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Polaronic effects on the energy levels of a double donor impurity in quantum wells in the presence of a magnetic field

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Abstract. In the presence of a magnetic field the Hamiltonian of the single or double polaron bound to a helium-type donor impurity in semiconductor quantum wells (QWs) are given in the case of positively charged donor center and neutral donor center. The couplings of an electron and the impurity with various phonon modes are considered. The binding energy of the single and double bound polaron in $Al_{x_l}Ga_{1-x_l}As/GaAs/Al_{x_r}Ga_{1-x_r}As$ QWs are calculated. The results show that for a thin well the cumulative effects of the electron-phonon coupling and the impurity-phonon coupling can contribute appreciably to the binding energy in the case of ionized donor. In the case of neutral donor the contribution of polaronic effects are not very important, however the magnetic field significantly modifies the binding energy of the double donor. The comparison between the binding energies in the case of the impurity placed at the quantum well center and at the quantum well edge is also given.

PACS. 71.38.+i Polarons and electron-phonon interactions – 63.20.Kr Phonon-electron and phonon-phonon interactions

1 Introduction

The ionized impurities play an important role in transport mechanisms at low temperatures in semiconductor physics. A detailed study of shallow impurities in QWs will provide useful information about their energy levels as well as the properties of the QWs themselves. Hence it is necessary to study the behavior of a bound polaron (an electron bound to an impurity center) in polar semiconductor QWs [1–3]. Although much of the attention is focused on hydrogenic impurities, the study of the state of a two-electron impurity center (double donor state) in QWs is of considerable interest too [4,5]. The present work deals with the polaronic effects on the binding energy of a helium-type impurity in QWs in the presence of a magnetic field in the case of the impurity placed at the quantum well center and at the quantum well edge. The non-parabolicity of the conduction band is taking into account in our calculations.

2 Theory

Consider a QWs composed of three different polar crystals. Layers of the materials l, w, and r are located at $z < 0$, $0 \leq z \leq L$ and $z > L$, respectively. Let z axis perpendicular to the interfaces which are located at $z = 0$ and L. For a double donor impurity, the total Hamiltonian can be written as

$$H = \sum_{b=1}^{2}(H^{\mathrm{e}}_{(b)} + H^{\mathrm{c}}_{(b)} + H'_{(b)} + H^{\mathrm{B}}_{(b)}) + H_{\mathrm{ee}} + H_{\mathrm{ph}}, \quad (1)$$

with

$$H^{\mathrm{e}}_{(b)} = -\frac{\hbar^2}{2m_{\parallel}}\left[\frac{1}{\rho_b}\frac{\partial}{\partial\rho_b}(\rho_b\frac{\partial}{\partial\rho_b}) + \frac{1}{\rho_b^2}\frac{\partial^2}{\partial\varphi_b^2}\right] - \frac{\hbar^2}{2}\frac{\mathrm{d}}{\mathrm{d}z_b}(\frac{1}{m(z_b)})\frac{\mathrm{d}}{\mathrm{d}z_b} + V(z_b), \quad (2)$$

where $H^{\mathrm{e}}_{(b)}$ is the energy operator of a bare electron (b) which is confined to the potential well $V(z)$. $V(z) = V_l$, for $z < 0$; $V(z) = V_w = 0$, for $0 \leq z \leq L$; $V(z) = V_r$, for $z > L$; and

$$H^{\mathrm{c}}_{(b)} = -\frac{2e^2}{4\pi\varepsilon_{\mathrm{f}}\epsilon_\infty r'}. \quad (3)$$

$H'_{(b)}$ corresponds to the Coulomb term between electron (b) and the impurity center which is localized at $(0, 0, z_{\mathrm{d}})$, ε_{f} is the permittivity of free space, ϵ_∞ is the high-frequency dielectric constant and

$$r'_b = \sqrt{\rho_b^2 + (z_b - z_{\mathrm{d}})^2}, \quad (4)$$

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$$H'_{(b)} = \sum_{\nu j\mathbf{k}_\parallel}\{[\Gamma_{\nu jk_\parallel}(z_b)\mathrm{e}^{\mathrm{i}\mathbf{k}_\parallel\cdot\rho_b} - \frac{1}{2}\Gamma^{(+)}_{\nu jk_\parallel}(z_\mathrm{d})\delta_{\nu w}]a_{\nu j\mathbf{k}_\parallel} + \mathrm{h.c.}\} + \sum_{i\mathbf{k}_\parallel}\{[\Gamma_{ik_\parallel}(z_b)\mathrm{e}^{\mathrm{i}\mathbf{k}_\parallel\cdot\rho_b} - \frac{1}{2}\Gamma^{(+)}_{ik_\parallel}(z_\mathrm{d})]a_{i\mathbf{k}_\parallel} + \mathrm{h.c.}\}. \quad (5)$$

