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Issue Article

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THE ANALYSIS OF THE NUMERICAL CALCULATION OF SHALLOW ACCEPTOR LEVELS OF $A^{III}B^{V}$ CRYSTALS IN A MAGNETIC FIELD

Abstract: *Using the method of invariants, a general formula is obtained for the energy of the Zeeman splitting of the acceptor shallow level for semiconductor crystals of the $A^{III}B^{V}$ type in an arbitrary direction of the magnetic field H. It is shown that if the value of g_2/g_1 is close to "singular" values, such as -4/7 and -4/7 or falls into the transition region [-4/13, -4/7], then it is necessary to carefully monitor the course of each magnetic sublevel $E_i^{(a)}$ of the acceptor. It is for such values of g_2/g_1 that pairwise merging or complex entanglement of sublevels and strong anisotropy of the Zeeman splitting are observed. This, in turn, leads to a strong anisotropy of the recombination radiation between the conduction band and the acceptor level in a "strong" magnetic field at $g_2 \neq 0$.*

Key words: *crystals $A^{III}B^{V}$, shallow acceptor, g-factor, symmetry of the centre of the Brillouin zone, regular wave functions, Zeeman splitting anisotropy.*

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Introduction

The method of magneto-photoluminescence spectroscopy makes it possible to study the influence of ultra-small defects and atomic inhomogeneities in semiconductor structures on the optical properties of impurity complexes, as well as free and bound excitons [1]. The spin-polarized electronic and optical properties of semiconductors enhanced by a magnetic field are of decisive importance for the manufacture of various spintronic devices [2]. Recently, there has been a significant increase in interest in the optical properties of quantum dots with A+ centres in a magnetic field, which is primarily due to the possibility of effectively controlling both the binding energy of impurity complexes A++e and the spectral curves of recombination radiation associated with the radiative transition of an excited electron to the level of the A+ centre [3].

This work is devoted to calculating the energy of the Zeeman splitting of the acceptor level in semiconductors of the GaAs type, which is fourfold degenerate with allowance for the spin at the centre of the Brillouin zone Γ, and to a theoretical analysis of the features of such splitting depending on the direction of the magnetic field and the values of the g factors of the acceptor.

As is known [4], in a solid body, free charge carriers and charges in impurity atoms (or ions) interact with an external magnetic field only with their spin and orbital magnetic moments (if their directed or Brownian motion is not taken into account). The spin orientation, which is responsible for such a well-known phenomenon as paramagnetism, manifests itself in the orientations of particle spins and is the cause of the occurrence of circularly polarized luminescence of crystals in a magnetic field.

The study of the polarization of the recombination radiation of semiconductors in a magnetic field is of great interest for obtaining information about the dynamics of a crystal lattice, in particular, about the g factors of its particles [5–9]. In [5], a detailed theoretical analysis was made of the formation of polarized radiation in direct-gap $A^{III}B^{V}$ semiconductors in weak magnetic fields (

$g_{e,h}\mu_0 H << kT$, ($\xi_{F_e,h}$ – in the case of degenerate semiconductors) where $g_{e,h}-g$ is the electron and hole factor, respectively, $\mu_0=\frac{e\hbar}{2m_0c}=0,92712\cdot10^{-20}erg/G$ – Bohr magneton, H is the magnetic field strength, k is the Boltzmann constant, T is the absolute temperature). It is shown that the corrugation (anisotropic geometry) of the constant energy surface of the valence band does not affect the results obtained. In the case when recombination radiation occurs with the participation of shallow acceptors in a nondegenerate semiconductor, a simple expression is obtained for the equilibrium value of the degree of circular polarization

$$P_{circ}=\frac{g_e\mu_0H}{4kT}+\frac{5g_h\mu_0H}{4kT}.$$

This shows that the polarization of the luminescence of a crystal in a weak magnetic field $H<3\div4kE$ (if then $H=3kE$, at $\mu_0H\approx5\cdot10^{-6}eV$, $T=2^0K$, $kT\approx5\cdot10^{-5}eV$.) is determined exclusively by the average induced spin magnetic moments of free electrons and acceptors, it depends linearly and isotropically on H and is inversely proportional to the first power of temperature.

