MAGNETO-OPTICS OF MULTI-WELL QUANTUM STRUCTURES WITH $D_2^-$-CENTRES

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The problem of electron binding states in field of two $D^0$ – centres in semiconductive quantum well (QW) in the presence of an external longitudinal magnetic field (along the QW growth axis) is studied within the framework of zero-range potential model. It is found that the magnetic field leads to a considerable change in positions of $g$ - and $u$-terms, and to a stabilization of the $D_2^-$-states in QW. It is shown that a form of impurity magneto-optical absorption spectrum essentially depends on the light polarization direction and on the spatial configuration of the $D_2^-$ molecular ion in QW.
1. Introduction

As it has been experimentally shown [1], reactions of the type $D^0 + e \rightarrow D^{-}$ are possible in low-dimensional systems under certain conditions. As the result of such reactions, neutral small donors bind an additional electron with the population formation of the so called “$D^{-}$-states”. Such states, which are confined by the structure potential, open new possibilities to study correlation effects in low-dimensional systems [1].

In the present paper we consider the following specific case: $D^0$-positions can not all be effectively filled by an electron transfer through a barrier [2]. In this case, a formation of the negative molecular ion $D_2^-$ is possible; this depends on the distance $R$ between the $D^0$-centers. It should be noted that the system consisting of a weakly bounded electron in the field of two equivalent potential centers appears in alkaline-halloids crystals [3]. This is the so called “dyeing center” $M^-$, which is electron in the field of neutral $M$-center (two neighbor $F$-centers). As it is known [4, 5], $D^-$-center is a simplest system, which can be simulated by an electron in the field of the zero-range potential. Earlier we have shown [6, 7] that the zero-range potential method allows to obtain analytical solution to the wave function and the binding energy of electron, which is localized on $D^0$-center. This method allows also to investigate the impurity magneto-optical absorption in nanostructures with a parabolic confinement potential.

The negative molecular ion $D_2^-$ simulation and investigation of its magneto-optical properties in QW are of much interest. Since $D_2^-$-system is symmetric with respect to the center, electron states (at fixed distance $R$ between $D^0$-centers) should be either symmetric ($g$-terms) or anti-symmetric ($u$-terms). Evidently, splitting of the $g$- and $u$-terms (which are degenerated at large $R$) is determined by the value of $R$ and by the QW-parameters (as a consequence of the
dimensional reduction). On the other hand, magnetic field (which is applied along the QW growth axis) plays the role of a variable parameter, which can change the system’s geometric confinement and, hence, to control energies of optical transitions. This gives some perspectives to develop molecular electronics, particularly, one-molecule devices with controllable characteristics.

The aim of this work is to investigate magneto-optical spectrum of QW within the framework of the zero-potential model. Structure of the spectrum is related to electron optical transitions from \( g \)-term state to QW hybrid-quantized states, depending on the light polarization direction and on the spatial configuration of the \( D_2^- \)-molecular ion.

2. \( D_2^- \)-molecular ion terms

To describe QW one-electron states one can use the parabolic confinement potential of the form

\[
U(z) = \frac{m^* \omega_b^2 z^2}{2},
\]

where \( m^* \) is the electron effective mass, \( |z| \leq \frac{L}{2} \), \( L \) is the width of QW, \( \omega_b \) is the confinement potential characteristic frequency of QW.

For one-electron states (which are undisturbed by impurities) under the longitudinal magnetic field \( \vec{B}(0,0,\vec{B}) \), Hamiltonian of the model is of the following form:

\[
\hat{\mathcal{H}} = -\frac{\pi^2}{2m^*} \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right) + \frac{\omega_b}{2} \hat{M}_z + \frac{m^* \omega_b^2 \rho^2}{8} + \hat{\mathcal{H}},
\]

where \( \omega_b = |\vec{e}|B/m^* \) is the cyclotron frequency, \( \hat{M}_z = -it\partial/\partial \varphi \) is the operator of orbital angular momentum projection on the \( z \)-axis;
\[ \hat{H}_z = -\left(\hbar^2 / 2m^*\right) \frac{\partial}{\partial z^2} + m^* \omega_0^2 z^2 / 2. \]

