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The theorem on the spin splitting of energy levels within the Kildal-Bodnar model

O.V. Dvornik and G.P. Chuiko
Kherson National Technical University, Department of General and Applied Physics
24, Beryslavske Shosse, 73008 Kherson, Ukraine; e-mail: olga_dvornik@mail.ru

Abstract. The semiconductor Cd_3As_2 is known as a zero-gap material like HgTe or α-Sn but with the tetragonal lattice and in various crystalline forms. One of the forms has no symmetry center, and just this form is stable under ordinary conditions. So, every of its energy bands is split into a pair of spin subbands owing to the removal of the Kramers degeneration. The theory predicts that the total sum of all spin splittings will be equal to zero, whereas the modeling shows the peculiar dependences of spin splittings on the direction and modulus of the wave vector.

Keywords: center of symmetry, spin splitting, Kramers degeneration.

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1. Introduction

A band model suitable for crystals with and without symmetry center has been presented in [1]. This model describes uniaxial semiconductors by taking into account their lattice deformations, spin-orbital interaction, and the splitting within the **kP**-approach. One of the features of the Hamiltonian in [1] is the account of removing the Kramers degeneration in a crystal modification without symmetry center. This allows the partition of some energy band into two subbands having opposite-spin states. The knowledge about this splitting is essential for the newest branches of electronics dealing with the opposite-spin states in crystals or nanostructures. We are going to prove here a general theorem on such a splitting within the model developed in [1].

The predictions of the theorem will be illustrated by the example of Cd_3As_2. We have two reasons for this:

1. This material has an inverted band structure like those in α-Sn, HgTe or HgSe what is interesting by itself [2].
2. This material can have few tetragonal structures, and one of them has no symmetry center ($I4_1cd$-C_{4v}^{12}) and is stable under normal conditions [3].

2. Theorem

It has been shown in [1] that the generalized **kP**-Hamiltonian for a uniaxial material can be presented in the rational canonical form (alias Frobenius' form):

$$H = \begin{pmatrix} H_\alpha & 0 \\ 0 & H_\beta \end{pmatrix}. \qquad (1)$$

It is worth to note that $H_\alpha = H_\beta$ if the symmetry center exists. Each of the submatrices has size [4×4]:

$$H_\alpha = \begin{pmatrix} 0 & 0 & 0 & -a_0 \\ 1 & 0 & 0 & -a_{1\alpha} \\ 0 & 1 & 0 & -a_2 \\ 0 & 0 & 1 & -a_3 \end{pmatrix}; \quad H_\beta = \begin{pmatrix} 0 & 0 & 0 & -a_0 \\ 1 & 0 & 0 & -a_{1\beta} \\ 0 & 1 & 0 & -a_2 \\ 0 & 0 & 1 & -a_3 \end{pmatrix}. \qquad (2)$$

Here, a_j are the coefficients of ε^j (j = 0, 1, 2, 3) in two characteristic polynomials in the spherical system of coordinates like that in [1]:

$$\begin{aligned} P_\alpha(\varepsilon,\theta) &= \varepsilon^4 - (\varepsilon_g - \Delta - \delta)\,\varepsilon^3 - \\ &- ((\sin^2\theta + \eta^{-4}\cos^2\theta)(Pk)^2 - \\ &- \left(\frac{2}{3}\right)\eta^{-1}\Delta\xi\sin(\theta)\,(Pk) + \left(\frac{2}{3}\right)\Delta\xi^2 + \\ &+ \left(\frac{2}{3}\right)\varepsilon_g\Delta\left(\delta + \frac{\Delta}{3}(1-\eta^{-2})\right)\times \\ &\times\varepsilon - \frac{\Delta}{3}\left(\delta + \frac{\Delta}{3}(1-\eta^{-2})\right)\sin^2\theta\,(Pk)^2, \end{aligned} \qquad (3)$$

$$\begin{aligned} P_\beta(\varepsilon,\theta) &= \varepsilon^4 - (\varepsilon_g - \Delta - \delta)\,\varepsilon^3 - \\ &- ((\sin^2\theta + \eta^{-4}\cos^2\theta)(Pk)^2 + \\ &+ \left(\frac{2}{3}\right)\eta^{-1}\Delta\xi\sin(\theta)\,(Pk) + \left(\frac{2}{3}\right)\Delta\xi^2 + \\ &+ \left(\frac{2}{3}\right)\varepsilon_g\Delta\left(\delta + \frac{\Delta}{3}(1-\eta^{-2})\right)\varepsilon - \\ &- \frac{\Delta}{3}\left(\delta + \frac{\Delta}{3}(1-\eta^{-2})\right)\sin^2\theta\,(Pk)^2. \end{aligned} \qquad (4)$$

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These polynomials are slightly different only for the structures without symmetry center.

