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INTERFACE STATES IN A CLASS OF HETEROJUNCTIONS BETWEEN DIATOMIC SEMICONDUCTORS *

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ABSTRACT

The theory of interface states in heterojunctions between diatomic semiconductors is developed in the framework of the S -matrix approach and on the basis of an one-dimensional model. The condition for the existence of interface states is explicitly derived for undeformed and deformed heterojunctions. Numerical analysis is performed and several particular cases are discussed in order to clarify the general features of the problem.

1. INTRODUCTION

Heterojunctions between diatomic semiconductors are subject of extensive research perhaps due to the fact that heterojunctions like GaP-GaAs [1),2)], CdS-CdSe [3),4)] and GaAs-ZnSe [5)] are of growing interest in solid state electronics. This had led to a number of theoretical studies, by various methods, of abrupt semiconductor heterojunctions [6)-8)]. As regards the theory of interfaces between two diatomic semiconductors, an attempt is made to approach this problem by using self-consistent pseudopotential calculations (see e.g. Ref.7). Although such calculations are of common usage now, some results they arrive at remain often "not yet well understood" [8)]. In this situation the development of rigorously treated one-dimensional models is a must [9)]. Let us mention that the treatment of one-dimensional models of semiconductor heterojunctions by the S -matrix method [10)] was recently succesfully applied to more complicated (and more realistic) cases of deformed heterojunctions [11)-13)].

It is the purpose of the present paper to develop the S -matrix approach to the theory of interface states in a class of heterojunctions between diatomic semiconductors. Attention is paid to the influence of the interface spacing and its changes on the condition for the existence of interface states.

2. THE MODEL AND THE RELEVANT WAVE FUNCTIONS

Let us consider a system of two epitaxially joined semi-infinite one-dimensional crystals. As usually [10),14)] the contact between the two crystals is characterised by a potential step $-eV_0$ at the interface. As a matter of fact we shall deal with the general case of deformed interface spacing (figure 1a), the particular case $\Delta a = \Delta b = 0$ (figure 1b) being of interest as an example of undeformed ideal heterojunction. The potential energy of the electron on the right and on the left of the interface is given by

$$(E_{pot})_r = \frac{a\hbar^2}{m}\left\{U_{1r}\sum_{n=0}^{\infty}\delta[x-(2n+1)a+\Delta a]+U_{2r}\sum_{n=0}^{\infty}\delta[x-(2n+2)a+\Delta a]\right\} \qquad x>0 \qquad (1)$$

and

$$(E_{pot})_l = \frac{b\hbar^2}{m}\left\{U_{1l}\sum_{n=0}^{\infty}\delta[x+(2n+1)b-\Delta b]+U_{2l}\sum_{n=0}^{\infty}\delta[x+(2n+2)b-\Delta b]\right\} \qquad x<0 \qquad (2)$$

respectively, $(E_{pot})_l$ being measured from $-eV_0$.

The general solution of the Schrödinger equation in the right-hand crystal is

$$\Psi_r(x) = \alpha_2\frac{\psi^*(x)}{\psi^*(a-\Delta a)} + \beta_2\frac{\psi(x)}{\psi(a-\Delta a)} \qquad (3)$$

where $\psi(x)$ and $\psi^*(x)$ are the two linearly independent Bloch waves moving to the right and to the left, respectively, and the constant α_2 (resp. β_2) is related to the amplitude of the incoming (resp. outgoing) wave - compare Refs.15 and 16. Straightforward calculations yield

$$\psi(x)=\frac{aU_{1r}}{k}\psi(a-\Delta a)\frac{\sin k(x+a+\Delta a)-e^{-2ia\mu}\sin k(x-a+\Delta a)}{\cos 2a\mu-\cos 2ak}+$$

$$+\frac{aU_{2r}}{k}\psi(2a-\Delta a)\frac{\sin k(x+2a+\Delta a)-e^{-2ia\mu}\sin k(x+\Delta a)}{\cos 2a\mu-\cos 2ak} \qquad (4)$$

where $\hbar\mu$ is the crystal momentum of the electron and $k^2=2mE/\hbar^2$. Substituting equation (4) and its complex conjugated expression in equation (3) leads to

$$\Psi_r(x)=$$

$$=\alpha_2\frac{\psi_{1r}^*\left[\sin\kappa(x+a+\Delta a)-e^{2ia\mu}\sin\kappa(x-a+\Delta a)\right]+\delta_r\psi_{2r}^*e^{2ia\mu}\left[\sin\kappa(x+2a+\Delta a)-e^{2ia\mu}\sin\kappa(x+\Delta a)\right]}{\psi_{1r}^*\sin 2a\kappa+\delta_r\psi_{2r}^*\left(1+e^{2ia\mu}\right)\sin a\kappa}+$$