Double-center potential \( V_\alpha(\varrho, \varphi, z; \varrho_{a_1}, \varphi_{a_1}, z_{a_1}; \varrho_{a_2}, \varphi_{a_2}, z_{a_2}) \) is modeled by the superposition of the zero-range potentials with intensity \( \gamma_i = 2\pi \gamma_i / (\alpha_i m^*) \) (\( i = 1, 2 \)):

\[
V_\alpha(\varrho, \varphi, z; \varrho_{a_1}, \varphi_{a_1}, z_{a_1}; \varrho_{a_2}, \varphi_{a_2}, z_{a_2}) = \sum_{i=1}^{2} \gamma_i \frac{\delta(\varrho - \varrho_{a_i}) \delta(\varphi - \varphi_{a_i}) \delta(z - z_{a_i}) \times}{\varrho} \left[ 1 + \left( \varrho - \varrho_{a_i} \right) \frac{\partial}{\partial \varrho} + \left( z - z_{a_i} \right) \frac{\partial}{\partial z} \right] \varrho, \tag{3}
\]

where \( \alpha_i \) is determined by the energy \( E_i = -\pi \alpha_i^2 / (2m^*) \) of electron localized states on the same \( D^- \)-centers in a bulk semiconductor.

The wave function \( \Psi_\lambda(\bar{r}; \bar{R}_{a_1}, \bar{R}_{a_2}) \) of the electron (\( \bar{R}_{a_i} = \varrho_{a_i}, \varphi_{a_i}, z_{a_i} \) is the impurity center coordinates), which is localized on \( D^- \)-centre, satisfying Lippman-Schwinger equation for the bound state, is a linear combination

\[
\Psi_\lambda(\bar{r}; \bar{R}_{a_1}, \bar{R}_{a_2}) = \sum_{i=1}^{2} \gamma_i c_i G(\bar{r}; \bar{R}_{a_i}; E_\lambda), \tag{4}
\]

where \( G(\bar{r}; \bar{R}_{a_i}; E_\lambda) \) is one-electron Green function corresponding to the source in point \( \bar{R}_{a_i} \) and to the energy \( E_\lambda = -\hbar^2 \lambda^2 / (2m^*) \) \( (E_\lambda \) is the electron binding energy in the field of \( D^0 \)-centers under longitudinal magnetic field (this energy is measured from the bottom of QW). From mathematical point of view, the double-center problem leads to finding of nontrivial solutions of the algebraic equations for \( c_i \) coefficients; this implies a transcendental equation for \( E_\lambda \). In the case when \( \gamma_1 = \gamma_2 = \gamma \), the latter equation is split in two equations, which determine the symmetric \( (g \)-term) and anti-symmetric \( (u \)-term) electron states. Accounting for the one-electron Green function for the case when the \( D^- \)-center axis is along the QW – growth axis \( \bar{R}_{a_1} (0,0,0) \) and \( \bar{R}_{a_2} (0,0,z_{a_2}) \), these equations become
where $\beta = L'/\left(4\sqrt{U_0^*}\right)$, $L = L/a_d$, $a_d$ is the effective Bohr radius, $U_0^* = U_0/E_d$, $U_0$ is the QW confinement potential amplitude; $E_d$ is the effective Bohr energy, $\eta_d^2 = |E_d|/E_d$, $\delta(t) = \exp(-\beta a_d^{-2}t)$, $a_d^2 = a_B/a_d$, $z_{a_d} = z_{a}/a_d$; upper sign in Eq. (5) corresponds to symmetric ($g$-term), and lower sign to anti-symmetrical ($u$-term) electron states.

In the case when $D_2^-$-center axis $(\bar{R}_n (0,0,0)$ and $\bar{R}_n (\rho_n, \varphi_n, 0))$ is transverse to the magnetic field direction, the corresponding equations can be written as

\[
-\frac{1}{2\sqrt{\pi}\eta_d} \int_0^\infty dt \exp\left(-\rho_n^2 \frac{1}{4a_n^2} t\right) \left[ 2^2 \beta a_n^{-2} \left(1 - e^{-2t}\right)^{1/2} \delta^{-1}(t) \sin^{-1}(\beta a_n^{-2} t) \right] \times
\]

where $\rho_{n} = \rho_{a_d}/a_d$.

