SPIN–ORBITAL BAND SPLITTING IN SYMMETRIC QUANTUM WELLS

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A spin–orbital splitting of the 2D spectrum of electrons and also of heavy and light holes in the GaAs quantum well caused by k^3-terms in the bulk dispersion law is calculated. At realistic parameter values of the quantum wells it has the scale 10^{-1}–1 meV which is quite available for experimental observation.

1. Introduction

A spin–orbital (SO) splitting of the electron (hole) spectrum in 2D gas may occur for two reasons. One of them is a low spacial symmetry of the confining layer (asymmetry of the space charge field in the heterojunction either in MIS-structure and the presence of the singular potential on the junction boundary). The second is the absence of an inversion centre in the bulk $A_{III}B_V$ material from which a heterostructure is made, resulting in the existence of k-odd terms in the hamiltonian of 3D-carriers. A contribution of the smooth asymmetric potential to SO-splitting has been considered in a number of papers (see refs. [1–5], for instance). The contribution of k-odd bulk terms was pointed out in ref. [6], and these terms were included in the electron spectrum of heterojunctions in ref. [7]. Experimentally lifting of degeneracy has been convincingly observed in refs. [8–11].

A splitting of the 2D spectrum occurs due to the presence of $\boldsymbol{K}$-odd terms in the 2D hamiltonian; here $\boldsymbol{K}$ is a two-dimensional wave vector. The simplest SO hamiltonian lifting a two-fold degeneracy is

$$H=\alpha[\boldsymbol{\sigma}\times\boldsymbol{K}]\boldsymbol{\nu}. \qquad (1)$$

It is linear in the quasimomentum $\boldsymbol{K}$. Here $\boldsymbol{\sigma}$ are the Pauli matrices and $\boldsymbol{\nu}$ is a normal to the junction (below $\boldsymbol{\nu}\parallel[001]$). It is on the basis of this hamiltonian that the results of refs. [8,9] were first interpreted in ref. [12]. For further discussion of the experimental data see refs. [13,14].

In the heterojunctions a contribution to a splitting of bands due to k-odd terms is masked by a competing contribution of the asymmetrical potential. However, in the symmetric quantum wells the situation is essentially simplified: the second contribution is absent. Thus, it is the quantum wells that are the optimal objects to separate a contribution of k-odd terms to SO splitting of 2D bands. At present there are no experiments where this splitting is observed in the symmetric wells. The authors of ref. [15] conclude it is absent. The authors of ref. [16] claimed initially that they observed the SO splitting of the 2D hole spectrum, however, later on they renounced this interpretation [17].

Thus, it is rather interesting to estimate the value of SO splitting theoretically. The GaAs quantum wells are appropriate for this purpose since the band structure of GaAs is rather well-known, including spin–orbital terms (data are summarized in the review article of Pikus et al. [18]).

Since SO splitting is considerably smaller than other energies entering the theory, k-odd terms will be considered by perturbation theory. We shall use the simplest boundary conditions for the wave function: $\psi=0$ on the boundaries of the well. The absence of a strict procedure to match wave functions and the existing uncertainty in the values of the hamiltonian parameters makes this rough approximation admissible.

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2. Electrons

A spin–orbital contribution into the electron hamiltonian has the form [21]

$$H_c = \alpha_c^*(\boldsymbol{\sigma}\cdot\boldsymbol{\kappa}),$$

$$\alpha_c^* = \alpha_c + \delta\alpha_c, \quad \kappa_x = k_x(k_y^2 - k_z^2), \tag{2}$$

κ_y and κ_z are obtained from κ_x by means of a cyclic permutation. For GaAs $\alpha_c^* = 35$ eV Å^3 [18] [#1].

Besides H_c the hamiltonian only contains the usual quadratic term $H_0 = \hbar^2\boldsymbol{k}^2/2m_e$. Thus, the ψ-function of the ground state in the well having width a is

$$\psi(z) = (2/a)^{1/2}\cos(qz), \quad q = \pi/a, \quad |z| \leqslant a/2.$$

A splitting $\Delta E(\boldsymbol{K})$, calculated in the linear approximation over H_c, is:

$$\Delta E(\boldsymbol{K}) = 2\alpha_c^*(\pi/a)^2 K[1 + \tfrac{1}{4}\beta(\beta-4)\sin^2 2\varphi]^{1/2}. \tag{3}$$

Here $\beta = (K/q)^2$ and φ is the angle between $\boldsymbol{K}$ and the axis [100]. SO splitting described by (3) is strongly anisotropic at $\beta \gtrsim 1$. At concentration $n \approx 5\times 10^{11}$ m^{-2}, $a = 100$ Å and $\varphi = 0$ we get $\Delta E \approx 1$ meV. Such a splitting is quite available for experimental observation. It is even unexpectedly large (as compared to the results calculated in ref. [7]). At a fixed value of Ka the splitting $\Delta E \propto a^{-3}$, i.e. it increases rapidly when a decreases.

