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Inversion asymmetry effect on quantum oscillations in 3D crystals with C_{nv} symmetry

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Abstract. The peculiarities of quantum oscillations in bulk semiconductors with C_{nv} symmetry caused by the lack of their symmetry centre are considered. A quasi-cubic model is used for finding the magnetic levels. The algorithm for numerical calculating the levels in the presence of the tilted magnetic field is suggested. Numerical estimations are performed for Cd_3As_2 and $Cd_{3-x}Zn_xAs_2$. It is shown that the most suitable conditions for observing the beating effect in these compounds are the high values of the electron concentrations and small angles between the direction of the magnetic field and crystal symmetry axis.

Keywords: spin splitting of bands, Fermi surface, quantum oscillations, beating effect, node, cadmium arsenide.

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1. Introduction

In the crystals without the symmetry center while straying from the Brillouin zone center, complete removing the energy band degeneracy may occur. The opposite signs of the electron spin projections onto the quantization axis correspond to the splitted states. For the crystals with C_{nv} symmetry class, such a splitting is linear in the wavevector \mathbf{k} . The appropriate isoenergetic surface is described by the following equation in the cylindrical coordinate system [1]:

$$\frac{(k_{\perp} \pm k_0)^2}{a^2} + \frac{k_z^2}{b^2} = 1, \quad (1)$$

where a , b are the semiaxes of the ellipse in which axial rotation along k_z produces the surface; k_0 is the nonzero (as a result of the symmetry center lack) value of the ellipse center shift from the origin of coordinates within the plane perpendicular to the crystal main axis.

Since a , b , k_0 depend on the band parameters as well as on the electron energy ε , the alteration of the latter one may lead to changes in the shape and topology of isoenergetic surface. When $k_0 > a$, the surface is topologically equivalent to the torus while for $k_0 < a$ it is the fourth order surface self-crossing in two conical points (Fig. 1).

The possibility to manifest peculiarities of isoenergetic surfaces (1) in quantum-oscillatory phenomena (Shubnikov – de Haas (SdH) and de Haas – van Alphen effects (dHvA)) was discussed in [2, 3]. However, these works dealt only with the cases when the magnetic field was parallel or perpendicular to the k_z -axis and the simple one-band parabolic model was used. In this paper, we present a more comprehensive study of this problem. In particular, we take into account the possible nonparabolicity of the energy spectrum and using the effective mass method consider the conditions for beating appearing in the case of different electron concentrations and orientations of magnetic field. Our theoretical analysis was accompanied by numerical calculations performed for Cd_3As_2 and $Cd_{3-x}Zn_xAs_2$ that have C_{4v}^{12} space group symmetry.

2. Theory and numerical calculations

It is known [4] that, in the quasi-classical approximation, the period of quantum oscillations is defined by the extreme in k'_z (k'_z is a component of the wavevector along the magnetic field \mathbf{B}) cross-section area S_m of the Fermi surface (FS) normal to the external magnetic field direction: $T = 2\pi e/\hbar S_m$. For FS which has more than one extreme cross-section area normal to a given magnetic field direction, there will be oscillatory effects associated with each such area.

