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The energy spectra of narrow-gap semiconductor heterostructures: spin splitting in the case of asymmetry

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Abstract. Using the two-band model, the energy spectrum is explicitly obtained as a function of the spin projection and transverse momentum for two abrupt semiconductor heterostructures of type II: (i) a double heterojunction and (ii) a system of two quantum wells, one in the valence band and one in the conduction band. The transverse motion of the carriers and the effective repulsion of the electron-like and hole-like energy levels give rise to effects which cannot be properly described in the framework of the single-band theory. The two special cases form the basis for a discussion of the properties of more general classes of heterostructures of any type. The spin splitting of the energy spectrum is found to be a characteristic property of asymmetric heterostructures. Degeneracy occurs in the case of spatially symmetric heterostructures and for a class of heterostructures which are spatially asymmetric but symmetric with respect to energy. The possibility of a new type of transition is discussed.

1. Introduction

The energy spectrum (ES) is one of the fundamental physical characteristics of semiconductor heterostructures. It is the basis for the theoretical calculation of optical and transport properties of a system, but it is also of interest in itself. Such features of the energy spectrum as the (direct or indirect) band gap and the effective masses of the carriers contain important information about the physical properties of the system.

Highly developed methods of heterostructure growth make it possible to construct virtually any predetermined band structure ('band engineering'). The parameters of semiconductors vary over wide ranges. This facilitates the construction of a large diversity of heterostructures by modifying the compositions of several semiconductors. Many different physical properties needed for particular applications can be achieved. For instance, it has been possible to build systems with negative differential conductivity, which give rise to oscillations.

Currently increasing interest is shown in the influence of the spin–orbit interaction on mesoscopic transport phenomena [1]. The spin–orbit interaction couples spin and spatial motion; this occurs in a two-dimensional electron gas with asymmetric potential wells [2].

Spin splitting is a well-known property of bulk semiconductors exhibiting bulk inversion asymmetry. In heterostructures, on the other hand, spin splitting also occurs as a result of structure inversion asymmetry, as was first pointed out by Bychkov and Rashba [3]. For two-dimensional hole systems such as GaAs/AlGaAs heterostructures, this leads to the emergence of spin-dependent hole spectra [4].

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The term 'structure' is used in the sense that the spatial dependence of the potential of the system considered, apart from its atomic periodicity, has some additional slowly varying modulation which is responsible for the special physical features of the system. If the energy gap of the semiconductors forming the structure is large compared to the magnitude of the modulation potential [5], then an energy level can be attributed to a single band. In this case the single-band effective Schrödinger equation is a good approximation. In the opposite case the effects of band hybridization become important. One should then make use of some model Hamiltonian which takes into account the interaction between adjacent bands. The III–V semiconductors (a typical representative is InSb) are well described by the Kane Hamiltonian [6]. However, the essential results can also be obtained with the simpler two-band model [7, 8].

In the present paper the ES of narrow-gap semiconductor heterostructures are investigated within the two-band approximation, with attention focused on the dependence on spin and transverse momentum. In section 2 we present the two-band model and discuss the structure of its solution. In the following sections we analyse the ES for two structures of type II [9]: (i) a double heterojunction and (ii) a system of two quantum wells, one in the valence band and one in the conduction band. The first structure, consisting of two semiconductors with an offset in the work function, was introduced in [10, 11], where systems of type I were considered. In section 3 we extend the analysis of [10, 11] to higher values of the offset, thus arriving at systems of type II. Some properties of the second structure were obtained in [12, 13]. In section 4 we present a complete analysis of this structure and show that the spin splitting of the ES is a specific feature of the ES of such a system. Our analysis of the ES for these special cases enables us to exhibit in section 5 some general properties of the ES of narrow-gap heterostructures. These results are valid for particular symmetries of a heterostructure, independently of its type.

2. The two-band model

The model that we are using was suggested by Keldysh for the description of deep levels in semiconductors, which cannot be attributed to any single band [7]. The Hamiltonian in this model is formally identical to that of Dirac and describes IV–VI semiconductors (such as PbSe, PbTe, SnTe) [14]:

$$H\Psi = \left[v\gamma^0\boldsymbol{\gamma}\cdot\boldsymbol{p} + \gamma^0\epsilon_g(z)/2 + \varphi(z)\right]\Psi = \epsilon\Psi \tag{1}$$

where the γ^i are the Dirac matrices, $\boldsymbol{p} = -\mathrm{i}\boldsymbol{\nabla}$, $\hbar = 1$ and the wave function Ψ consists of two spinors, assigned to two interacting bands. The interband velocity matrix element v is responsible for the hybridization of the bands; it is the analogue of the velocity of light in the Dirac Hamiltonian. The energy gap ϵ_g and work function φ depend only on the coordinate z along the growth axis. This implies that the transverse two-dimensional momentum $\boldsymbol{k}_\perp$ (perpendicular to z) is a good quantum number.