It is interesting to make a comparison with the results of Malcher et al. [7] who calculated $\Delta E(\boldsymbol{K})$ for the heterojunctions GaAs/AlGaAs. An important conclusion of ref. [7] consists in the fact that for these heterojunctions a cubic nonparabolicity (2) makes the main contribution to ΔE. It is remarkable that the value of ΔE obtained in ref. [7] is smaller than the one found by us for the comparable value of the concentration of the 2D-electrons and despite a smaller value of the effective width of the 2D layer.

3. Holes

The hamiltonian of the holes, quadratic over k, is described by the three Luttinger constants. For GaAs $\gamma_1 = 6.85$, $\gamma_2 = 2.1$, $\gamma_3 = 2.9$ [20]. We shall consider it as the hamiltonian of the zero approximation H_0. The eigenfunctions Ψ are four-component spinors, $\Psi(\pm a/2) = 0$. It is convenient to choose the eigenfunctions of the operator H_0 as odd or even with respect to reflection in the plane $z = 0$. Under the usual choice [21] of the matrices of the angular momentum $J = 3/2$ this operation is produced by means of the substitution $z \to -z$ in the wave functions and the action of the matrix

$$\Sigma_z = \begin{Vmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{Vmatrix}$$

on them. Here even and odd functions look like, respectively,

$$\Psi_1 = \begin{pmatrix} c_1 \\ s_1 \\ c_2 \\ s_2 \end{pmatrix} \exp(\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{\rho}),$$

$$\Psi_2 = \begin{pmatrix} s_1' \\ c_1' \\ s_2' \\ c_2' \end{pmatrix} \exp(\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{\rho}), \quad \boldsymbol{\rho} \perp \mathbf{z}. \tag{4}$$

The functions $c_1(z)$, $c_2(z)$, $c_1'(z)$ and $c_2'(z)$ entering here are even functions of z, consisting of the two terms of the type $\cos(q_i z)$, where $q_i(\boldsymbol{K})$, $i = 1, 2$ are the solutions of the dispersion equation [22,23]. The functions $s_1(z)$, $s_2(z)$, $s_1'(z)$ and $s_2'(z)$ are odd functions containing $\sin(q_i z)$.

Since H_0 is invariant relative to spatial inversion, its spectrum $E(\boldsymbol{K})$ is two-fold degenerate. The function with the same values of $\boldsymbol{K}$ and the energy but with opposite parity with respect to reflection in the plane $z = 0$ may be put into correspondence to each of the functions Ψ_1 and Ψ_2. These functions are obtained from Ψ_1 and Ψ_2 by the action of the operators of the Kramers conjugation K and the inversion I. As applied to Ψ_1 it is equivalent to the action of the matrix

$$\Sigma_x = \begin{Vmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{Vmatrix},$$

complex conjugation and the substitution $\boldsymbol{\rho} \to -\boldsymbol{\rho}$. For Ψ_2 it is necessary to use the matrix $-\Sigma_x$.

The perturbation hamiltonian reflecting the noninvariance of the bulk hamiltonian with respect to

[#1] All the parameters denoted in ref. [18] as γ are denoted here and below as α with the corresponding subscripts.