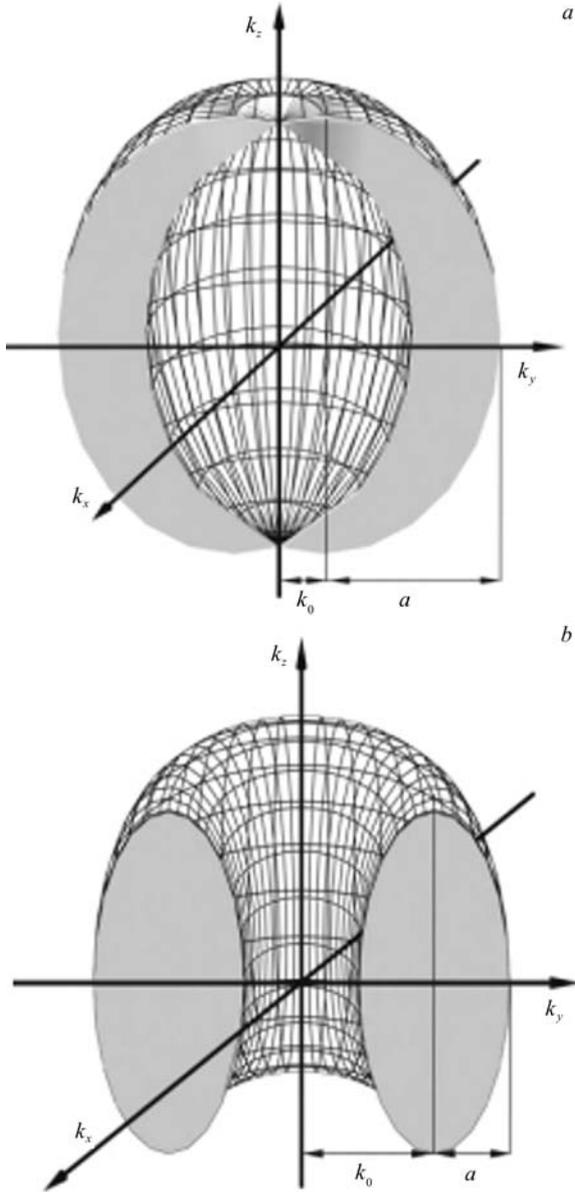


Fig. 1. Shape of the isoenergetic surfaces described by equation (1): $k_0 < a$ (a), $k_0 > a$ (b).

For the majority of semiconductors, the characteristic of the deviation of FS (1) from an ellipsoidal shape $r = k_0/a \ll 1$. The quasi-classical theory developed for this case [2, 3] predicts the existence of regular “beats” in quantum oscillations connected with the existence of two close central cross-section areas of FS. It is easy to derive the expression for finding the beating period in the form

$$\begin{pmatrix}
 \varepsilon_1 & 0 & iP\hat{k}_z + \xi & 0 & 0 & iP\hat{k}_- & 0 & iP\hat{k}_+ \\
 0 & \varepsilon_1 & 0 & iP\hat{k}_z + \xi & -iP\hat{k}_+ & 0 & iP\hat{k}_- & 0 \\
 -iP\hat{k}_z + \xi & 0 & \varepsilon_2 & 0 & \Delta_1 & 0 & 0 & 0 \\
 0 & -iP\hat{k}_z + \xi & 0 & \varepsilon_2 & 0 & \Delta_1 & 0 & 0 \\
 0 & iP\hat{k}_- & \Delta_1 & 0 & \varepsilon_3 & 0 & 0 & 0 \\
 -iP\hat{k}_+ & 0 & 0 & \Delta_1 & 0 & \varepsilon_3 & 0 & 0 \\
 0 & -iP\hat{k}_+ & 0 & 0 & 0 & 0 & -\varepsilon & 0 \\
 -iP\hat{k}_- & 0 & 0 & 0 & 0 & 0 & 0 & -\varepsilon
 \end{pmatrix}
 \begin{pmatrix}
 \varphi_1 \\
 \varphi_2 \\
 \varphi_3 \\
 \varphi_4 \\
 \varphi_5 \\
 \varphi_6 \\
 \varphi_7 \\
 \varphi_8
 \end{pmatrix}
 = 0. \quad (3)$$

$$T_B = \pi T_0 / 8r\mathbf{E}(\kappa) \quad (2)$$

where $T_0(\varepsilon_F) = (2e\sqrt{b^2 \cos^2 \theta + a^2 \sin^2 \theta} / \hbar a^2 b)_{\varepsilon=\varepsilon_F}$ is the oscillatory period obtained by ignoring the inversion asymmetry; ε_F is the Fermi energy; $\mathbf{E}(\kappa)$ is the complete elliptic integral of the second kind with the parameter $\kappa = 1/\sqrt{1 + (b^2/a^2) \cot^2 \theta}$; θ is the angle between the field direction and k_z -axis. It should be noted, however, that within the limits of quasi-classical approach the interaction between the electron spins and magnetic field (Zeeman’s term) is not taken into account. Very often such an interaction complicates the beating pattern [5, 6]. So, to correctly describe this effect one should use the quantum-mechanical approach.