In the simplest case of constant ϵ_g and φ one obtains the dispersion of the bulk semiconductor

$$\epsilon^{(\pm)}(k_\perp) = \varphi \pm \sqrt{\epsilon_g^2/4 + v^2k_\perp^2}. \tag{2}$$

The conduction band $\epsilon^{(+)}(k_\perp) = \varphi + \sqrt{(\epsilon_g^2/4 + v^2k_\perp^2)}$ and the valence band $\epsilon^{(-)}(k_\perp) = \varphi - \sqrt{(\epsilon_g^2/4 + v^2k_\perp^2)}$, viewed as branches of a single analytic function, correspond to the electron and positron branches of the Dirac spectrum. The energy gap of the semiconductor corresponds to the forbidden energy region between these two branches.

It can be verified that the 'pseudoparity' operator $P = \mathrm{i}\gamma_0\gamma^3(\boldsymbol{\gamma}_\perp \cdot \boldsymbol{k}_\perp)/k_\perp$ commutes with the Hamiltonian (1) [15]. This operator, with eigenvalues $\lambda = \pm 1$, is the analogue of the helicity operator for the Dirac Hamiltonian. Then, defining the γ-matrices as in [16], we can rewrite (1) in the form of two pairs (one for each λ-value) of coupled equations

$$\begin{pmatrix} \epsilon_g(z)/2 + \varphi(z) & vk_\perp\lambda - v\,\partial_z \\ vk_\perp\lambda + v\,\partial_z & -\epsilon_g(z)/2 + \varphi(z) \end{pmatrix} \begin{pmatrix} \psi_\lambda \\ \chi_\lambda \end{pmatrix} = \epsilon_\lambda \begin{pmatrix} \psi_\lambda \\ \chi_\lambda \end{pmatrix} \tag{3}$$

with two scalar envelope functions ψ_λ and χ_λ. The x-axis is chosen along the direction of the transverse motion, so from now on $k_\perp$ is a scalar, with both positive and negative values. The term $vk_\perp\lambda$ plays a role similar to that of the spin–orbit interaction in the single-band problem. The use of the Dirac Hamiltonian greatly facilitates the treatment of the spin dependence, because the Hamiltonian intrinsically incorporates it and one does not have to introduce the spin–orbit interaction separately.

Thus, the ES of a system described by the Hamiltonian (1) is a double-valued function of $k_\perp$ analogous to (2), which we denote by $\epsilon^{(\pm)}_{i,\lambda}(k_\perp)$, where the index i labels the energy level. From (3) one immediately obtains the general relation $\epsilon^{(\pm)}_{i,\lambda}(k_\perp) = \epsilon^{(\pm)}_{i,-\lambda}(-k_\perp)$. Below we shall derive some other properties of the ES for some particular forms of $\epsilon_g(z)$ and $\varphi(z)$.

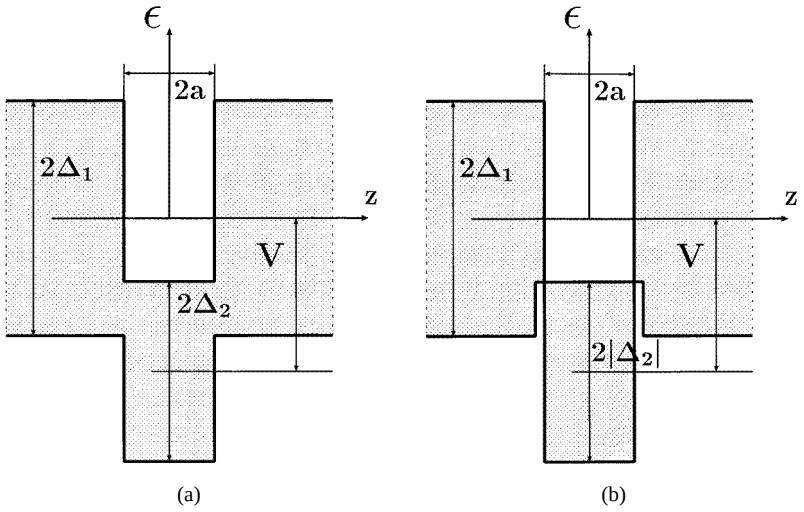

Figure 1. The valence and conduction bands as functions of the coordinate z along the axis of growth for the two heterostructures considered in section 3. The region of the energy gap is shaded. (a) The system with band gaps $2\Delta_1$ and $2\Delta_2$, and an offset V in the work function. (b) The system with band inversion, $\Delta_2 < 0$.