Our numerical analysis for Eqs. (5) and (6) shows that the magnetic field leads to a considerable change in positions of the terms and to a stabilization of the QW $D_2^-$-states. With the transfer from Eq. (5) to Eq. (6) the role of spatial configuration for the QW
$D^-_2$-center becomes apparent: the closeness of QW boundaries for the configuration (5) leads to the energy levels break (cleavage), for degenerated $g$- and $u$-states.

3. Spectral dependence for the impurity magneto-optical absorption coefficient for the multi-well quantum structure

In this Section, we calculate the impurity magneto-optical absorption coefficient $K_B(\omega)$ for the semiconductive structure, which consists of the tunnelly non-binding QWs taking into account their width dispersion $u = L/\bar{L}$, where $\bar{L}$ is the mean value of the QW width. It is supposed that in every QW there is one $D^-_2$-centre, with two possible spatial configurations, which are described by Eqs. (5) and (6). In the general case, the light absorption coefficient $K_B(\omega)$ can be represented as

$$K_B(\omega) = \frac{2\pi}{\hbar I_0 E_c L_c S} \sum_{m \in n_{\min}, n_{\max}} \sum_{n=0}^{N} P[u^*] |M^{(j,k)}_{f,A}|^2 \beta^{\nu \nu'} \left[ \bar{B}(n + \frac{1}{2}) \right]^{-1}, \quad (7)$$

Where $M = [C_1]$ is even part of the number $C_1 = (X - \eta^-_B - \bar{B})^{-1} \cdot u_{\max}^{-1} (n_{\min} + 1/2)/(2a^+_B)^{-1/2}$; $n_{\min} = 0$ or $n_{\min} = 1$ depending on selection rules; $N = [C_2]$ is even part of the number $C_2 = (X - \eta^-_B - a^+_B (|m| + m + 1)) \beta u_{\max}^{-1/2}$; $N_1 = [C_3]$ is even part of the number $C_3 = (X - \eta^-_B - \bar{B})^{-1} \cdot u_{\max}^{-1} (n + 1/2)/(2a^+_B)^{-1} (|m| + m + 1)/2$; $X = \hbar \omega/E_c$ is the photon energy, in effective Bohr energy units; $I_0$ is the light intensity; $L_c$ is the mean value of structure period; $S$ is the area of QW in the plain, which is perpendicular to the growth axis; $u^* = (\bar{B})^{-1} (n + 1/2)(X - \eta^-_B - a^+_B (2n + |m| + m + 1))^{-1}$; $\beta^* = \bar{B} \cdot u^*$; $u_{\min}, u_{\max}$ are minimal and maximal dispersion values of $u$; $n_{\nu} = 0, 1, 2, \ldots$ is the ra-
dial quantum number corresponding to the Landau level; 
\( m = 0, \pm 1, \pm 2, \ldots \) is the magnetic quantum number; \( n = 0, 1, 2, \ldots \) is the oscillator quantum number; \( \mathcal{B} = \frac{\mathcal{E}}{4\sqrt{U_0}} \); \( P(u) \) is the distribution function for the QW width dispersion,

\[
P(u) = 2 \left[ \sqrt{\pi} (\Phi(u_{\text{max}}) - u_0) + \Phi(u_0 - u_{\text{min}}) \right] e^{-\left( u - u_0 \right)^2}, \tag{8}
\]

where \( \Phi(z) \) is the error function \([8]\); \( u_0 = (u_{\text{min}} + u_{\text{max}})/2 \).

The upper indices \( j, k \) in matrix element \( M_{j,k}^{(i,i)} \), which determines the oscillator force value for the dipole optical transition from \( g \)-state to the state of the QW quasi-discrete spectrum, denote the light polarization direction (with respect to the QW growth axis, \((j = s, t)\)) and the molecular ion \( D_2^+ \) spatial configuration, which is described by Eqs. \((5)\) and \((6)\), \( K_1 = (0,0,0 \text{ and } 0,0,z_{a_1}) \); \( K_2 = (0,0,0 \text{ and } \rho_{a_2}, \varphi_{a_2}, 0) \), correspondingly. For the optical transition with maximal oscillator force \((n_i = 0, m = 0, n = 0)\), the expression for \( M_{j,k}^{(i,i)} \) can be written as