It is known [4] that the harmonics amplitudes of the SdH(dHvA)-signal contain the multiplicative factor $\cos(j\pi\nu)$ (j is the harmonic number; $\nu = (\varepsilon_n^+ - \varepsilon_n^-) / \hbar\omega_c$, where ε_n^\pm is the energy of the Landau magnetic subband with the extreme value k'_z , ω_c is the cyclotron frequency). When the ν -factor magnetic field dependence is available, the harmonics amplitudes may turn into zero for certain values of the magnetic field – a “node” appears in the oscillatory curve. As a rule, these peculiarities manifest themselves in the range of the magnetic fields where it is possible to detect only the first harmonic. The condition of the node appearing for it is written as $|\nu| = i - 0.5$, where i is the node number.

To determine the subband energies, we use the quasi-cubic band model [7], which properly describes the effects of spin splitting, anisotropy and nonparabolicity of bands energy. In the eight-band effective mass approximation, the electronic wavefunction can be chosen in the following form:

$$\Psi = \begin{pmatrix} \Psi \uparrow \\ \Psi \downarrow \end{pmatrix} = \frac{1}{\sqrt{N}} \begin{pmatrix} \varphi_1 S + \varphi_3 Z + \varphi_6 R_- + \varphi_8 R_+ \\ \varphi_2 S + \varphi_4 Z - \varphi_5 R_+ + \varphi_7 R_- \end{pmatrix},$$

where N is the number of a unit cell in crystal; $R_\pm = (X \pm iY) / \sqrt{2}$ and the symbols \uparrow and \downarrow mean the spin-up and spin-down functions, respectively. S, X, Y, Z are the periodic Bloch amplitudes transformed like atomic s - and p -functions under the operations of the tetrahedral group at Γ point. φ_i are envelope functions satisfying the set of eight coupled differential equations, which in the case of quasi-cubic approximation can be represented in the following matrix form [8]:

Here $\varepsilon_1 = \varepsilon_g - \varepsilon$, $\varepsilon_2 = -(\varepsilon + \delta + \Delta/3)$, $\varepsilon_3 = -(\varepsilon + 2\Delta/3)$, $\Delta_1 = \sqrt{2}\Delta/3$; $\hat{k}_\pm = (1/\sqrt{2})(\hat{k}_x \pm i\hat{k}_y)$, where $\hat{k}_x, \hat{k}_y, \hat{k}_z$ are the components of the operator $\hat{k} = -i\nabla + (e/\hbar)\mathbf{A}$, \mathbf{A} is the vector-potential of field. Hence the model along with the optical energy gap ε_g needs to know the values of spin-orbit splitting of the valence band Δ and interband momentum matrix element P , crystal field splitting the valence band at Γ point δ , and ξ is the parameter defined by "interaction" between S and Z states via the asymmetric part of the crystal potential [8, 9].

Let us introduce the axis transformation $x' = \cos\theta x - \sin\theta z$, $y' = y$, $z' = \sin\theta x + \cos\theta z$, and choose the "Landau" gauge in the form $\mathbf{A}' = B(-y', 0, 0)$. In this case, we have the next commutation relations

$$[\hat{k}_x, \hat{k}_y] = -\frac{i}{l^2} \cos\theta, \quad [\hat{k}_y, \hat{k}_z] = -\frac{i}{l^2} \sin\theta, \quad [\hat{k}_x, \hat{k}_z] = 0, \quad (4)$$

where $l = \sqrt{\hbar/eB}$ is the cyclotron radius. Let us express $\varphi_3 \dots \varphi_8$ in terms of φ_1 , φ_2 and eliminate them by substituting in the first two equations of the set (3). Then using (4) we obtain