Additionally, we mention that ε_g, P, Δ are three known parameters of Kane's model [4]: the energy gap, impulse matrix element, and spin-orbital interaction parameter, respectively; δ is the crystal field parameter introduced by Kildal [5]; ξ is the another crystal field parameter which can be either non-zero in the absence of a symmetry center or equal to zero otherwise [1]; and η is the parameter of the uniaxial lattice deformation [1]. The energy ε is reckoned from the top of the highest valence band. The subscripts (α, β) for the coefficient $a_{1\alpha,\beta}$ correlate with two opposite spin states.

The model [1] ($\xi \neq 0$, $\eta \neq 0$, $\delta \neq 0$) generalizes both the model for cubic crystals [4] ($\xi = 0$, $\eta = 0$, $\delta = 0$) and the model for uniaxial crystals with symmetry center [5] ($\xi = 0$, $\eta = 0$, $\delta \neq 0$) to the crystals without symmetry center and with axial deformations of lattices.

Let us to denote the solutions of Eqs. (3) and (4) as $\varepsilon_{n,\alpha}$ and $\varepsilon_{n,\beta}$, respectively ($n = 1, 2, 3, 4$). It is well known that the sum of these solutions is equal to a_3 (as it is the trace of a submatrix). Thus, we have

$$\sum_n \varepsilon_{n,\alpha} = \sum_n \varepsilon_{n,\beta} = \varepsilon_g - \Delta - \delta \qquad (5)$$

simply for the reason that this coefficient is identical for both polynomials. Moreover, it follows from relation (5) that

$$\sum_n \left(\varepsilon_{n,\alpha} - \varepsilon_{n,\beta}\right) = \sum_n s_n = 0. \qquad (6)$$

Rule (6) is trivial if the center of symmetry exists, because each element of the sum is zero ($s_n = 0$). Nevertheless, this rule would be operating even if the symmetry center is absent and elements of the sum are non-zeros ($s_n \neq 0$). Now we can formulate the following proposition:

Table.

ε_g, eV	P, eV·m	Δ, eV	δ, eV	ξ, eV	η	a, Å	c, Å
–0.13	$7.0\times$ $\times 10^{-10}$	0.27	0.095	0.035	1.005648	12.6461	25.4908

Theorem. *The total sum of the spin splittings of all subbands must be zero with Hamiltonian* (*1*).

This theorem is true under condition that the absence of symmetry, which is the reason for removing the degeneration by spin, does not change anyway the sum of parameters presented by (5): $\varepsilon_g - \Delta - \delta = a_3$.

The numerical values of the parameters characterizing Cd_3As_2 which were used in our computations are presented in the Table according to [1].

3. Results of computations and their discussion

Equations (3), (4) allow the direct solutions. We calculated the dependences of the elements of sum (6) (i.e., $s_n = \varepsilon_{n,\alpha} - \varepsilon_{n,\beta}$) on the modulus and direction of the wave vector by using the numerical values of parameters given in the table. The results are shown in Figs. 1 and 2.

The direct computer verification of the obtained rule (6) showed their correctness within the limits of the computing accuracy. It is clearly visible even from the different signs of these splittings.

Each sheet of Fig. 1 which corresponds to one of the energy bands demonstrates an extremum depending on the modulus of the wave vector **k**, whereas the dependences of the splittings on the directions are monotonic: they simply increase from the main axis direction ($\theta = 0$) up to the directions normal to them $\left(\theta = \frac{\pi}{2}\right)$.