(5)

$$+\beta_2\frac{\psi_{1r}\left[\sin\kappa(x+a+\Delta a)-e^{-2ia\mu}\sin\kappa(x-a+\Delta a)\right]+\delta_r\psi_{2r}e^{-2ia\mu}\left[\sin\kappa(x+2a+\Delta a)-e^{-2ia\mu}\sin\kappa(x+\Delta a)\right]}{\psi_{1r}\sin 2a\kappa+\delta_r\psi_{2r}\left(1+e^{-2ia\mu}\right)\sin a\kappa}$$

with

$$\psi_{1r}=\psi(a-\Delta a),\quad \psi_{2r}=\psi(2a-\Delta a),\quad \delta_r=U_{2r}/U_{1r} \tag{6}$$

and ψ_{1r} , ψ_{2r} are connected by the relation

$$\psi_{1r}=\psi_{2r}\frac{\cos a\mu\, e^{-ia\mu}}{\cos a\kappa+\frac{aU_{1r}}{\kappa}\sin a\kappa} \tag{7}$$

Analogically, for the wave function in the left-hand crystal we obtain

$$\Psi_\ell(x)=$$

$$=\alpha_1\frac{\psi_{1\ell}\left[e^{2ib\nu}\sin\lambda(x+b-\Delta b)-\sin\lambda(x-b-\Delta b)\right]+\delta_\ell\psi_{2\ell}e^{2ib\nu}\left[e^{2ib\nu}\sin\lambda(x-\Delta b)-\sin\lambda(x-2b-\Delta b)\right]}{\psi_{1\ell}\sin 2b\lambda+\delta_\ell\psi_{2\ell}\left(1+e^{2ib\nu}\right)\sin b\lambda}+$$

(8)

$$+\beta_1\frac{\psi_{1\ell}^*\left[e^{-2ib\nu}\sin\lambda(x+b-\Delta b)-\sin\lambda(x-b-\Delta b)\right]+\delta_\ell\psi_{2\ell}^*e^{-2ib\nu}\left[e^{-2ib\nu}\sin\lambda(x-\Delta b)-\sin\lambda(x-2b-\Delta b)\right]}{\psi_{1\ell}^*\sin 2b\lambda+\delta_\ell\psi_{2\ell}^*\left(1+e^{-2ib\nu}\right)\sin b\lambda}$$

where $\hbar\nu$ is the crystal momentum of the electron in the left-hand crystal,

$$\lambda^2=\kappa^2+(2me V_0)/\hbar^2 \tag{9}$$

$$\psi_{1\ell}=\psi(-b+\Delta b),\quad \psi_{2\ell}=\psi(-2b+\Delta b),\quad \delta_\ell=U_{2\ell}/U_{1\ell} \tag{10}$$

$$\psi_{1\ell}=\psi_{2\ell}\frac{\cos b\nu\, e^{ib\nu}}{\cos b\lambda+\frac{bU_{1\ell}}{\lambda}\sin b\lambda} \tag{11}$$

and α_1 (resp. β_1) corresponds to the amplitude of the incoming (resp. outgoing) wave.

The expression (5) for $\Psi_r(x)$ holds in the region $0<x<a-\Delta a$ and, analogically, the expression (8) for $\Psi_\ell(x)$ holds for $-b+\Delta b<x<0$. Now we are in a position to construct the relevant S - and $\mathcal{R}$ -matrices, characterising the interface as a scatterer, thus arriving at the $\mathcal{R}$ -matrix formulation of the condition for the existence of interface states.

3. $\mathcal{R}$ -MATRIX OF THE HETEROJUNCTION AND THE CONDITION FOR THE EXISTENCE OF INTERFACE STATES

As it is well known the condition for the existence of interface states is given by the requirement for singularity of the relevant S -matrix characterising the heterojunction together with the restriction the levels so obtained to lie in common energy gap (see e.g. Refs.10 and 13).

It is convenient to introduce the relevant $\mathcal{R}$ -matrix of the heterojunction

$$\begin{pmatrix}\beta_2\\ \alpha_2\end{pmatrix}=\begin{pmatrix}\mathcal{R}_{11} & \mathcal{R}_{12}\\ \mathcal{R}_{21} & \mathcal{R}_{22}\end{pmatrix}\begin{pmatrix}\alpha_1\\ \beta_1\end{pmatrix} \tag{12}$$

Since

$$S = R_{22}^{-1} \begin{pmatrix} -R_{21} & 1 \\ \det R & R_{12} \end{pmatrix} \tag{13}$$

the requirement for singularity of S implies $R_{22}=0$, while the second requirement leads to

$$\mu = n_r \frac{\pi}{2a} + i\xi\,, \quad \xi>0, \quad n_r = 1, 2, \ldots$$
$$\nu = n_\ell \frac{\pi}{2b} + i\chi, \quad \chi>0, \quad n_\ell = 1, 2, \ldots \tag{14}$$

Here n_r and n_ℓ enumerate the energy gaps of the two crystals.