$$\begin{pmatrix} \gamma - f_1(\hat{k}_x^2 + \hat{k}_y^2) - f_2\hat{k}_z^2 + \frac{f_{\parallel}\cos\theta}{l^2} & -2if_3(\hat{k}_x - i\hat{k}_y) + \frac{f_{\perp}\sin\theta}{l^2} \\ 2if_3(\hat{k}_x + i\hat{k}_y) + \frac{f_{\perp}\sin\theta}{l^2} & \gamma - f_1(\hat{k}_x^2 + \hat{k}_y^2) - f_2\hat{k}_z^2 - \frac{f_{\parallel}\cos\theta}{l^2} \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} = 0, \quad (5)$$

where

$$\gamma(\varepsilon) = \varepsilon(\varepsilon - \varepsilon_g)[\varepsilon(\varepsilon + \Delta) + \delta(\varepsilon + 2\Delta/3)],$$

$$f_{\parallel} = P^2(\varepsilon + \delta)\Delta/3, \quad f_{\perp} = P^2\varepsilon\Delta/3,$$

$$f_1(\varepsilon) = P^2[\varepsilon(\varepsilon + 2\Delta/3) + \delta(\varepsilon + \Delta/3)],$$

$$f_2(\varepsilon) = P^2\varepsilon(\varepsilon + 2\Delta/3), \quad f_3(\varepsilon) = P\varepsilon\xi\Delta/3.$$

From (5) it follows that a, b, k_0 may be expressed in terms of polynomials γ , f_i as

$$a^2 = (\gamma f_1 + f_3^2)/f_1^2, \quad b^2 = (\gamma f_1 + f_3^2)/f_1 f_2, \quad k_0 = f_3/f_1.$$

It is convenient to perform a unitary transformation $U\hat{H}U^{-1}$,

$$U = \begin{pmatrix} \cos\frac{\beta}{2} & \sin\frac{\beta}{2} \\ -\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \quad \tan\beta = f_{\perp}/f_{\parallel},$$

in order to make a new two-component quasi-Hamiltonian to be a diagonal one up to the terms proportional to f_3 . Expand now the new components φ_1 , φ_2 into an infinite series of linear harmonic oscillatory functions:

$$\varphi_1 = \exp(i(k'_x x' + k'_z z')) \sum_n a_n \phi_n,$$

$$\varphi_2 = \exp(i(k'_x x' + k'_z z')) \sum_n b_n \phi_n,$$

and introduce the creation and annihilation operators according to [10]:

$$\hat{a}^\dagger(\hat{a}) = \frac{l}{\sqrt[4]{4AB}} (A\hat{k}'_x + i(-i)B\hat{k}'_y + C\hat{k}'_z), \quad [\hat{a}, \hat{a}^\dagger] = 1,$$

where

$$A = f_1 \cos^2 \theta + f_2 \sin^2 \theta, \quad B = f_1,$$

$$C = \frac{(f_1 - f_2) \sin \theta \cos \theta}{\sqrt{f_1 \cos^2 \theta + f_2 \sin^2 \theta}}.$$

It is possible to express the components of the wavevector operator via these operators as follows:

$$\hat{k}_x = \frac{\sqrt[4]{4AB} \cos \theta}{2l\sqrt{A}} (\hat{a}^\dagger + \hat{a}) + \left(\sin \theta - \frac{C}{\sqrt{A}} \cos \theta \right) \hat{k}'_z,$$

$$\hat{k}_y = -\frac{i\sqrt[4]{4AB}}{2l\sqrt{B}} (\hat{a}^\dagger - \hat{a}),$$

$$\hat{k}_z = -\frac{\sqrt[4]{4AB} \sin \theta}{2l\sqrt{A}} (\hat{a}^\dagger + \hat{a}) + \left(\cos \theta + \frac{C}{\sqrt{A}} \sin \theta \right) \hat{k}'_z.$$