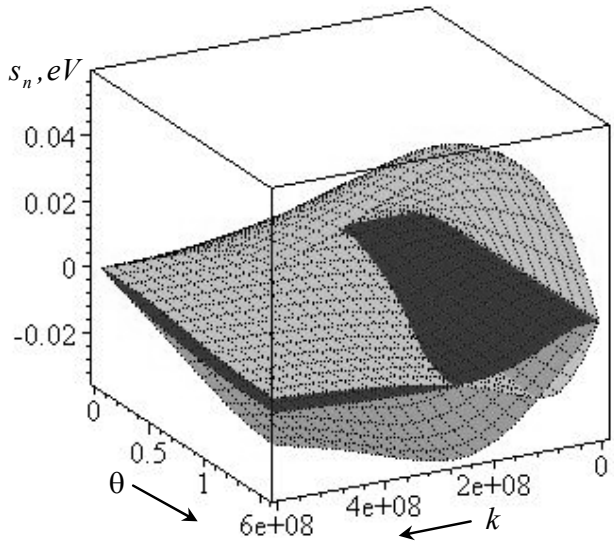

Fig. 1. Dependences of s_i on the direction (θ) and modulus of the wave vector.

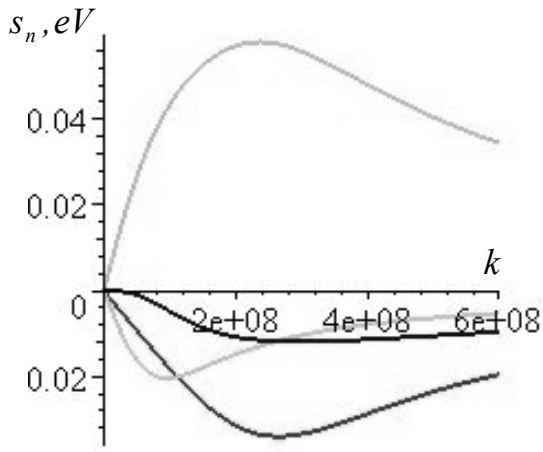

Fig. 2. Dependences of s_n on the modulus of the wave vector.

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The magnitudes s_n of the spin splitting are comparable with the magnitude of the parameter $\xi \approx 0.035$ eV. Our calculations convince us also that they depend on this parameter much stronger than on the parameter δ or η.

So, both the theoretical analysis and the computation testify that the absence of a symmetry center is not able to create such a splitting of energy levels, for which the total sum could be non-zero, within the model [1].

Let us also to remark that an analogous statement can be proved as for the influence of a tetragonal deformation on shifts of the energy levels. Indeed, such a deformation (η) cannot change the coefficient $a_3 = \varepsilon_g - -\Delta - \delta$, generally speaking. It would be right if none of them does not depend on such a deformation directly. However, sometimes it may take place, for instance, for $\delta = \delta(\eta)$ [6].

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References

1. G.P. Chuiko, V.V. Martyniuk, and V.K. Bazhenov, Basic peculiarities of energy band spectra within generalized Kildal's model for semiconductors with one main axis // *Semiconductor Physics, Quantum Electronics & Optoelectronics* **8**(2), p. 28-31 (2005).
2. G.P. Chuiko, I.A. Teplinskaya, Topological transition and related with it singularity in the density of states of conduction band as features of the inverse tetragonal semiconductor – cadmium arsenide // *Fizika, Tekhnika Poluprovodnikov* **17**(6), p. 1123-1125 (1983) (in Russian).
3. G.P. Chuiko, N.L. Don, and V.V. Ivchenko, Ordering and polytypism in $A_3^{II}B_2^{V}$ crystals // *Functional Materials* **12**(3), p. 454-460 (2005).
4. E.O. Kane, Band structure of indium antimonide // *J. Phys. Chem. Solids* **1**, p. 249-261 (1957).
5. H. Kildal, Band structure of $CdGeAs_2$ near $k = 0$ // *Phys. Rev. B* **10**(12), p. 5082-5087 (1974).
6. G.P. Chuiko, O.V. Dvornik, Coupling between crystal splitting of valence bands and tetragonal deformation of lattice for compounds $A_3^{II}B_2^{V}$ // *Fizika, khimiya tverdogo tela* **3** (4), p. 682-686 (2002) (in Russian).

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