The matrix elements of the R -matrix of the heterojunction are obtained from the boundary condition at the interface

$$\Psi_\ell(0) = \Psi_r(0)\,, \qquad \Psi_\ell'(0) = \Psi_r'(0) \tag{15}$$

Then the requirement $R_{22}=0$ leads to

$$\lambda \frac{\left[\cos\lambda(b+\Delta b) - e^{-2ib\nu}\cos\lambda(b-\Delta b)\right] + \delta_\ell \frac{\psi_{2\ell}^*}{\psi_{1\ell}^*} e^{-2ib\nu}\left[\cos\lambda(2b+\Delta b) - e^{-2ib\nu}\cos\lambda\Delta b\right]}{\left[\sin\lambda(b+\Delta b) + e^{-2ib\nu}\sin\lambda(b-\Delta b)\right] + \delta_\ell \frac{\psi_{2\ell}^*}{\psi_{1\ell}^*} e^{-2ib\nu}\left[\sin\lambda(2b+\Delta b) - e^{-2ib\nu}\sin\lambda\Delta b\right]} =$$

(16)

$$= -K \frac{\left[\cos K(a+\Delta a) - e^{-2ia\mu}\cos K(a-\Delta a)\right] + \delta_r \frac{\psi_{2r}}{\psi_{1r}} e^{-2ia\mu}\left[\cos K(2a+\Delta a) - e^{-2ia\mu}\cos K\Delta a\right]}{\left[\sin K(a+\Delta a) + e^{-2ia\mu}\sin K(a-\Delta a)\right] + \delta_r \frac{\psi_{2r}}{\psi_{1r}} e^{-2ia\mu}\left[\sin K(2a+\Delta a) - e^{-2ia\mu}\sin K\Delta a\right]}$$

What remains to be done is to substitute in the above condition μ and ν from the Kronig-Penney relations for diatomic crystals

$$\cos^2 a\mu = \left(\cos aK + \frac{aU_{1r}}{K}\sin aK\right)\left(\cos aK + \frac{aU_{2r}}{K}\sin aK\right)$$
$$\cos^2 b\nu = \left(\cos b\lambda + \frac{bU_{1\ell}}{\lambda}\sin b\lambda\right)\left(\cos b\lambda + \frac{bU_{2\ell}}{\lambda}\sin b\lambda\right) \tag{17}$$

taking into account that μ and ν belong to the relevant gaps, i.e. equations (14) hold.

Introducing the new variables

$$x = aK \qquad \varepsilon_r = \Delta a/a \qquad A_{ir} = -a^2 U_{ir}$$
$$y = a\lambda \qquad \varepsilon_\ell = \Delta b/b \qquad A_{i\ell} = -b^2 U_{i\ell} \qquad i = 1, 2 \tag{18}$$
$$B = b/a$$

where A_{ir}, $A_{i\ell} \in (0, 1)$, after some cumbersome calculations, equation (16) may be presented as

$$W_\pm(By, A_{1\ell}, A_{2\ell}, \varepsilon_\ell) = -B\,W_\pm(x, A_{1r}, A_{2r}, \varepsilon_r) \tag{19a}$$

$$W_\pm(By, A_{1\ell}, A_{2\ell}, \varepsilon_\ell) = -B\,W_\pm(x, A_{1r}, A_{2r}, \varepsilon_r) \tag{19b}$$

The functions $W_\pm$ have the form

$$W_\pm(z, A_{1j}, A_{2j}, \varepsilon_j) = \tag{20}$$
$$= z\frac{(-1)^{n_j}\sqrt{\frac{\sigma_j}{S_{1j}S_{2j}}}\left(z+\delta_j S_{ij}\right) - \left(z\tan z\varepsilon_j + \delta_j S_{ij}\cot z\right) + \delta_j\frac{z^2}{S_{2j}}\left(-\tan z\varepsilon_j + \cot z\right)}{(-1)^{n_j}\sqrt{\frac{\sigma_j}{S_{1j}S_{2j}}}\left(z+\delta_j S_{ij}\right)\tan z\varepsilon_j + \left(z - \delta_j S_{ij}\cot z\tan z\varepsilon_j\right) + \delta_j\frac{z^2}{S_{2j}}\left(1+\cot z\tan z\varepsilon_j\right)}$$

where

$$S_{1j} = z - A_{1j}\tan z \quad , \quad S_{2j} = z - A_{2j}\tan z$$

$$\sigma_j = A_{1j}A_{2j} - z^2 - z(A_{1j} + A_{2j})\cot z$$

$$\delta_j = A_{2j}/A_{1j}$$

and $j = c \Longrightarrow z = X$, $j = \ell \Longrightarrow z = By$, respectively. The expression W_+ holds for even energy gaps (n_j even), and W_- holds for odd energy gaps (n_j odd).