Taking into account these remarks, it is easy to show that the system (5) is reduced to the infinite system of algebraical equations, a fragment of which has the form:

$$\begin{pmatrix} \Lambda_{n-1} & -iL_n & [0] \\ iL_n^\top & \Lambda_n & -iL_{n+1} \\ [0] & iL_{n+1}^\top & \Lambda_{n+1} \end{pmatrix} \begin{pmatrix} a_{n-1} \\ b_{n-1} \\ a_n \\ b_n \\ a_{n+1} \\ b_{n+1} \end{pmatrix} = 0, \quad (6)$$

where

$$\Lambda_n = \begin{pmatrix} \frac{1}{T_0 B} - \left(n + \frac{1}{2} \right) + \frac{\nu_0}{2} & 0 \\ 0 & \frac{1}{T_0 B} - \left(n + \frac{1}{2} \right) - \frac{\nu_0}{2} \end{pmatrix},$$

$$L_n = \frac{2f_3 l}{\nu_0 (4f_1 (f_1 \cos^2 \theta + f_2 \sin^2 \theta))^{3/4}} \sqrt{\frac{n}{f_1}} \times \begin{pmatrix} f_{\perp} \sin \theta & (f_{\parallel} + f_1 \nu_0) \cos \theta \\ (f_{\parallel} - f_1 \nu_0) \cos \theta & -f_{\perp} \sin \theta \end{pmatrix},$$

$$v_0(\varepsilon_F) = \left(\frac{(f_{\parallel}^2 \cos^2 \theta + f_{\perp}^2 \sin^2 \theta)}{f_1(f_1 \cos^2 \theta + f_2 \sin^2 \theta)} \right)_{\varepsilon=\varepsilon_F} \quad \text{is the value of}$$

ν -factor in the limit of strong magnetic fields (in (6) we put $k'_z = 0$, because it corresponds to the extreme FS cross-section).

It is possible to derive the analytical expression for finding the energy levels from (6) only in the case when $\xi\theta = 0$. With $\xi = 0$ ($f_3 = 0$), we have the result first obtained in [11]. If $\theta = 0$ one gets

$$1/T_0 B = n + \frac{1}{2} \sqrt{8nl^2 k_0^2 + (1 + \nu_0)^2}, \quad (7a)$$

$$1/T_0 B = n + 1 - \frac{1}{2} \sqrt{8(n+1)l^2 k_0^2 + (1 + \nu_0)^2} \quad (7b)$$

(while obtaining the expressions (7), we performed $n \rightarrow n+1$ shift for the system of “-” levels, because this numeration is more preferable from the physical point of view).

Using the formulae (7) and applying the method for ν -factor calculation suggested in [11] for this direction of the magnetic field, one obtains

$$\nu(\varepsilon_F, B) = \left[\sqrt{(4r/BT_0)^2 + (1 + \nu_0)^2} - 1 \right]_{\varepsilon=\varepsilon_F} \quad (8)$$

The dependence of electron ν -factor on the magnetic field can be explained in this case by complicated nature of the spin-orbit interaction and as a result of it, the spin splitting of the Landau levels is no longer linear dependent on the magnetic field. When $i \gg 1$ (i.e., for relatively weak fields), from (8) it follows that $B_{i+1}^{-1} - B_i^{-1} = T_0/4r$. Hence, the nodes with large numbers are periodically located along the scale B^{-1} with the period (2). As the magnetic field increases, the location of the nodes turns to be irregular (the Zeeman subbands splitting reveals itself). If we take into account the fact that with the lowering the node number the difference between the magnetic field values corresponding to two neighbour nodes grows rapidly, it becomes obvious that only some first nodes

can be observed in the fields where quantum oscillations start to manifest themselves.

Let us perform the specific calculations for Cd_3As_2 and $\text{Cd}_{3-x}\text{Zn}_x\text{As}_2$. For this purpose, we use the rank values of their band parameters suggested in [8]. Since the value of the parameter ξ is known only by its order [8], all the calculations are made for several values of this parameter.

Fig. 2 shows the concentration dependences of the first nodes' location calculated for three different values of the parameter ξ . The characteristic feature of all these curves is the increase (which is more or less smooth depending on ξ value) of the field value corresponding to the node when increasing the electron concentration.