Theoretical results [5] were experimentally confirmed in [6], where, in particular, using the methods of the optical orientation of the spins of nonequilibrium carriers, their contributions to the polarization was measured. The work [7] is devoted to the experimental study and theoretical explanation of the formation mechanism of the 0,709 eV spectral line of polarized luminescence in germanium in a wide range of magnetic field values (up to $50kE\to\mu_0H=8\cdot10^{-5}eV\approx10^{-4}eV$). Although the experimental results have shown that in weak fields the radiation polarization is indeed isotropic and depends linearly on the value of H, however, at high magnetic fields, a significant anisotropy and a deviation from the linear dependence P_{circ} appear (in the general case, the anisotropy is not related to only the conduction band of the crystal, but also its valence band).

Therefore, the theoretical analysis of the anisotropy of the Zeeman splitting of the shallow level of an acceptor in semiconductors of the H type and the theoretical calculation of the intensity and degree of polarization of luminescence in a magnetic field in arbitrary directions of the crystal is of particular interest. Using the method of Picus-Beer invariants [4], we will try to obtain general formulas for the splitting energy of the acceptor level, as well as to analyze the features of splitting anisotropy depending on g_1 and g_2 constants of the acceptor g-factor.

Statement of the problem and its solution

Let us consider a $A^{III}B^V$ ($GaAs$, $ZnSb$, ...) type semiconductor placed in a uniform magnetic field in which nonequilibrium carriers are created, and their radiative recombination proceeds through the magnetic sublevels of shallow acceptors. Due to the orientation of the spins of electrons in the conduction band and holes in the acceptor levels under the action of an external magnetic field, the luminescence of a semiconductor turns out to be circularly polarized.

Semiconductors $A^{III}B^V$ are direct-gap, the symmetry of the centre ($\vec{k}=\vec{k}_0=\vec{0}$) of the Brillouin zone is determined by the group T_d. The quantum states in the conduction band and in the valence band are twice and four times degenerate, respectively, with spin taken into account. They are described by wave functions transforming accordingly according to the irreducible representations Γ_6, Γ_8 and in the notation of Luttinger and Kohn they can be represented as [10-13].

$$\Gamma_6\to\begin{cases}\psi_{1/2}^{1/2}=\frac{1}{\sqrt{3}}\left[\left(X+iY\right)\beta+Z\alpha\right]=S_\alpha\,,\\ \psi_{-1/2}^{1/2}=\frac{1}{\sqrt{3}}\left[-\left(X-iY\right)\alpha+Z\beta\right]=S_\beta\,,\end{cases}\qquad(1)$$

$$\Gamma_8\to\begin{cases}\psi_{3/2}^{3/2}=\frac{1}{\sqrt{2}}(X+iY)\alpha,\quad \psi_{1/2}^{3/2}=\frac{i}{\sqrt{6}}\left[\left(X+iY\right)\beta-2Z\alpha\right],\\ \psi_{-1/2}^{3/2}=\frac{1}{\sqrt{6}}\left[\left(X-iY\right)\alpha+2Z\beta\right],\quad \psi_{-3/2}^{3/2}=\frac{i}{\sqrt{2}}\left(X-iY\right)\beta,\end{cases}$$

Where $S=\begin{Vmatrix}\psi_1\\ \psi_2\end{Vmatrix}-$ is the electron spinor of the free zone; α,β -th spin matrix functions: $\alpha=\begin{Vmatrix}1\\0\end{Vmatrix}$, $\beta=\begin{Vmatrix}0\\1\end{Vmatrix}$, $\alpha\alpha^*=\beta\beta^*=1$; $X,Y,Z-$ Blokh functions $U_n(\vec{k}=\vec{0})$ at the point Γ of the Brillouin zone, transforming under operations of the cubic group as x,y,z respectively.