The presence of deformations in the interface spacing has as its result, that for such heterojunctions there is no parity-check selection rule at all (compare Ref.13 for the analogical situation of heterojunctions between monatomic semiconductors).

It is worth noting, that even for the case of an ideal undeformed heterojunction (figure 1b), interface states may appear in a common gap obtained from two odd gaps. A straightforward generalization of Aerts' parity-check selection rule for heterojunctions between monatomic semiconductors [10], which cancels the appearance of interface states in a common gap obtained from two energy gaps of the same parity, remains valid only for the case of contact between two even energy gaps.

More specifically, for equations (19) to hold it is necessary the functions $W_\pm$ defined by (20), which for the case of undeformed interface spacing reduce to

$$W_\pm(z, A_{1j}, A_{2j}) = \frac{(-1)^{n_j}\sqrt{\frac{\sigma_j}{S_{1j}S_{2j}}}(z + \delta_j S_{1j}) - \delta_j S_{1j}\cot z + \delta_j \frac{z^2}{S_{2j}}\cot z}{1 + \delta_j \frac{z}{S_{2j}}} \qquad (21)$$

to have opposite signs for the two crystals in contact. If n_j is even, then $S_{1j} > 0$, and $\cot z < 0$. Since we are

interested in such values of z which correspond to a forbidden energy band, we arrive at the additional inequality $S_{1j} > z^2/S_{2j}$. Thus the function W_+ is always positive for an even energy gap. For n_j odd $\cot z > 0$ and either

$$A_{1j} < A_{2j} \Longrightarrow S_{1j} > 0 \,, \quad S_{2j} < 0 \qquad (22a)$$

or

$$A_{1j} > A_{2j} \Longrightarrow S_{1j} < 0 \,, \quad S_{2j} > 0 \qquad (22b)$$

In the case (22a) the denominator in (21)

$$1 + \delta_j \frac{z}{S_{2j}} = \frac{1}{S_{2j}}(z + \delta_j S_{1j})$$

is always negative, and consequently $W_- > 0$. In the case (22b) $W_- \gtrless 0$ depending on

$$\delta_j \cot z\left(-S_{1j} + \frac{z^2}{S_{2j}}\right) \gtrless \sqrt{\frac{\sigma_j}{S_{1j}S_{2j}}}\,(z + \delta_j S_{1j})$$

The assymptotic behaviour of W_+ when $z \to \pi$ is of certain interest. For the case of an ideal undeformed heterojunction

$$\lim_{z\to\pi} W_+(z, A_{1j}, A_{2j}) = \sqrt{A_{1j}A_{2j} - z^2 - z(A_{1j} + A_{2j})\cot z} \qquad (23)$$

while for a deformed heterojunction

$$\lim_{z\to\pi} W_+(z, A_{1j}, A_{2j}, \varepsilon_j) = \frac{z}{\tan z\,\varepsilon_j} \qquad (24)$$

Evidently in the undeformed case the expression (23) is invariant under the substitution $A_{1j} \rightleftarrows A_{2j}$, while for the deformed case the expression for W_+ does not depend on A_{ij} at all.

4. NUMERICAL RESULTS AND DISCUSSION

It is convinient to formulate the condition for the existence of interface states in terms of quantities which naturally characterise the heterojunction under consideration, e.g. the ratio of the lattice constants $B = b/a$ and the interface potential step $-eV_0$. On account of (18), equation (9) takes the form

$$y^2 = x^2 - 2\gamma^2 \qquad (25)$$

where $\gamma^2 = -a^2 m e V_0 / \hbar^2$. Then, from (19a) and (19b) and making use of (25) we can obtain the $B - \gamma^2$ relation for any fixed value of X. By this way we obtain the manyfold of heterojunctions in which an interface state with this X, that is with this energy, exists. In other words, if an interface state with given energy does exist in a particular heterojunction characterised with the pair (B, γ^2), then the point (B, γ^2) must lie on the $B - \gamma^2$ curve for this value of X and the relevant A_{ij} $(i = 1,2\ ;\ j = r, \ell)$. Obviously, γ^2 can take positive as well as negative values depending on the sign of the internal contact potential difference.