Let us now examine the behaviour of ν -factor in the tilted magnetic field. The difficulty of this task is caused by the fact that it is impossible to apply the standard perturbation theory to the parameter f_3 because the combination $f_3\sqrt{n}$ being a part of (4.7) is not small [12]. Besides, the additional difficulties in comparison with 2D systems are connected with the fact that only the magnetic field component normal to the 2D layer effects on the orbital moment, while in the bulk crystal such an interaction is determined as a whole by the field.

For defining the energy spectrum when $\theta, \xi \neq 0$, let us use the technique of folding the determinants of the block matrixes. Applying the well-known Schur formula it is possible to show that

$$\det(\Lambda_n - L_{n+1}(\Lambda_{n+1}^I)^{-1}L_{n+1}^T - L_n^T(\Lambda_{n-1}^{II})^{-1}L_n) = 0,$$

where the matrixes Λ_{n+1}^I , and Λ_{n-1}^{II} are determined using the following recurrent relations:

$$\Lambda_{n+1}^I = \Lambda_{n+1} - L_{n+2}(\Lambda_{n+2}^I)^{-1}L_{n+2}^T,$$

$$\Lambda_{n-1}^{II} = \Lambda_{n-1} - L_{n-1}^T(\Lambda_{n-2}^{II})^{-1}L_{n-1}.$$

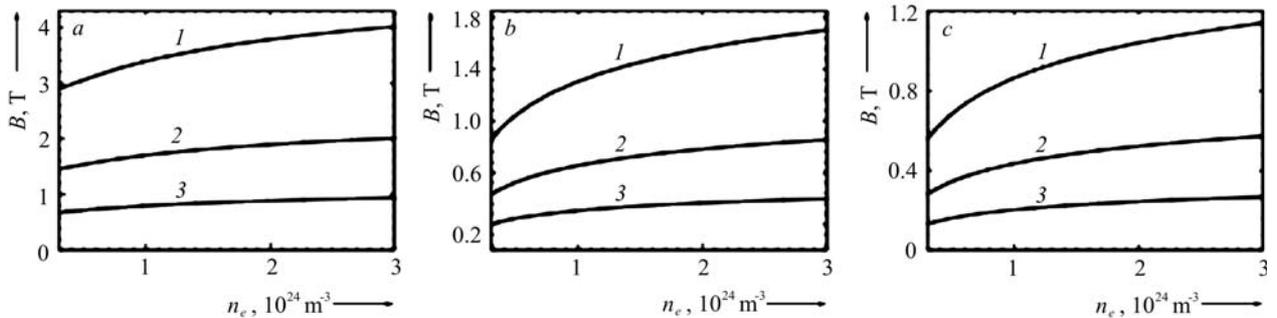


Fig. 2. Theoretical dependence of the first (a), second (b) and third (c) node location on the electron concentration for Cd_3As_2 : $\xi = 30$ meV (1); $\xi = 15$ meV (2); $\xi = 7$ meV (3).