The Hamiltonians of the interaction of a free electron and a bound hole on an acceptor with an external magnetic field of strength $\vec{H}$ in the linear approximation are described by the following matrices [4]

$$\hat{\mathrm{H}}^{(c)}=\frac{1}{2}g_e\mu_0(\hat{\vec{\sigma}}\vec{H}),\qquad (2a)$$

$$\hat{\mathrm{H}}^{(a)}=\mu_0\sum_i(g_1\hat{J}_i+g_2\hat{J}_i^3)H_i,\ (i=x,y,z).\qquad (2b)$$

Here $\hat{\sigma}_i-$Pauli 2x2 matrices; $\hat{J}_i-$Luttinger and Kohn matrices of order 4x4 (see [4], Table 26.3); $g_1,\ g_2-$constants of the Zeeman splitting of the acceptor level in the ground state, which determines the g_h-factor of holes at these levels. They are expressed in terms of (both paramagnetic and diamagnetic constants) the valence band parameters k,q and A,B,D [4]. Potentials (2) are considered as small perturbations of the first order concerning the potentials of intercrystalline interactions (in particular,

$$\Delta E_{ij}^{(a)}\approx g_1\mu_0H<<E_0^{(a)}=\frac{m_0e^4}{2\varepsilon^2\hbar^2}\cdot\frac{m^*}{m_0}=R\frac{m^*}{\varepsilon^2m_0};$$

where $\Delta E_{ij}^{(a)}$ is the splitting energy between i- and j-sublevels; $E_0^{(a)}$ is the energy of the ground state of the ionized acceptor; $R=13,607\,eV$ is the Rydberg energy; $m_0=9,1\cdot10^{-31}kg$ is the mass of a free electron, and m^* is its effective mass in the acceptor state, ε is the static dielectric constant, $\hbar=1,054\cdot10^{-34}J\cdot c$ is the Planck constant). As a result of these perturbations, the degeneracies in the states of a free electron (2-fold) and an acceptor (4-fold) are completely removed. The correct wave functions of these states in the zeroth approximation of the perturbation theory are determined, respectively, by the relations

$$\Psi_M^{(c)}=\sum_m C_m^{(M)}\psi_m^{1/2}\quad\left(m=\pm\frac{1}{2},M=\pm1\right),$$

$$\Psi_N^{(a)}=\sum_n C_n^{(N)}\psi_n^{3/2}\quad\left(n=\pm\frac{3}{2},\pm\frac{1}{2};\ N=1,2,3,4\right).$$

Expansion coefficients (over complete sets of orthonormal functions $\psi_n^{3/2}$) $C_m^{(M)}$, $C_n^{(N)}$ (they are column matrices of the order of 2:1, 4:1, respectively) and the values of split energy sublevels $E_M^{(c)}$, $E_N^{(a)}$ (in electronic language, but in fact for bound holes $\xi_N^{(a)}=-E_N^{(a)}$) are found from the following matrix equations

$$\left\|\hat{\mathrm{H}}^{(c)}-E_M^{(c)}\hat{I}'\right\|\cdot\left\|\hat{C}^{(M)}\right\|=0,\qquad (3a)$$

$$\left\|\hat{\mathrm{H}}^{(a)}-E_N^{(a)}\hat{I}\right\|\cdot\left\|\hat{C}^{(N)}\right\|=0,\qquad (3b)$$

where $\hat{I}'$ and $\hat{I}-$ are identity matrices of order 2x2 and 4x4.