Figure 2 shows the relevant $B - \gamma^2$ relations for two heterojunctions, $AB-CD$ and $AB-DC$, for $X = 0.9$. Figure 3 shows the same for another value of X, namely $X = 2.9$. From a physical point of view the interval $0.5 < B < 2$ is of a particular interest. Generally speaking, the shape of the $B - \gamma^2$ curves is analogical to those characterising heterojunction between two monatomic semiconductors (compare Ref.13).

As regards the curves corresponding to the undeformed heterojunctions, the influence of the nature of the end atoms at the interface is especially clear from figures 2a and 2b. It appears that, by this particular choice of the two crystal potentials in epitaxial contact, an interface state with a value of X from the first energy gap on the right-hand

crystal can exist in the common gap of the $AB-CD$ heterojunction if and only if this gap is obtained from the first gaps of the two crystals. For the heterojunction $AB-DC$ an interface state with the same X may exist only if the common gap is obtained from the first energy gap of the right-hand crystal and the second energy gap of the left-hand crystal. As regards the situation in figures 3a and 3b, an interface state with a value of X from the second energy gap of the right-hand crystal may exist if to the common gap belong this gap and the first energy gap of the left-hand crystal. This remains valide for $AB-CD$ heterojunction and for $AB-DC$ heterojunction as well. The appearance of interface states in a common gap obtained from two even energy gaps is forbidden for indeformed heterojunction (see §3).

Figures 2 and 3 show the change in the $B - \gamma^2$ curves due to deformations. Even small and symmetrical deformations may lead to significant deviations from the undeformed case.

The $B - \gamma^2$ curves for an $AB-CD$ heterojunction, computed for a value of X near the top of the second energy gap of the right-hand crystal is shown in figure 4. For the relevant $AB-DC$ heterojunction the corresponding curves remain almost the same, in agreement with equations (23) and (24).

Having in mind heterojunctions like GaP-GaAs and CdS-CdSe, let us especially consider the particular case of an $AB-AC$ heterojunction. More specifically we have to consider the two subcases $AB-AC$ and $AB-CA$ depending on the end atomic planes at the interface. As far as atoms of one type are characterised by one and the same strength of the δ-function potential, we obtain $A_{2\ell}$ for fixed values of A_{1r}, A_{2r} and $A_{1\ell}$ through $A_{2\ell}/b = A_{1r}/a$ for the $AB-AC$ heterojunction, and through $A_{2\ell}/b = A_{2r}/a$ for the $AB-CA$ heterojunction, respectively. Tables 1 and 2 visualize the dependence between the characteristic parameters B, γ^2 and X for the above two heterojunctions. The influence of the deformation is also clearly seen.

Table 1. Relation between characteristic parameters for $AB-AC$ heterojunction ($A_{1r} = 0.125$, $A_{2r} = 0.750$, $A_{1\ell} = 0.950$, $A_{2\ell} = A_{1\ell}B$)

Case I : common gap obtained from gaps with the same parity (equation (19b))

Case II: common gap obtained from gaps with opposite parity (equation (19a))

X	B	γ^2			
		$\varepsilon_r = \varepsilon_\ell = 0$		$\varepsilon_r = 0.1$, $\varepsilon_\ell = 0.5$	
		I	II	I	II
0.9	0.9	-0.55	-	-	-5.60
	1.0	-0.30	-	-	-4.44
	1.1	-0.12	-	-	-3.59
	1.5	0.22	-	-0.05	-1.69
1.4	0.9	0.76	-	-0.25	-4.48
	1.0	0.82	-	0.05	-3.35
	1.1	0.86	-	0.27	-2.53
	1.5	0.93	-	0.69	-0.78
2.9	0.9	-	3.76	-1.75	-
	1.0	-	3.90	-0.59	-
	1.1	-	3.98	0.26	3.30
	1.5	-	4.13	2.15	3.77
3.14	0.9	-	4.84	0.15	4.18
	1.0	-	4.85	1.09	4.37
	1.1	-	4.87	1.77	4.49
	1.5	-	4.90	-	4.74

Table 2. Relation between characteristic parameters for $AB-CA$ heterojunction ($A_{1r} = 0.750$, $A_{2r} = 0.125$, $A_{1\ell} = 0.950$, $A_{2\ell} = A_{2r}B$)

Case I : common gap obtained from gaps with the same parity (equation (19b))

Case II: common gap obtained from gaps with opposite parity (equation (19a))