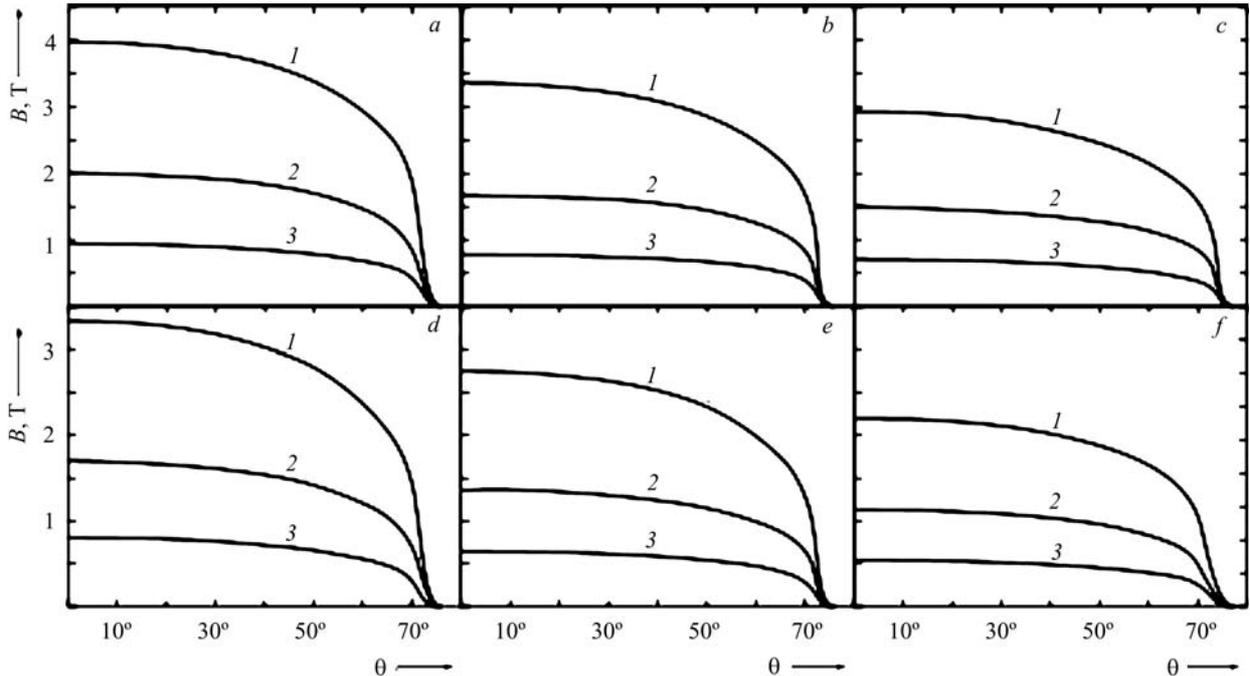


Fig. 3. Theoretical dependence of the maximal magnetic field corresponding to the nodes of oscillation on the azimuth angle for $\text{Cd}_{3-x}\text{Zn}_x\text{As}_2$: $\varepsilon_g = -0.1$ eV (a-c), $\varepsilon_g = 0.1$ eV (d-f); $n_e = 3 \times 10^{24} \text{ m}^{-3}$ (a),(d); $n_e = 10^{24} \text{ m}^{-3}$ (b), (e); $n_e = 4 \times 10^{23} \text{ m}^{-3}$ (c), (f); $\xi = 30$ meV (1), $\xi = 15$ meV (2), $\xi = 7$ meV (3).

While performing the specific numerical calculations, this algorithm is realized through the truncating the infinite matrix on the both sides of the fixed block Λ_{n_0} . In our calculations, the convergence for the eigenvalues was attained for the truncated matrix of 20×20 size.

Fig. 3 shows the results of numerical calculations for the dependence of the maximal magnetic field corresponding to the nodes on the azimuth angle. The following features are clearly seen:

1. With the increasing θ the magnetic field decreases monotonously.
2. Beating disappears in the case of large values θ ; the critical angle ($\sim 70^\circ$) at which the beating starts to disappear has a weak dependence on the band parameters and the carrier concentration.
3. With the decreasing ξ and rising ε_g , the values of the magnetic field reduce and locate within the narrower range.

4. Conclusions

The investigations carried out in this work show that the beating patterns in crystals with C_{nv} symmetry have their own specific character. Particularly, for $A_3^{\text{II}}B_2^{\text{V}}$ compounds one should expect the decrease of the maximal magnetic field corresponding to the nodes of oscillation when the electron concentration decreases and the field tilting about the symmetry axis increases. Moreover, starting from a certain azimuth angle the

beatings should disappear. The mentioned peculiarities are supposed to help in specifying the value of the parameter ξ which defines the magnitude of zero spin splitting of bands when studying the beating effect in $A_3^{\text{II}}B_2^{\text{V}}$ semiconductors (in which it has already been observed experimentally [13]).

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