The compatibility condition for the system of linear algebraic equations (3a) (where the unknowns are $C_m^{(M)}$), as well as (3b) lead to secular equations

$$\left|\hat{\mathrm{H}}^{(c)}-E_M^{(c)}\hat{I}'\right|=0,$$

$$\left|\hat{\mathrm{H}}^{(a)}-E_N^{(a)}\hat{I}\right|=0.$$

The first of them, taking into account (2a), allows us to find the energies of the Zeeman splitting of spin energy subbands for electrons at the bottom of the conduction band

$$E_M^{(c)}=\frac{1}{2}Mg_e\mu_0H\qquad (E_m^{(c)}=mg_e\mu_0H),\ (4a)$$

and from the second, taking into account (2b), we find the expressions for the energy of acceptor sublevels $E_N^{(a)}$

$$E_{1,4}^{(a)} = \pm g_1\mu_0 H\sqrt{\frac{1}{8}\left[9(1+\frac{9}{4}\frac{g_2}{g_1})^2+(1+\frac{1}{4}\frac{g_2}{g_1})^2\right]+(1+\frac{7}{4}\frac{g_2}{g_1})\sqrt{(1+\frac{13}{4}\frac{g_2}{g_1})^2-\frac{9}{4}\frac{g_2}{g_1}(1+\frac{5}{2}\frac{g_2}{g_1})\gamma}}\ , \quad (4b)$$

$$E_{2,3}^{(a)} = \pm g_1\mu_0 H\sqrt{\frac{1}{8}\left[9(1+\frac{9}{4}\frac{g_2}{g_1})^2+(1+\frac{1}{4}\frac{g_2}{g_1})^2\right]-(1+\frac{7}{4}\frac{g_2}{g_1})\sqrt{(1+\frac{13}{4}\frac{g_2}{g_1})^2-\frac{9}{4}\frac{g_2}{g_1}(1+\frac{5}{2}\frac{g_2}{g_1})\gamma}}\ ,$$

где $$\gamma = 4(h_x^2h_y^2 + h_y^2h_z^2 + h_z^2h_x^2) = \sin^2 2\theta + \sin^4\theta\sin^2 2\varphi \qquad (5)$$

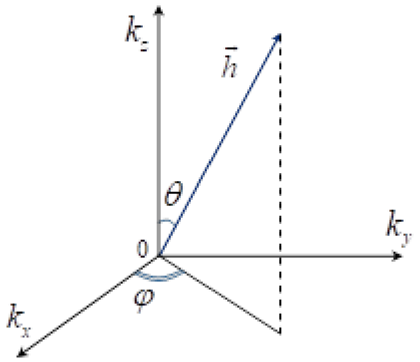

Fig.1. The geometry of the direction of the magnetic field vector.

– anisotropy factor, polar θ and azimuthal φ angles determine the direction of the unit vector $\vec{h} = \vec{H}/H$ along the magnetic field in the wave vector space (Brillouin zones, Fig.1).

The discussion of the results

In the general case, the Zeeman splitting for the acceptor level, as can be seen from formulas (4b), has a complex dependence on g_1, and g_2 and is anisotropic due to the factor γ at nonzero values of the constant g_2. If $g_2 = 0$, then there is no anisotropy and we have only an isotropic splitting with double degenerations $E_{1,4}^{(a)} = \pm\frac{3}{2}g_1\mu_0 H$, $E_{2,3}^{(a)} = \pm\frac{1}{2}g_1\mu_0 H$. A similar situation also occurs for the values $g_2/g_1 = -4/7$ ($E_{1,2}^{(a)} = \frac{3}{7}g_1\mu_0 H$, $E_{3,4}^{(a)} = -\frac{3}{7}g_1\mu_0 H$) and $g_2/g_1 = -2/5$ ($E_{1,4}^{(a)} = \pm\frac{9}{20}g_1\mu_0 H$, $E_{2,3}^{(a)} = \pm\frac{3}{20}g_1\mu_0 H$). At γ=0 (for example, θ=0, i.e. $\vec{H}\parallel OZ \parallel [001]$) from (4b) it can be seen that the structure of levels $E_i^{(a)}$ exactly coincides for two values of g_2/g_1 equal to -4/7 and -4/13: $E_{1,2}^{(a)} = \frac{39}{8}g_1\mu_0 H$, $E_{3,4}^{(a)} = -\frac{39}{8}g_1\mu_0 H$. Such characteristic features of the Zeeman splitting of the acceptor level in cubic crystals of the type $A^{III}B^{V}$ are clearly illustrated in Figures 2-4.