inversion contains terms linear and cubic over k [21]. However, a contribution of the linear terms in the spectrum of 2D carriers is small [6,24] and we omit it. Firstly, among the terms of the order of k^3 [25] there is a nonrelativistic invariant

$$H_h^{(1)} = \alpha_v (\boldsymbol{J}\cdot\boldsymbol{\kappa}) \tag{5}$$

similar to H_e; $\boldsymbol{J}$ are the matrices of the angular momentum $J=3/2$. In the widely-accepted seven-band scheme of the spectrum of GaAs the other invariants of the order of k^3 enter as a combination [18]:

$$H_h^{(2)} = \tfrac{1}{2}\delta\alpha_v \Big(\tfrac{13}{4}\boldsymbol{J}\cdot\boldsymbol{\kappa} - \sum_j J_j^3 \kappa_j + \sum_j \kappa_j(\boldsymbol{J}) k_j (k_j^2 - \tfrac{1}{3}k^2) \Big), \tag{6}$$

where

$$\kappa_x(\boldsymbol{J}) = J_y J_x J_y - J_z J_x J_z \,. \tag{7}$$

According to the results summarized in ref. [18] we get

$$\alpha_v \approx -39 \text{ eV Å}^3 \quad \text{and} \quad \delta\alpha_v \approx -35 \text{ eV Å}^3 .$$

A splitting of the spectrum induced by the SO interaction is found from the secular equation obtained by means of calculation of the matrix elements of $H_h = H_h^{(1)} + H_h^{(2)}$ on the functions Ψ_1 and $K|\Psi_1$ (or Ψ_2 and $K|\Psi_2$).

Two general statements follow from this secular equation. First, the scale relationship $\Delta E_i(\boldsymbol{K}, a) \propto a^{-3}\varphi_i(Ka)$ holds, the explicit appearance of the functions φ_i is different for different branches of the spectrum. Second, one can get an explicit expression for ΔE_i in the region $Ka \ll 1$. For the upper band of "heavy" holes h_0 we get

$$\Delta E_{h_0}(\boldsymbol{K}) = \delta\alpha_v \left[\xi \left(1 - \frac{2\zeta}{\pi} \operatorname{ctg}\left(\frac{\pi\zeta}{2}\right) \frac{1+\zeta^2}{1-\zeta^2} \right) - 1 \right] \left(\frac{\pi}{a}\right)^2 K, \tag{8}$$

and for the upper band of "light" holes ℓ_0 we have

$$\Delta E_{\ell_0}(\boldsymbol{K}) = \left\{ \delta\alpha_v \xi \left[\frac{2}{\pi\zeta} \operatorname{ctg}\left(\frac{\pi}{2\zeta}\right) \frac{\zeta^2+1}{\zeta^2-1} \right] - (2\alpha_v + \delta\alpha_v) \right\} \left(\frac{\pi}{a}\right) K. \tag{9}$$

Here

$$\xi = \frac{\gamma_3}{\gamma_2}, \quad \zeta = \left(\frac{\gamma_1 - 2\gamma_2}{\gamma_1 + 2\gamma_2} \right)^{1/2}. \tag{10}$$

Numerical calculations were made in the axial approximation [26]. Moreover, the exact solution for $\boldsymbol{K} \| \langle 1, 0 \rangle$ has been found. In fig. 1 the dispersion law in the upper subbands of heavy and light holes at $H_h = 0$ is represented. In fig. 2 the SO splitting of the spectrum for the upper subbands of heavy (a) and light (b) holes is given. The comparison shows that these splittings are comparable with the splitting of the electron spectrum. One should emphasize that a splitting is a nonmonotonous function of K.

We point out that a spectrum of the holes ℓ_0 in GaAs possesses an anomaly high sensitivity to the details of the chosen model. It relates to the specific numeric value of the parameter ζ which at the values of γ_1 and γ_2 given above is equal to $\zeta = 0.49$. Hence the argument of the cotangent entering (9) is very close to π, i.e. in fact we are in the vicinity of a singular point. Similarly, $\operatorname{tg}(\pi/4\zeta)$ enters the formulae for the effective mass at small K in the subband ℓ_0 [22], i.e. the same singularity manifests itself. Thus, the spectrum of the subband ℓ_0 is very sensitive to

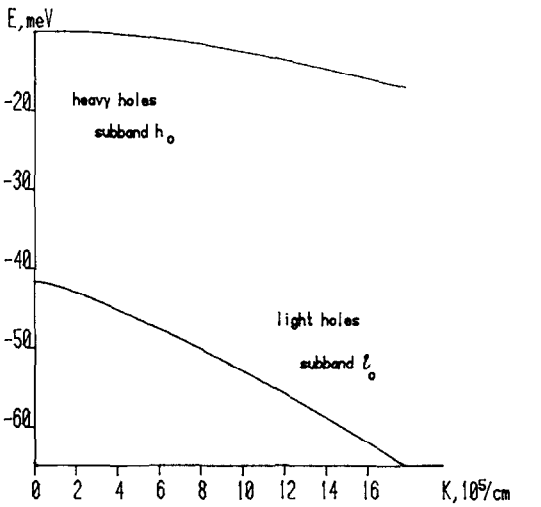

Fig. 1. Dispersion law in the upper subbands of heavy (h_0) and light (ℓ_0) holes in quantum well with a width $a = 100$ Å in GaAs. The maximal value of K is equal to the Fermi momentum at the concentration 5×10^{11} cm^{-2}.