X	B	γ^2			
		$\varepsilon_r = \varepsilon_\ell = 0$		$\varepsilon_r = 0.1$, $\varepsilon_\ell = 0.5$	
		I	II	I	II
0.9	0.9	-	-5.21	0.10	-
	1.0	-	-4.19	0.15	-
	1.1	-	-3.42	0.19	-
	1.5	-	-1.70	0.29	-
1.4	0.9	-	-3.79	-	-
	1.0	-	-2.87	-	-
	1.1	-	-2.20	-	-
	1.5	-	-0.72	-	-
2.9	0.9	-	3.49	-1.85	-
	1.0	-	3.70	-0.69	-
	1.1	-	3.84	0.16	-
	1.5	-	4.09	2.05	-
3.14	0.9	-	4.84	0.15	4.18
	1.0	-	4.85	1.09	4.37
	1.1	-	4.87	1.77	4.49
	1.5	-	4.90	-	4.74

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CAPTIONS FOR THE FIGURES

Figure 1. One-dimensional model of heterojunction between two diatomic semiconductors with lattice constants $2a$ and $2b$, respectively. U_{ij} ($i=1,2$; $j=r,l$) characterise the strength of the corresponding δ-potential.
(a) heterojunction with deformations Δa and Δb.
(b) undeformed heterojunction

Figure 2. $B-\gamma^2$ relations for $X = 0.9$
——— $\varepsilon_r = \varepsilon_l = 0$
—·—·— $\varepsilon_r = \varepsilon_l = 0.1$
— — — $\varepsilon_r = 0.1$, $\varepsilon_l = 0.5$
(a) heterojunction $AB-CD$
($A_{1r} = A_{2l} = 0.125$, $A_{2r} = 0.750$, $A_{1l} = 0.950$)
(b) heterojunction $AB-DC$
($A_{1r} = 0.750$, $A_{2r} = A_{2l} = 0.125$, $A_{1l} = 0.950$)

Figure 3. $B-\gamma^2$ relations for $X = 2.9$
——— $\varepsilon_r = \varepsilon_l = 0$
— — — $\varepsilon_r = 0.1$, $\varepsilon_l = 0.5$
(a) heterojunction $AB-CD$
(b) heterojunction $AB-DC$

Figure 4. $B-\gamma^2$ relations for heterojunction $AB-CD$ for $X = 3.14$
——— $\varepsilon_r = \varepsilon_l = 0$
— — — $\varepsilon_r = 0.1$, $\varepsilon_l = 0.5$

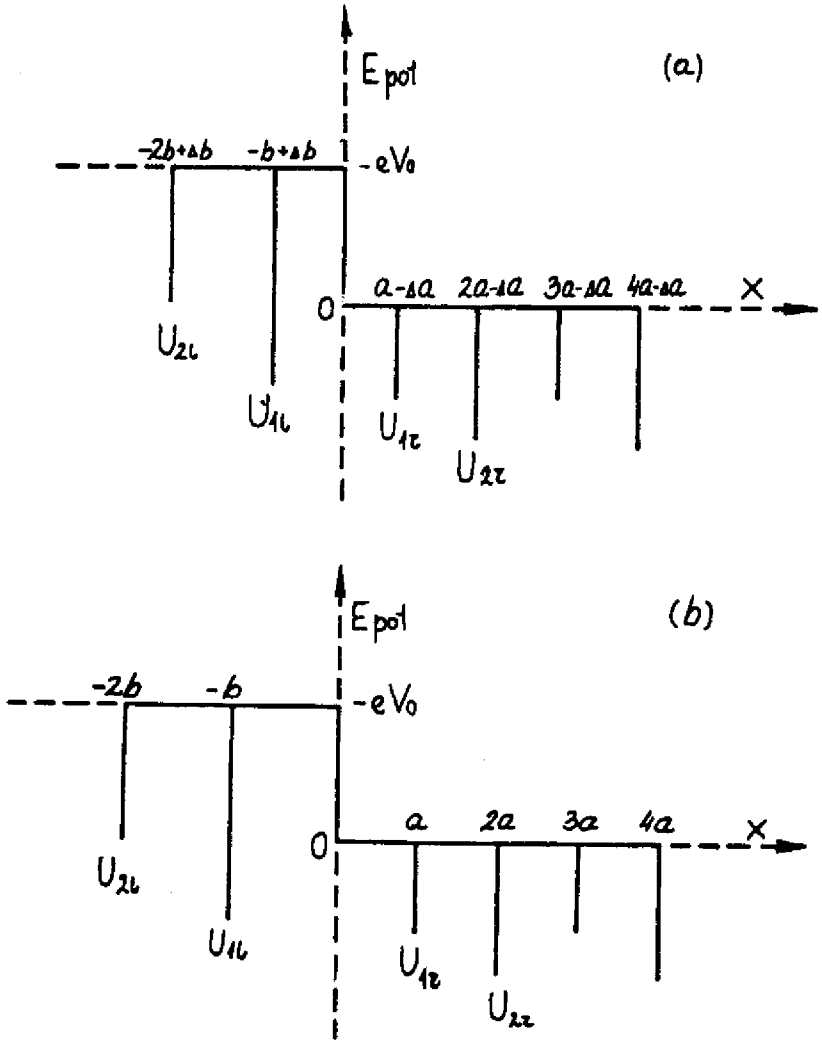
E pot
(a)
-2b+Δb
-b+Δb
-eV₀
0
a-Δa
2a-Δa
3a-Δa
4a-Δa
X
U2l
U1l
U1r
U2r
E pot
(b)
-2b
-b
-eV₀
0
a
2a
3a
4a
X
U2l
U1l
U1r
U2r