Impact Factor:

ISRA (India)	= **6.317**	**SIS** (USA)	= **0.912**	**ICV** (Poland)	= **6.630**
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GIF (Australia)	= **0.564**	**ESJI** (KZ)	= **8.771**	**IBI** (India)	= **4.260**
JIF	= **1.500**	**SJIF** (Morocco)	= **7.184**	**OAJI** (USA)	= **0.350**

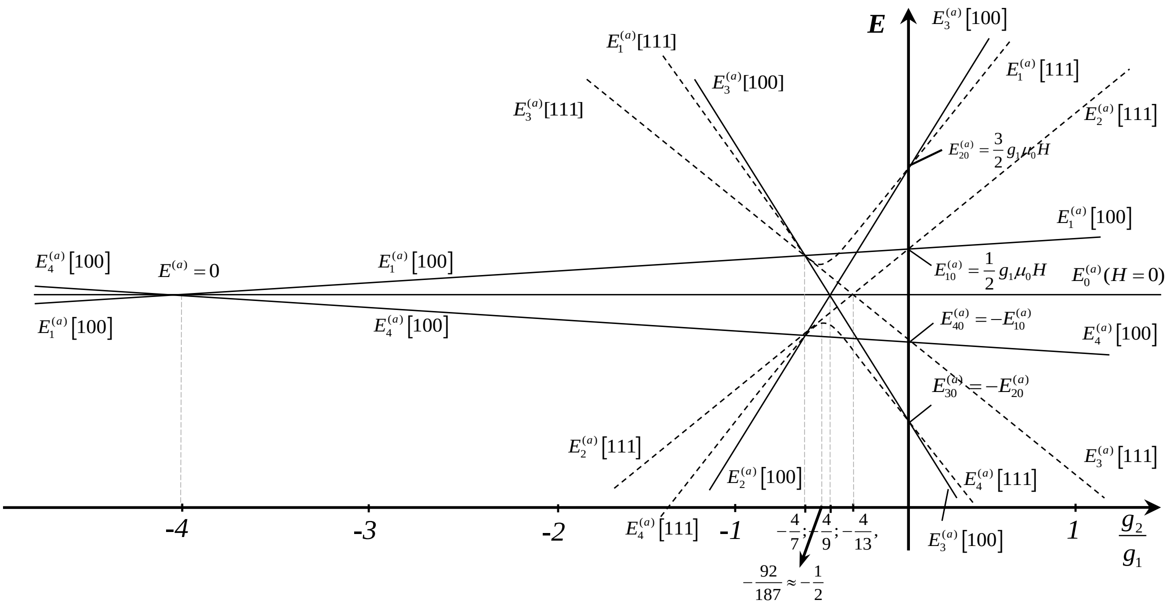

Fig. 2. Zeeman splitting of the energy level of the ground state of a shallow acceptor of a GaAs crystal as a function of the value of the parameter g_2 / g_1 along the crystallographic directions [100]-solid lines and [111]-dotted lines.

On fig. 2 solid and dotted lines show dependence $E_i^{(a)} = E_i^{(a)}(g_2 / g_1)$ for crystallographic directions [100] and [111] respectively (when γ=0 and γ=4/3), constructed using formula (4. b). It can be seen that for the direction (100) the course of the straight lines $E_1^{(a)}$ and $E_4^{(a)}$, $E_2^{(a)}$ and $E_3^{(a)}$ in pairs qualitatively coincide: each pair intersects at an angle different from π/2 at one negative critical value q_2 / q_1 (equal to -4 and -4/9), where the Zeeman splitting for these pairs vanishes and then its sign is inverted.