3. The double heterojunction

In [10, 11] an abrupt double heterojunction of type I, consisting of two semiconductors with an offset in the work function, was considered. Here we deal with type-II structures. One distinguishes two types of system: without (figure 1(a)) and with band inversion (figure 1(b)) [15, 17]. The functions $\varphi(z)$ and $\epsilon_g(z)$ for the two types of system are given by

$$\begin{aligned} &\varphi = 0 \qquad \epsilon_g = 2\Delta_1 \qquad \text{for } |z| > a \\ &\varphi = -V \qquad \epsilon_g = 2\Delta_2 \qquad \text{for } |z| < a \end{aligned} \tag{4}$$

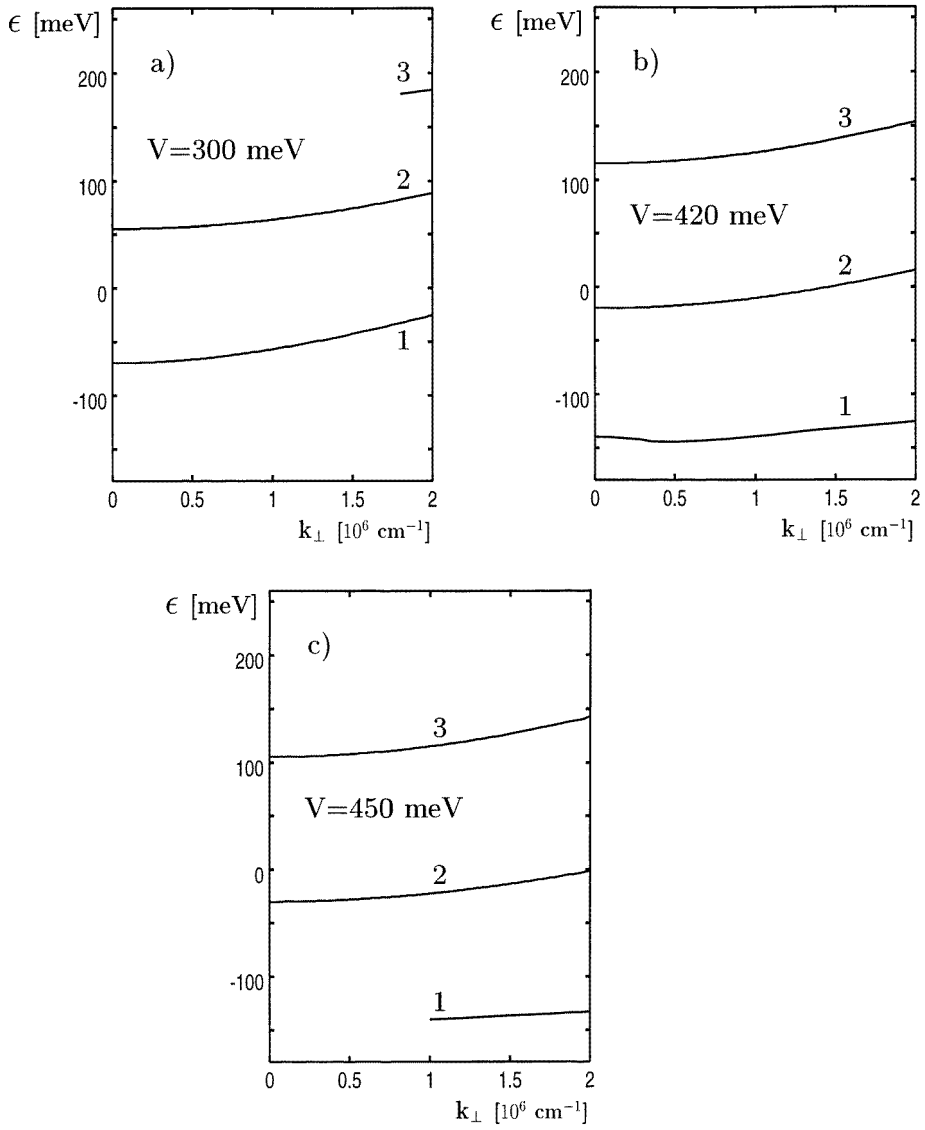

Figure 2. The dispersion along the direction perpendicular to the growth axis in the heterostructure of figure 1(a) for $\Delta = 150$ meV and several values of the parameter V. (a) $V = 2\Delta$; the upper level (curve 3) is an MDBS. (b) $V = 2.8\Delta$; the minimum of the ground state (curve 1) lies at $k_\perp \neq 0$. (c) $V = 3\Delta$; the ground state (curve 1) becomes an MDBS. (It is understood that the curves in figures 2–4 are continued symmetrically across $k_\perp = 0$.)

where $\Delta_1 > 0$, and $\Delta_2 > 0$ for figure 1(a) and $\Delta_2 < 0$ for figure 1(b).

The dispersion curves of such a system have been shown in [10, 11] to describe 'motionally dependent bound states' (MDBS) with terminal points (cf. below).