Fig. 1

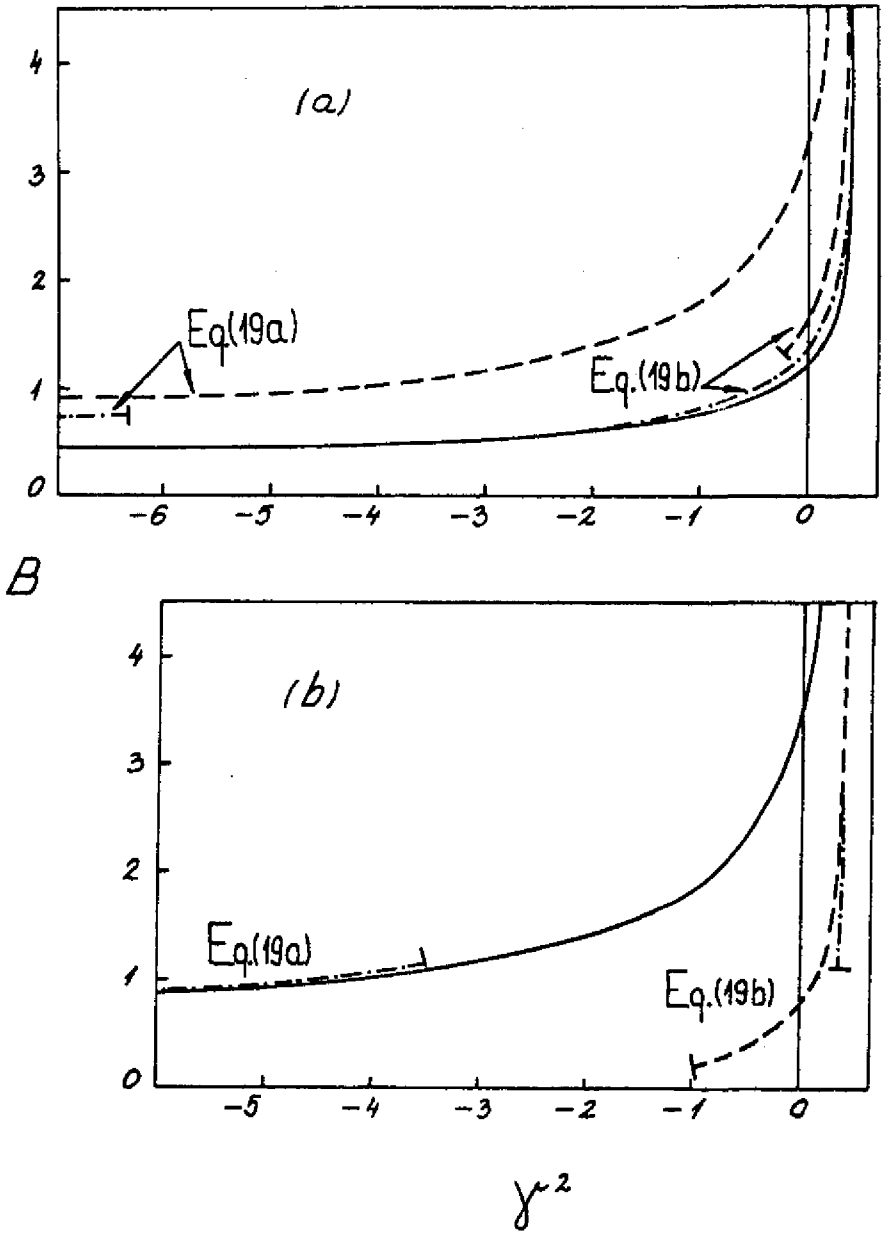
(a)
Eq.(19a)
Eq.(19b)
B
(b)
Eq.(19a)
Eq.(19b)
γ²