Note that at a small distance from the critical point $q_2 / q_1 = -4/9$ on the left and right, the absolute value of the splitting between the Zeeman sublevels $E_1^{(a)}$ $E_4^{(a)}$ is significantly less than the value for the sublevels $E_2^{(a)}$ nd $E_3^{(a)}$, in the interval $-4/7 < q_2 / q_1 < -4/13$, the opposite relationship is observed, i.e. $\left| \Delta E_{14}^{(a)} / \Delta E_{23}^{(a)} \right| > 1$. However, such a picture of the Zeeman splitting depending on the parameter q_2 / q_1 is somewhat violated for the [111] direction.

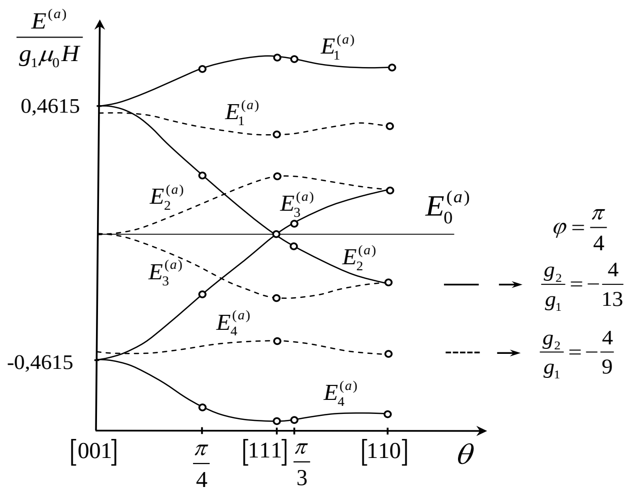

Fig. 3. Angular dependence of the splitting energy of acceptor sublevels $E_i^{(a)}$ in a magnetic field for two values of g_2 / g_1 .

Firstly, although the character of the straight line, the course of the lines $E_2^{(a)}(q_2/q_1)$ and $E_3^{(a)}(q_2/q_1)$ is qualitatively preserved, however, the critical point for them is shifted by the value $q_2/q_1=-4/13$ and the slope coefficients are slightly reduced. Secondly, the course of the lines $E_1^{(a)}(q_2/q_1)$ and $E_4^{(a)}(q_2/q_1)$ is qualitatively rearranged: these lines are anticrossed at the critical point $q_2/q_1=-92/187$, where the lines are repulsed and a "forbidden energy band" with a width of, proportional to H, in the middle of which corresponds the value of the initial energy level of the accetor $E_0^{(a)}(H=0)$. Lines $E_1^{(a)}(q_2/q_1)$ and $E_4^{(a)}(q_2/q_1)$ on the plane (q_2/q_1, E) have two axes of symmetry: the horizontal axis coincides with the position of the acceptor level at H=0, and the vertical axis passes through the minimum and maximum of the lines $E_1^{(a)}(q_2/q_1)$ and $E_4^{(a)}(q_2/q_1)$.

Figure 2 highlights the region (-4/7, -4/13) of q_2/q_1 values, where a relatively complex pattern of $E_i^{(a)}=E_i^{(a)}(g_2/g_1)$ lines is observed - the entanglement of the split sublevels of the ground state of the acceptor. In this regard, in Fig. Figure 3 separately demonstrates the anisotropy $E_i^{(a)}=E_i^{(a)}(\theta)$ for fixed values of $g_2/g_1=-4/9,\ -4/13$ lying in the indicated region. It can be seen that the sublevels $E_2^{(a)}(\theta)$ and $E_3^{(a)}(\theta)$ at $g_2/g_1=-4/13$ exhibit the greatest anisotropy, while in other cases we see a flatter dependence on θ for all levels with extrema in the [111] direction, with the maximum splitting energy $\Delta E_{14}^{(a)}$ is observed between sublevels $E_1^{(a)}(\theta)$ and $E_4^{(a)}(\theta)$ for $g_2/g_1=-4/13$ along the [111] direction, and at the same time $\Delta E_{23}^{(a)}=0$. Except for a small neighborhood of the value θ=0, the above inequality $\left|\Delta E_{14}^{(a)}/\Delta E_{23}^{(a)}\right|>1$ is strictly fulfilled for the remaining values of θ inclusive up to θ=π/2.