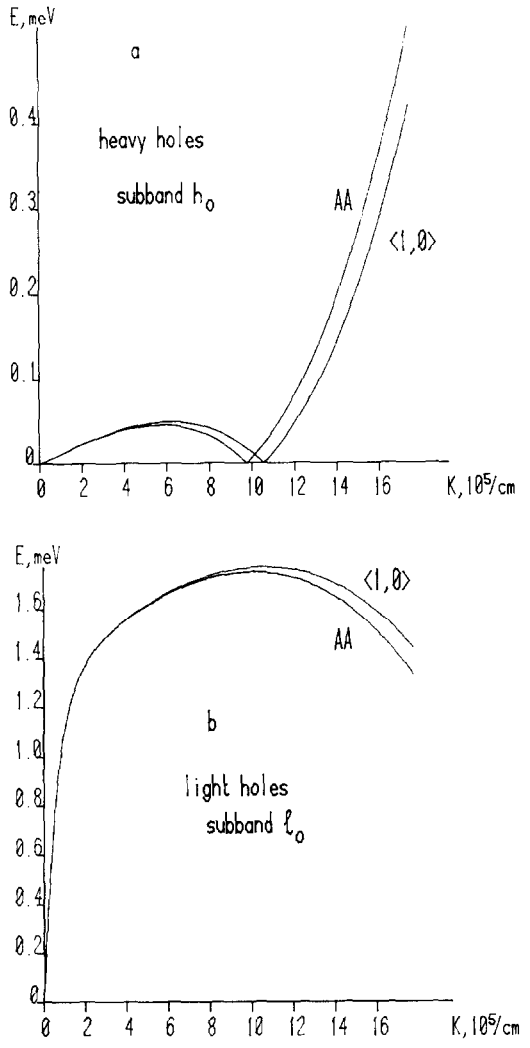

Fig. 2. Spin–orbital splitting of the spectrum in the upper subbands of heavy (a) and light (b) holes. The curves obtained in the axial approximation: AA, the exact solution: ⟨1, 0⟩. The maximal value of K is the same as in fig. 1.

the details of the chosen model, for the boundary conditions, in particular. This seems to be the reason for the fact that the electron curvature sign has been obtained for $E_{\ell_0}(\boldsymbol{K})$ in ref. [26] (which seems to be in agreement with a number of experiments) in contrast to the spectrum in fig. 1. One can also see an extreme sensitivity of the spectrum to the parameters of the model from the figures given in ref. [26]. This sensitivity can also account for the anomalies which made the authors of ref. [27] reconsider the values of the effective masses of the holes which is equivalent to the change of the choice of the parameters γ_i. From our point of view the data given above testify to the fact that no calculations of the ℓ_0 band in GaAs made by the effective mass method can be truthful, at least in the small K region.

The results of the calculation are essentially connected with the choice of the face (001). In this case there is a linear term in the spectrum for both subbands (h_0 and ℓ_0). It only vanishes in the band h_0 at $\delta\alpha_v = 0$. While chosing face (111) a linear term in the subband h_0 always vanishes as it follows from the symmetry group C_{3v} [28].

4. Conclusion

The results of the calculations show that the SO splitting of the spectrum of 2D electrons and holes in the GaAs quantum wells caused by k^3-terms in the bulk dispersion law of the carriers has a value quite accessible for experimental observation. The accuracy of the numerical results is restricted by both the accuracy with which the set of SO parameters α_c^*, α_v and $\delta\alpha_v$ is now known and by the abnormal sensitivity of the results for the ℓ_0 band to the details of the accepted model. As applied to the electron band and the h_0 band the error within a factor two seems natural. For the ℓ_0 band the error might be markedly higher and one should expect that our results give an upper bound of the SO splitting. However, as a whole, the accuracy is quite enough to substantiate the statement made above.

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