The eigenvalue equation is obtained from the continuity of the envelope functions ψ_λ and χ_λ at the interfaces and has the following form (for both signs of Δ_2):

$$2v^2 q\kappa \left\{(\epsilon - V)^2 + \epsilon^2 - 2v^2 k_\perp^2 - 2\Delta_1\Delta_2 - V^2\right\}^{-1} = \tan(2a\kappa) \tag{5}$$

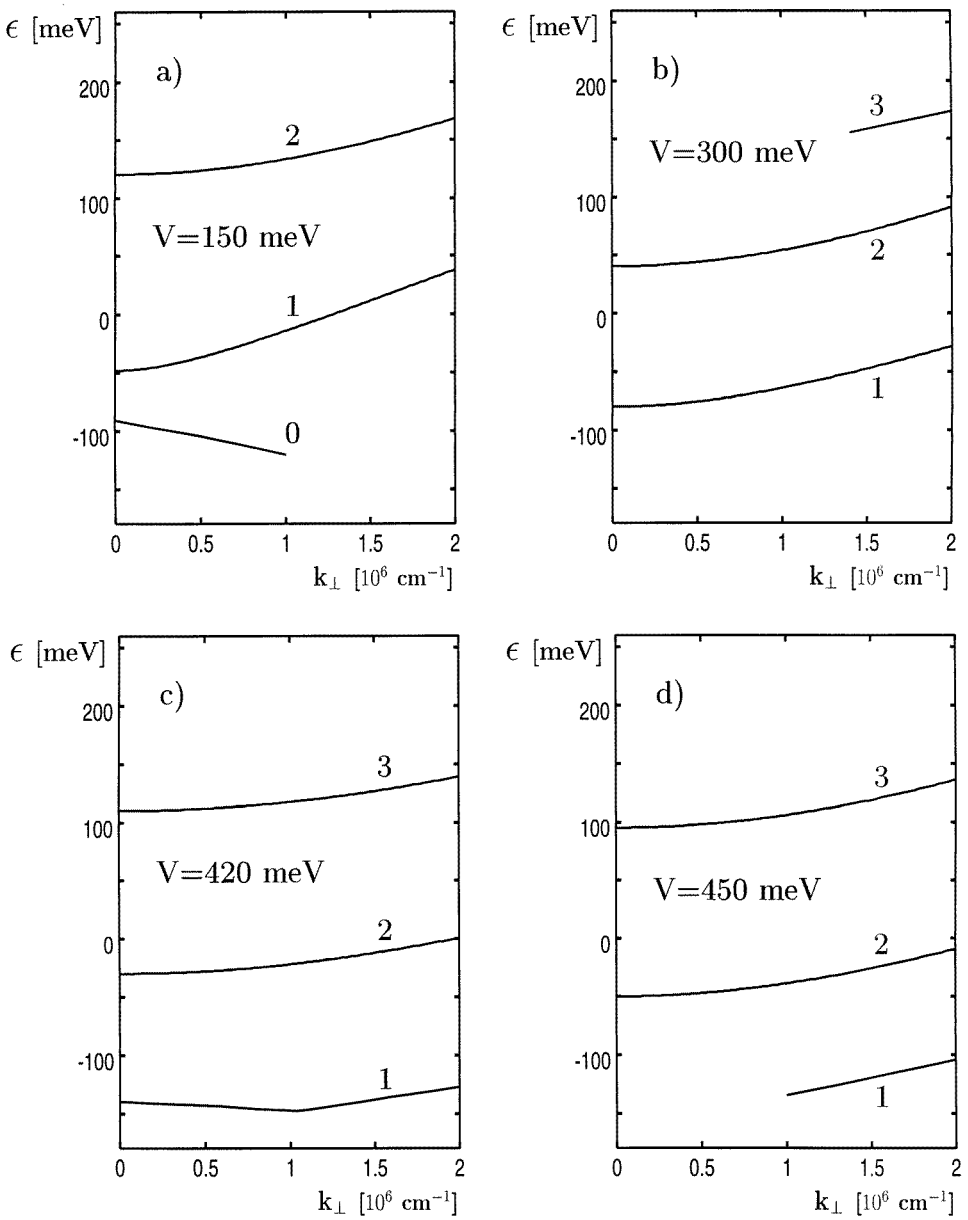

Figure 3. As figure 2, but for the heterostructure of figure 1(b). (a) $V = |\Delta|$; the ground state of the system (curve 0) is an MDBS. (b) $V = 2\Delta$; a new MDBS (curve 3) is observed. (c) $V = 2.8\Delta$. (d) $V = 3\Delta$; the dispersion reveals a behaviour similar to that of the heterostructure without inversion.

where $q^2v^2 = \Delta_1^2 + v^2k_\perp^2 - \epsilon^2$, $\kappa^2v^2 = (\epsilon - V)^2 - v^2k_\perp^2 - \Delta_2^2$ and the other notation is introduced in figure 1(a).

Equation (5) is valid for both choices, $\lambda = \pm 1$. Moreover, the dispersion curves are symmetric under a change of sign of the momentum $k_\perp$. In this section we therefore restrict ourselves to positive values of $k_\perp$.