Fig. 2

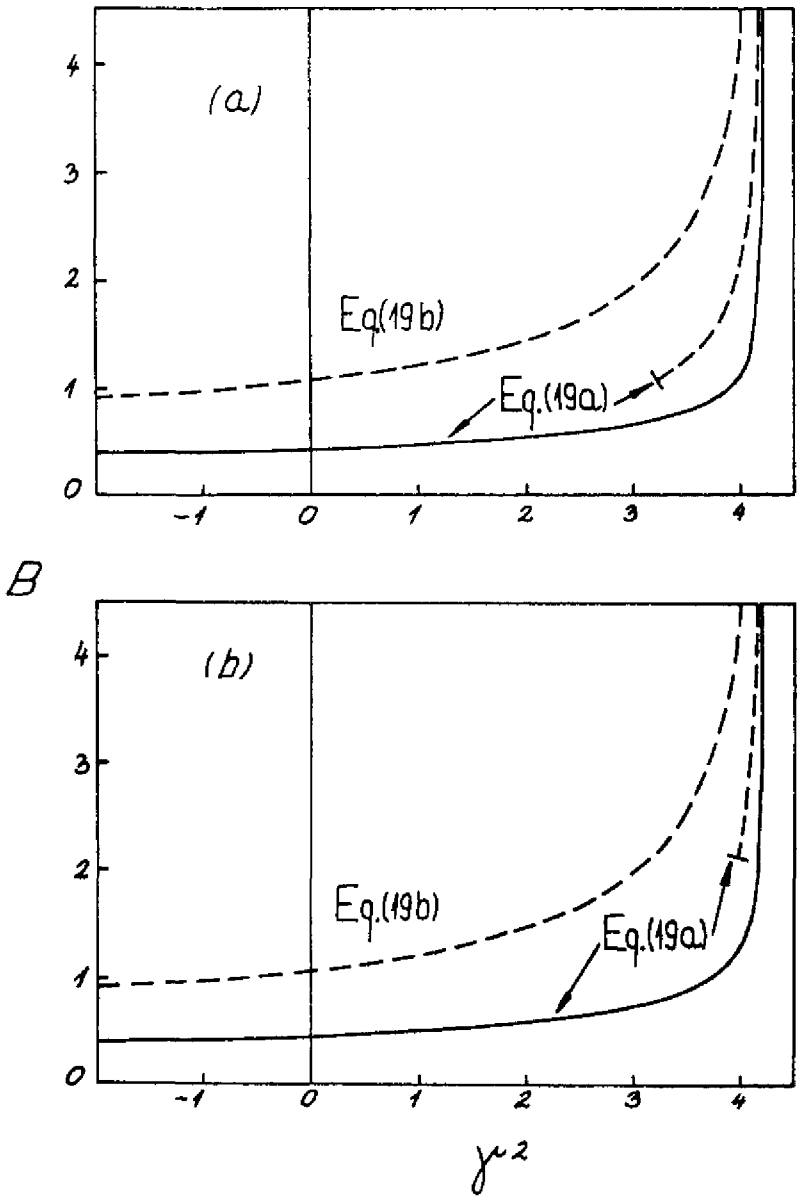

Fig. 3

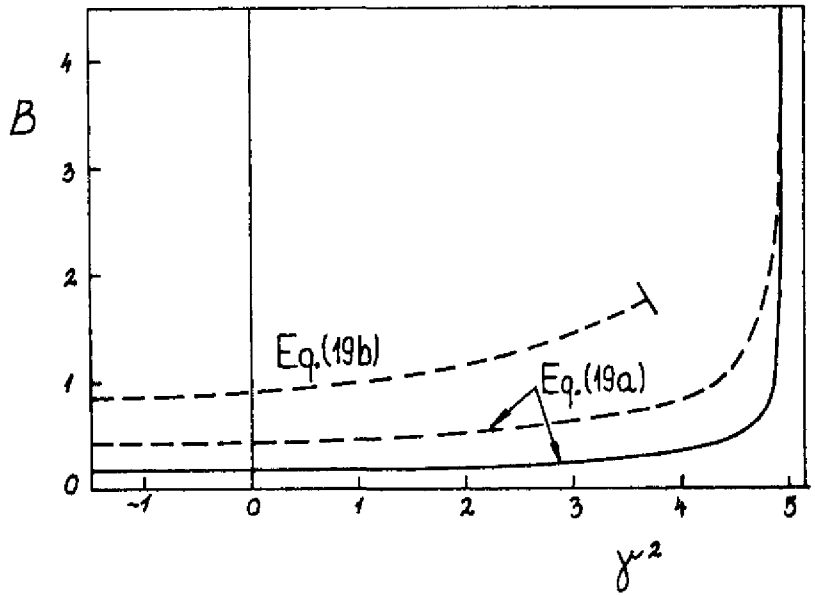

Fig. 4

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