Figure 4 clearly demonstrates the location of the magnetic sublevels of a shallow acceptor along the energy axis for some values of the parameter g_2/g_1 and at a fixed H, where the above-mentioned main features of the splitting dynamics are clearly seen.

Note that magneto-optical phenomena in semiconductor nanostructures have been intensively studied lately (see, for example, [10–13]) and further it makes sense to develop the problem considered above for such materials.

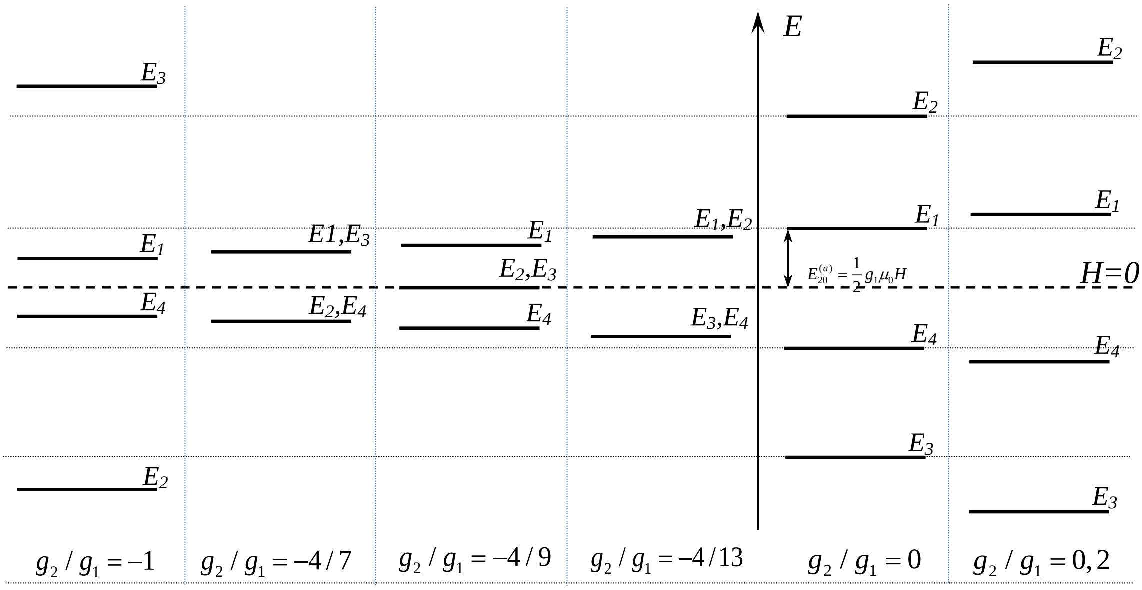

Fig.4. Dynamics of the Zeeman splitting of a 4-fold degenerate level of a shallow crystal acceptor $A^{III}B^{V}$ in the crystallographic direction [100] depending on the value of the parameter g_2/g_1 and at a fixed H.

Conclusion

In conclusion, we note once again that if in crystals of the GaAs type for an acceptor impurity in a quantum state with a total mechanical moment $L = 3/2\hbar$ the value of g_2 / g_1 is close to "special" values, like $-4/13$ and $-4/7$, or falls into the transition region $[-4/7, -4/13]$, then it is necessary to carefully monitor the course of each magnetic sublevel of the acceptor $E_i^{(a)}$. It is for such values of g_2 / g_1 that pairwise merging or complex entanglement of sublevels and a strong anisotropy of the Zeeman splitting are observed. This, in turn, leads to a strong anisotropy of the recombination radiation between the conduction band and the acceptor level in a "strong" magnetic field at $g_2 \neq 0$, to which a separate article will be devoted.

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