We have studied (5) for both situations (without and with band inversion) with the parameter V varying over a wide range: from small values $V < \Delta_1$ gradually increasing up to $V > \Delta_1 + |\Delta_2|$. For simplicity we shall consider the case of identical gaps, $\Delta_1 = |\Delta_2| = \Delta$. The physical results do not depend upon this assumption.

The dispersion curves of the non-inverted heterostructure are presented in figure 2 (figure 3 for the inverted system). The following parameters were used: $\Delta = 150$ meV, $2a = 100$ Å and $v = (\Delta/m_{\text{eff}})^{1/2}$ with $m_{\text{eff}} = 0.01m_0$ (m_0 is the mass of the free electron).

For small values of V, $V \leqslant 2\Delta$, the behaviour of the energy levels is similar to that obtained in [10, 11]. Without band inversion, all of the curves reveal electron-like behaviour (figure 2(a)). Curve 3 exhibits the feature of an MDBS: it corresponds to a state localized in the well only for values of the momentum $k_\perp$ above some terminal point; below this point the electrons are motionally unbound. Similarly, in the case of band inversion the ground state has a hole-like behaviour, being localized for momenta $k_\perp$ below some terminal point (curve 0 in figure 3(a)); this state corresponds to the zeroth (supersymmetric) mode which is specific to heterostructures with band inversion [17].

With increasing V, an MDBS becomes localized for all values of $k_\perp$ in the non-inversion case (figure 2(b)). For the system with inversion the terminal point moves to $k_\perp = 0$, so eventually the MDBS becomes delocalized for all values of $k_\perp$ and the corresponding curve 0 disappears (figure 3(b)).

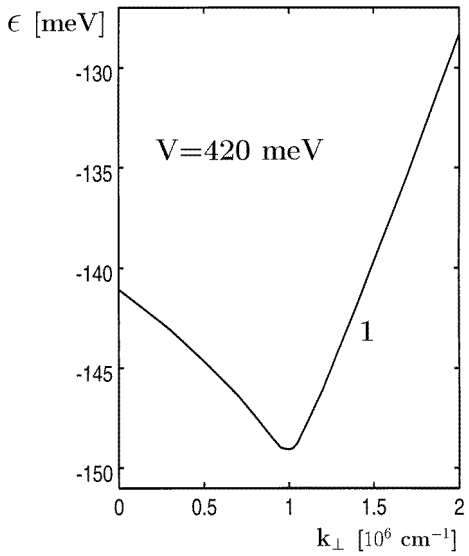

Figure 4. Curve 1 from figure 3(c), on a larger scale.

For higher values of V, $V > 2\Delta$, several new effects can be observed. In the region $2.5\Delta \leqslant V \leqslant 3\Delta$ the electron-like valley in the non-inversion case becomes gradually flatter with increasing V, and at $V_c \approx 2.8\Delta$ an 'indirect' valley appears at some momentum $k_\perp^{\min} \neq 0$ (curve 1 in figure 2(b)). In the case of band inversion a new MDBS appears at $V \approx 2\Delta$ (curve 3 in figure 3(b)). With further increase of V, the ground-state curve reveals a behaviour similar to that in the previous case: it becomes flatter and at $V_c \approx 2.8|\Delta|$ an indirect valley can be seen (curve 1 in figure 3(c), which is repeated in figure 4 on a larger scale).

Another peculiarity of the system was observed for $V \geqslant 3|\Delta|$. In contrast to the situation

considered in [10], where the MDBS always lies above the other eigenstates (which are localized for all $k_\perp$), here the MDBS is the ground state in this range of parameters, as revealed by curve 1 in figure 2(c) and curve 1 in figure 3(d). These curves start at some terminal point $k_\perp \neq 0$ and extend towards larger values of $k_\perp$. A ground-state MDBS encompassing the point $k_\perp = 0$ would be favourable for semiconductor lasers; however, we have not found such states.

In concluding this section, we discuss which of the ES considered above correspond to heterostructures which can be realized in practice. The typical materials taken for type-II structures are InAs/GaSb [18]. Band inversion occurs in PbTe/SnTe, PbSe/SnSe and HgTe/CdTe [11, 17]. Unfortunately, for all of these materials, the offset V is not large enough to give rise to the new features exhibited in figures 2(b), 2(c) and figures 3(c), 3(d). It remains to be seen whether new materials with larger offsets V can be found or, conversely, whether more realistic Hamiltonians may be employed which would give rise to these features for smaller V.

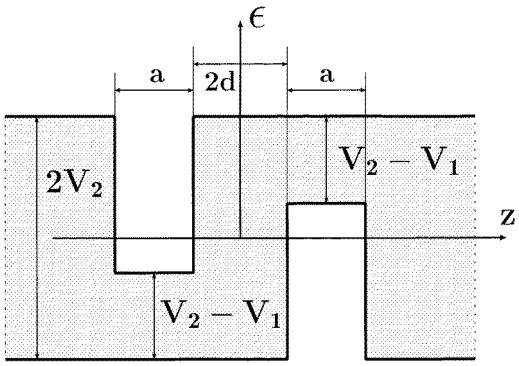

Figure 5. The valence and conduction bands as functions of the coordinate z along the axis of growth for the two-well structure considered in section 4.

