another interesting result of the numerical analysis is that in certain cases interface states exist only in second-type heterojunctions (e.g. Fig. 5a for potential steps in the interval 0–0.5 eV). In certain cases there are no interface states at all. Such a situation arises e.g. in heterojunctions characterized by  $A_{r1} = 0.1$ ;  $A_{r2} = 0.75$ ;  $A_{l1} = 0.95$ ;  $A_{l2} = 0.75$  and interface potential steps in the interval from –3.8 eV to –5.6 eV, provided the common gap is formed from the first gap of the right-hand crystal and the second gap of the left-hand crystal.

#### 4. Conclusions

The first-type interface can be considered as a particular case from the second-type interface. Correspondingly, the  $R$ -matrix of the second-type interface can be factorized in a product of two matrices, one of which is just the  $R$ -matrix of first type interface. Nevertheless, the determinants of the  $R$ -matrices for the two types of interfaces are equal, i.e.

$$\det R_{II} = \det R_I = \det R_{ps} = \frac{\lambda_l}{\lambda_r}.$$

This points to the fact that in both cases the relevant scattering matrices are unitary in the generalised sense of Buslaev and Fomin [1].

It is worth noting that the condition  $\det R_{ps} \neq 1$  for steplike potentials is sometimes interpreted in the sense that the  $S$ -matrix of the potential step is not unitary (see e.g. the first paper by Cohen in [2]). In fact, the deviation of  $R_{ps}$  from unimodularity leads to deviation of the relevant  $S$ -matrix from symmetry, i.e. in our notation

$$S_{21}^{(ps)} = S_{12}^{(ps)} \det R_{ps}.$$

Consequently, the precise statement is that in the case of steplike potentials the well-known condition for unitarity of bumplike potentials has to be replaced by its generalised form derived by Buslaev and Fomin [1, 5, 29]. For the particular case of abrupt potential step and real basis unitarity reduces to orthogonality. What is

more, Mora et al. [10] have even worked out a generalisation of the transfer matrix in one dimension, which enables to treat a wide class of problems on the basis of both Schrödinger and Dirac equations. Their transfer matrix is redefined in such a way that it remains unimodular even for a steplike scatterer, a fact especially useful by numerical calculations. The advantage of the traditionally defined transfer matrix we are used here is that it makes more transparent the specific physics characterising the difference in scattering from steplike and bump-like potentials.

In addition to the above general results, a more detailed physical interpretation follows from the numerical analysis performed. Thus, in addition to the Aerts-type interface states which may appear only in a common energy gap at the interface of an even and an odd gaps, in the model under consideration interface states can exist in a common gap formed from two odd gaps (e.g. Fig. 5a). Second-type interface states are forbidden for common gaps from two even gaps, but this selection rule does not hold for first type interface states.

In all of the numerically investigated cases for a given pair of crystals with fixed interface potential step, the energy of second-type interface state is below the energy of the relevant first-type interface state when both  $AB-BC$  and  $AB-CB$  heterojunctions can be realized.

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