\[
M_{j,k}^{(i,i)} = -2 \frac{5}{4} \pi^{\frac{5}{2}} i \lambda_0 \sqrt{\frac{\alpha^4}{\omega}} \beta \beta^2 a_\beta^{-1} a_\beta^{1} \left[ \left( \beta \eta_\beta^2 + \beta a_\beta^{-2} + \frac{1}{2} \right)^{-1} + \left( \beta \eta_\beta^2 + \beta a_\beta^{-2} + \frac{5}{2} \right)^{-1} \right] \times
\]

\[
\times 2 \pi \exp \left( \frac{z_{a_1}^2}{(2a_1^2)} \right) \left[ \left( \beta \eta_\beta^2 + \beta a_\beta^{-2} + \frac{1}{2} \right)^{-1} + \left( \beta \eta_\beta^2 + \beta a_\beta^{-2} + \frac{5}{2} \right) \left( 1 - 2 \left( \frac{z_{a_1}}{a_1} \right)^2 \right) \right] \right] \right] \right], \tag{9}
\]

\[
M_{j,k}^{(i,i)} = -2 \frac{1}{4} \pi^{\frac{1}{2}} i \lambda_0 \sqrt{\frac{\alpha^4}{\omega}} \beta \beta^2 a_\beta^{-1} a_\beta^{3} \left[ 1 + \exp \left( -\frac{z_{a_1}^2}{(2a_1^2)} \right) \right] \times
\]

\[
\times \left[ e^{-i\psi} \delta_{m,1} \left( \beta \eta_\beta^2 + \beta a_\beta^{-2} + \frac{1}{2} \right)^{-1} + e^{i\psi} \delta_{m,-1} \left( \beta \eta_\beta^2 + 3 \beta a_\beta^{-2} + \frac{1}{2} \right) \right], \tag{10}
\]

\[
M_{j,k}^{(i,k)} = 2 \frac{5}{4} \pi^{\frac{5}{2}} i \lambda_0 \sqrt{\frac{\alpha^4}{\omega}} \beta \beta^2 a_\beta^{-1} a_\beta^{2} \left[ \left( \beta \eta_\beta^2 + \beta a_\beta^{-2} + \frac{1}{2} \right)^{-1} + \left( \beta \eta_\beta^2 + \beta a_\beta^{-2} + \frac{5}{2} \right)^{-1} \right] +
\]

\[
\times \left[ e^{-i\psi} \delta_{m,1} \left( \beta \eta_\beta^2 + \beta a_\beta^{-2} + \frac{1}{2} \right)^{-1} + e^{i\psi} \delta_{m,-1} \left( \beta \eta_\beta^2 + 3 \beta a_\beta^{-2} + \frac{1}{2} \right) \right],
\]
\[ + \left( \frac{\rho_\alpha}{\sqrt{2}a_B^2} \right)^{\frac{\alpha}{2}} \exp \left\{ - \frac{\rho_\alpha^2}{\beta a_B^2} \left( \beta\eta_B^2 + \beta a_B^{-2} (\beta m + m + 1) + \frac{1}{2} \right) \right\} + \\
+ \left( \beta\eta_B^2 + \beta a_B^{-2} (\beta m + m + 1) + \frac{5}{2} \right) \right\}, \]

\[ M_f^{(\alpha, \delta)} = -2^{-\frac{1}{4}} \pi^{-\frac{1}{2}} i \lambda_0 \sqrt{\frac{\alpha}{\omega}} B \right) \beta^2 a_B^2 a_d^2 \chi i \alpha^2 \cdot \left| e^{-i\varphi} \delta_{m+1} \right( \beta\eta_B^2 + \beta a_B^{-2} + \frac{1}{2} \right) + \\
e^{-i\varphi} \delta_{m-1} \left( \beta\eta_B^2 + 3\beta a_B^{-2} + \frac{1}{2} \right)^{-1} + a_B^{-2} \left( \beta a_B^{-2} \right) \exp \left( - \frac{\rho_\alpha^2}{4a_B^2} \right) \cdot e^{-im\varphi} \left[ \Theta(m)(m) \right]^{\frac{1}{2} \times} \]