4. The system of two quantum wells

The essential feature of the two-band description [7], namely that electron-like and hole-like states in narrow-gap systems are described by a single equation, is especially useful for the theoretical analysis of the semimetal–semiconductor transition. We have studied such a transition in [12] for the system of figure 5, which is described by the following functions $\varphi(z)$ and $\epsilon_g(z)$:

$$\begin{array}{lll} \varphi = 0 & \epsilon_g = 2V_2 & \text{for } |z| > d + a \text{ and } |z| < d \\ \varphi = -(V_1 + V_2)/2 & \epsilon_g = V_2 - V_1 & \text{for } -(d + a) < z < -d \\ \varphi = (V_1 + V_2)/2 & \epsilon_g = V_2 - V_1 & \text{for } d < z < d + a. \end{array} \tag{6}$$

It was found that for any choice of parameters there always exists an energy gap between two neighbouring energy levels. This effect is analogous to the level splitting in two identical quantum wells and is due to an effective interaction (repulsion) of energy levels.

In [12] the discussion was restricted to the case where $k_\perp = 0$. In this section we shall take the dependence of the ES on the transverse momentum $k_\perp$ into account. The

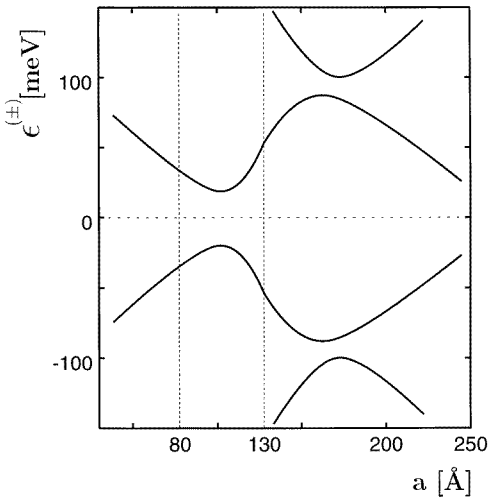

Figure 6. The dependence of the energy levels on the well width a for $k_\perp = 0$ and $\lambda = 1$ for the heterostructure of figure 5 with $V_1 = 100$ meV and $V_2 = 300$ meV.

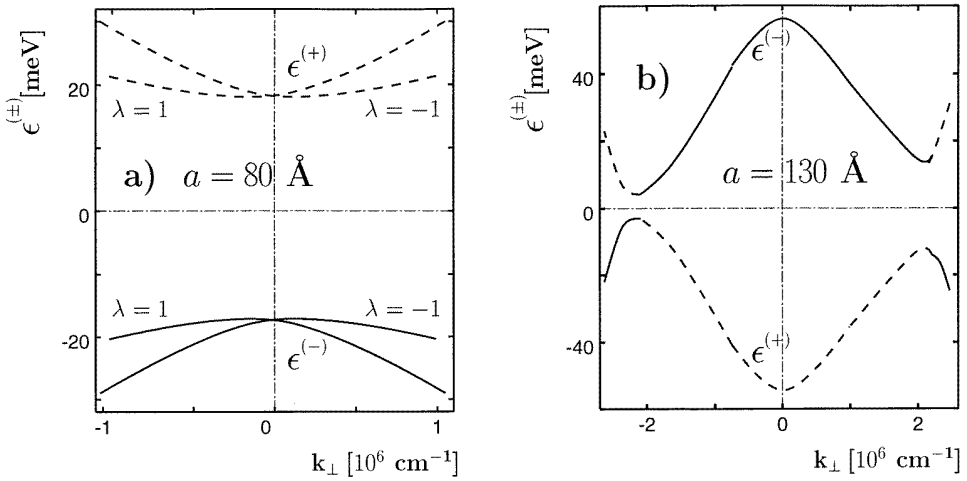

Figure 7. Dispersion curves for the heterostructure of figure 5 with $V_1 = 100$ meV, $V_2 = 300$ meV, (a) for $a = 80$ Å and (b) for $a = 130$ Å. In (a) the spin-split dispersion curves are drawn explicitly with $\epsilon^{(\pm)}_{i,-\lambda}(k_\perp) = \epsilon^{(\pm)}_{i,\lambda}(-k_\perp)$. (b) corresponds to $\lambda = -1$. Solid and dashed lines correspond to hole-like and electron-like levels, respectively.

eigenvalues of this problem are determined by the equation

$$\begin{aligned}[q\cosh(dq) + k_\perp\lambda\sinh(dq)][&\tan(a\kappa_1)\tan(a\kappa_2)(q^4+\kappa_1^2\kappa_2^2)\\ &+ \tan(a\kappa_1)(q^2-\kappa_1^2)q\kappa_2 + \tan(a\kappa_2)(q^2-\kappa_2^2)q\kappa_1 + 2q^2\kappa_1\kappa_2]\\ &+ [k_\perp\lambda\cosh(dq) + q\sinh(dq)][-\tan(a\kappa_1)\tan(a\kappa_2)q^2(\kappa_1^2+\kappa_2^2)\\ &+ \tan(a\kappa_1)(q^2-\kappa_1^2)q\kappa_2 + \tan(a\kappa_2)(q^2-\kappa_2^2)q\kappa_1 + 2q^2\kappa_1\kappa_2] = 0 \qquad (7)\end{aligned}$$

where $\kappa_1^2v^2 = (\epsilon + V_1)(\epsilon + V_2) - v^2k_\perp^2$, $\kappa_2^2v^2 = (\epsilon - V_1)(\epsilon - V_2) - v^2k_\perp^2$ and $q^2v^2 = v^2k_\perp^2 + V_2^2 - \epsilon^2$. In figure 6 the resulting ES is plotted as function of a for $k_\perp = 0$. Figure 7

displays the dispersion for two well widths, $a = 80$ Å and $a = 130$ Å. The following typical parameter values have been used: $V_1 = 150$ meV, $V_2 = 450$ meV, $v = 3 \times 10^8$ cm s^{-1} and $d = 300$ Å.

The dependence of the eigenenergies $\epsilon^{(+)}$ and $\epsilon^{(-)}$ on the well widths a reveals an oscillatory behaviour [12] (cf. figure 6). For $a = 80$ Å the wave functions corresponding to $\epsilon^{(+)}$ are localized in the conduction band well and have an *electron-like* behaviour: the energy diminishes with increasing a. This is also confirmed by the dispersion of this level (dashed curves in figure 7(a)). The spectrum of the carriers in the valence band well, $\epsilon^{(-)}(k_\perp)$, is represented by the pair of solid curves in figure 7(a). It is mirror symmetric to the curves $\epsilon^{(+)}(k_\perp)$ (cf. case (ii) in section 5).

For $a = 130$ Å the upper level has a *hole-like* behaviour: the energy increases with increasing a. The dependence of the energy on $k_\perp$ is shown in figure 7(b). This figure can also be regarded as showing the dispersion of two quantized levels: the hole-like level $\epsilon^{(-)}$ (represented by the solid line) and the electron-like level $\epsilon^{(+)}$ (represented by dashed line). The gaps at $k_\perp \approx 2 \times 10^6$ cm^{-1} are due to hybridization. The electron-like level $\epsilon^{(+)}$ at small values of $k_\perp$ lies below the hole-like level $\epsilon^{(-)}$, proving that a transition has indeed taken place as a increases from 80 Å to 130 Å. This is also confirmed by the behaviour of the wave functions corresponding to $\epsilon^{(-)}$ for these values of $k_\perp$: they are now localized in the valence band well. Figures 6 and 7 exhibit clearly the avoided crossing (repulsion) of levels.

Recently the InAs/GaSb system has attracted much interest due to its application as an infra-red device and because of its bipolar conduction [19]. For thick layers the InAs/GaSb system is a broken-gap type-II system where charge is transferred forming a two-dimensional electron gas in the InAs layer and a two-dimensional hole gas in the GaSb layer. These carriers are strongly confined in both energy and coordinate space, and the strong mixing between electrons and holes will be important. In [13] dispersions were obtained which were similar to the ones shown in our figures 7(a) and 7(b). However, the authors of [13] did not give an explicit derivation of their results. Neither did they treat the spin dependence accurately. The curves obtained in [13] appear to be symmetric under $k_\perp \to -k_\perp$, whereas our analysis shows that this is not the case. Nevertheless, the results of [13] demonstrate that the avoided-crossing behaviour of the ES obtained in [12, 13] and in the present paper occurs also in more general forms of heterostructures, where the widths of the two wells are not equal.

We close with some remarks concerning the experimental observation of the effects described in this section. The structures having the suggested behaviour are typically built from III–V semiconductors, e.g. GaAs/InAs/GaAs/GaSb/GaAs. In fact, our two-band model is not quite suited for these materials; they are more appropriately described by the Kane model [6]. However, the peculiar avoided-crossing behaviour would also be obtained there. Experimental tests could, for example, make use of optical properties of the system. A comparison of the characteristic energies associated with the effects with typical values of the temperature and the Fermi energy shows that their practical observation may be possible.

5. General properties

It is well known that in the single-band approximation the states in a symmetric one-dimensional potential can be classified according to their parity: the wave functions are symmetric or antisymmetric. The wave functions of the Hamiltonian (1) generally do not have this property. Instead, as mentioned above, they are classified according to the eigenvalues $\lambda = \pm 1$ of the helicity operator P. For some heterostructures with additional

symmetries the energies can become degenerate. In this section we shall prove several general properties of the ES for heterostructures of this kind.