\times \left\{ m \left( \frac{\rho_\alpha^2}{2a_B^2} \right)^m e^{i\alpha - \varphi} \left( \rho_\alpha^2 \right)^{m-1} \left( \frac{\rho_\alpha^2}{2a_B^2} \left( \beta a_B^{-2} \right)^{-1} \right)^m + \rho_\alpha^2 \left( \beta a_B^{-2} \right)^{-1} \right\}, \]

where \( v_0 = \left( \beta\eta_B^2 + \frac{1}{2} \right)^{-1} \left( \beta a_B^{-2} \right) \); \( \lambda_0 \) is the local field coefficient; \( \alpha = |e|^2 / (4\pi\varepsilon_0\sqrt{\epsilon}c/h) \) is the fine structure constant which accounts for the static relative dielectric permeability \( \epsilon \); \( c \) is the speed of light in vacuum; \( \delta_{l, \alpha} \) is Kronecker symbol; \( \Theta(x) \) is Havside function;

\[ B_1 = \left( \frac{\beta a_B^{-2} a d}{\gamma^2 \beta^2} \right)^{1/2} \left( \sqrt{\pi} \sum_{l=0}^{\infty} \Gamma \left( \frac{d}{2} \right) G\Psi(d) \right) \left( \frac{4\Gamma \left( \frac{d+1}{2} \right) + \beta^2 a_B^{-2} \exp \left( - \frac{\rho_\alpha^2}{4a_B^2} \right) \right) \right] \times \\
\times \left( \frac{\beta a_B^{-2} a d}{\gamma^2 \beta^2} \right)^{1/2} G_2 \left( \frac{\beta a_B^{-2} a d}{\gamma^2 \beta^2} \right)^{1/2} \left( \frac{\rho_\alpha^2}{4a_B^2} \right) \right]^{1/2} \]

where \( G_2 (\alpha, \gamma, z) \) is the degenerate hypergeometric function of the second kind [8]; \( \Psi(x) \) is the logarithmic derivative of Euler gamma-function; \( d = \beta\eta_B^2 \); \( G \approx 0.916 \) is the Katalane constant [8]; \( \psi \) is the polar angle for the polarization unit vector \( \vec{e}_\alpha \) in the cylindrical system of reference.
Figures 1 (a, b) and 2 (a, b) show the spectral dependences $K^{(s,k)}_{\beta}(\omega)$, $K^{(z,k)}_{\beta}(\omega)$ and $K^{(r,k)}_{\beta}(\omega)$, $K^{(l,k)}_{\beta}(\omega)$, which are correspondingly calculated due to Eq. (7) for the multi-well quantum structure based on InSb. As seen from Figs. 1 and 2, the change of direction of the light polarization leads to a drastic modification of the profile of absorption spectral curve (compare (a) and (b) in Figs. 1 and 2). This is partially related with the change of selection rules for the magnetic quantum number. From a comparison of Figs. 1(a) and 2(a), and Figs. 1(b) and 2(b) one can observe an essential role of the spatial configuration for the QW $D_{2}^{−}$ molecular ion. Namely, one can see not only spatial curve profile, but also the absorption value too.

In summary, we have shown that the magneto-optical absorption anisotropy in multi-well quantum structure is related with not only the light polarization direction but also with the $D_{2}^{−}$-ion spatial configuration.
Fig. 1. The spectral dependence for the magneto-optical impurity absorption coefficient: (a) the transversal polarization case \( K_{B}^{(\mathbf{t},\mathbf{K}_t)}(\omega) \); (b) the longitudinal polarization case \( K_{B}^{(\mathbf{s},\mathbf{K}_s)}(\omega) \); \( |E_i| = 5.5 \cdot 10^{-2} \text{eV} \), \( \mathcal{L} = 71.6 \text{nm} \), \( U_0 = 0.2 \text{eV} \), \( z_{a_2}^* = 0.25 \), \( B = 5 \text{T} \), \( \mathbf{R}_{a_1} = (0,0,0) \), \( \mathbf{R}_{a_2} = (0,0,z_{a_2}) \).
Fig. 2. The spectral dependence for the magneto-optical impurity absorption coefficient: (a) the transversal polarization case \( K_{B}^{(s,K_{2})}(\omega) \); (b) the longitudinal polarization case \( K_{B}^{(t,K_{2})}(\omega) \); \(|E_{i}| = 5.5 \times 10^{-2} \text{ eV}, L = 71.6 \text{ nm}, U_0 = 0.2 \text{ eV}, \rho_{\nu_{s}} = 0.25, B = 5 \text{ T}, \vec{R}_{\nu} = (0,0,0), \vec{R}_{\nu_{s}} = (\rho_{\nu_{s}}, \varphi_{\nu_{s}}, 0)\).
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