(i) Comparing (5) and (7) for the ES we notice a rather important difference: equation (7) contains terms proportional to the first power of $\lambda k_\perp$, while (5) does not. From this one can immediately conclude that for (5) the equalities $\epsilon_{i,\lambda}^{(\pm)}(k_\perp) = \epsilon_{i,-\lambda}^{(\pm)}(k_\perp)$ are valid, whereas for (7) they are not.

In fact, it is seen quite generally that the degeneracy with respect to the helicity quantum number λ holds for *any* heterostructure which is symmetrical under spatial inversion. Let us consider a system in which the bottom of the conduction band $E_c(z) = \varphi(z) + \epsilon_g(z)/2$ and the top of the valence band $E_v(z) = \varphi(z) - \epsilon_g(z)/2$ are symmetric under $z \to -z$. Then, if the functions

$$\begin{pmatrix} \psi_{k_\perp,\lambda}(z) \\ \chi_{k_\perp,\lambda}(z) \end{pmatrix} \tag{8}$$

satisfy (3) for some ϵ, λ, the functions

$$\begin{pmatrix} \psi_{k_\perp,\lambda}(-z) \\ -\chi_{k_\perp,\lambda}(-z) \end{pmatrix}$$

will also be solutions of (3) for the same value of ϵ, but opposite value of λ.

(ii) As (7) contains $\lambda k_\perp$ linearly, there is no degeneracy with respect to the sign of $k_\perp$ in the corresponding ES for fixed λ. Instead, we may suspect that for a system with $E_v(z) = -E_c(-z)$ the energies occur in pairs, $\pm\epsilon$. This can be proved with the aid of the transformation properties of the solutions of Hamiltonian (1), found in [12]. Indeed, it can be checked that if the functions (8) are solutions of (3) with eigenvalue ϵ, then the functions

$$\begin{pmatrix} \chi_{k_\perp,\lambda}(-z) \\ -\psi_{k_\perp,\lambda}(-z) \end{pmatrix}$$

will also be solutions for the same values of $k_\perp$ and the same λ but with the energy $-\epsilon$.

(iii) On the other hand, when $E_v(z) = -E_c(z)$, the situation is the following. Here only the relation $\epsilon_{i,\lambda}^{(+)}(k_\perp) = -\epsilon_{i,\lambda}^{(-)}(-k_\perp)$ is generally valid. Combined with the relations $\epsilon_{i,\lambda}^{(\pm)}(k_\perp) = \epsilon_{i,-\lambda}^{(\pm)}(-k_\perp)$, which hold for any system, it yields $\epsilon_{i,\lambda}^{(+)}(k_\perp) = -\epsilon_{i,-\lambda}^{(-)}(k_\perp)$. However, if we restrict ourselves to piecewise-constant functions $E_v(z)$ and $E_c(z)$, degeneracy with respect to λ again holds. This fact can be checked if one fixes some particular choice of the Dirac matrices [15, 17] and then matches the wave functions on either side of a heterojunction. As a result, the terms containing $\lambda k_\perp$ linearly will cancel each other everywhere, so the eigenvalue equation is invariant under $k_\perp \to -k_\perp$.

6. Conclusions

In the present work we have studied type-II heterostructures within the two-band model. Several new effects were found. For the double heterojunction, formed by semiconductors with an offset in the work function (figure 1), the dispersion curves have very different shapes, depending on the choice of the parameter values. Conditions were found under which the MDBS becomes the ground state of the system. For a system of two wells, one in the valence band, the other in the conduction band (figure 5), the gap between electron-like and hole-like energy levels has been calculated for all possible values of $k_\perp$ and all types of heterostructure.

The behaviour of the dispersion curves under a change of parameters resembles to a large extent the change of the thermodynamic potential in a second-order phase transition.

Thus, we suggest that a new type of transition may occur in semiconductor heterostructures, which is different from the usual semimetal–semiconductor transition. In such a transition the character of the energy gap changes, so the position of the ES minimum moves from $k_\perp = 0$ to $k_\perp \neq 0$. However, more work is needed to determine what physical consequences this can bring about. Since we are using a one-particle approach, we cannot predict how many-particle effects could mask this transition.

Some general properties of the ES were investigated for several classes of heterostructure. For an arbitrary heterostructure, the ES is generally split with respect to the helicity λ. In the case where $E_v(z) = -E_c(-z)$ one finds that the gap between hole-like and electron-like energy levels survives also for $k_\perp \neq 0$ (level repulsion). The ES of such a structure is symmetric: if ϵ is an energy level then so is $-\epsilon$. For systems with $E_v(z) = E_v(-z)$ and $E_c(z) = E_c(-z)$, as well as for systems with $E_v(z) = -E_c(z)$ (with $E_v(z)$, $E_c(z)$ piecewise constant), the energy eigenvalues have been shown to be degenerate with respect to the helicity λ.

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