$H'_{(b)}$ stands for the electron-phonon interaction as well as the interaction of the point positive charge of the impurity with the phonon field. The first series corresponds to the confined and half-space longitudinal optical (LO) phonons, the second to the interface phonons. The definition of $\Gamma_{\nu jk_\parallel}(z)$ is given as in reference [7]. It describes the intensity of the interaction between an electron and the confined phonons or the half-spaced LO phonons. $\Gamma_{ik_\parallel}(z)$ in equation (5) describes the intensity of the interaction between an electron and the interface phonons in QW and has been given in reference [6]. While $\Gamma^{(+)}(z_\mathrm{d})$ describes the intensity of the interaction between the impurity and the phonon fields. It can be obtained from Γ by replacing e in Γ with $2e$. The coefficient in front of $\Gamma^{(+)}$ comes from the double counting due to the sum of the series for (b).

H_ee is the electron-electron interaction term,

$$H_\mathrm{ee} = \frac{e^2}{4\pi\varepsilon_\mathrm{f}\epsilon_\infty|\mathbf{r}_1 - \mathbf{r}_2|}\cdot \quad (6)$$

The free-phonon Hamiltonian is

$$H_\mathrm{ph} = \sum_{\nu j\mathbf{k}_\parallel}\hbar\omega_{L\nu}a^+_{\nu j\mathbf{k}_\parallel}a_{\nu j\mathbf{k}_\parallel} + \sum_{i\mathbf{k}_\parallel}\hbar\omega_{i\mathbf{k}_\parallel}a^+_{i\mathbf{k}_\parallel}a_{i\mathbf{k}_\parallel}, \quad (7)$$

which includes the confined bulk-like LO, the half-space LO and the interface phonons; $\hbar\omega_{L\nu}$ is the bulk LO phonon energy in material $\nu(\nu = l, w, r)$; $\hbar\omega_{i\mathbf{k}_\parallel}$ is the interface phonon energy, and $m(z)$ is the electron effective mass [8]. Considering the subband nonparabolicity, m(z) is given by

$$m(z) = \begin{cases} m_l(E) = m_l[1 - (V_l - E)/E_{gl}], & z < 0, \\ m_w(E) = m_w[1 - (V_w - E)/E_{gw}], & 0 \le z < L, \\ m_r(E) = m_r[1 - (V_r - E)/E_{rw}], & z > L \end{cases}$$

where $E_{g\nu}(\nu = l, w, r)$ is the energy gap between the conduction and light-hole valence bands in the material ν, E is the electron energy level which can be obtained by solving the following subband energy equation (17), m_ν is the mass constant in the material ν. For simplicity, we assumed that $m_\parallel = m(z)$.

$$H^\mathrm{B}_{(b)} = \frac{e}{2m}\mathbf{B}\cdot\mathbf{L} + \frac{e^2}{2m}A^2_{(b)} \quad (8)$$

where the vector potential $\mathbf{A}$ is defined as $\mathbf{A} = \mathbf{B}\times\mathbf{r}/2$, $\mathbf{B}$ and $\mathbf{L}$ are the magnetic induction intensity and the angular momentum respectively.

By introducing the canonical transformations

$$a_{\nu j\mathbf{k}_\parallel} \longrightarrow a_{\nu j\mathbf{k}_\parallel} + \Gamma^*_{\nu jk_\parallel}(z_\mathrm{d})/(\hbar\omega_{L\nu}), \quad (\text{where} \quad \nu = w) \\ a_{i\mathbf{k}_\parallel} \longrightarrow a_{i\mathbf{k}_\parallel} + \Gamma^*_{ik_\parallel}(z_\mathrm{d})/(\hbar\omega_{ik_\parallel}), \quad (9)$$

and then ignoring the consequent infinite constant terms, which correspond to the infinite constant self-energy contributions, the Hamiltonian (1) is reduced to

$$H = \sum_{b=1}^{2}\left(H^\mathrm{e}_{(b)} + H^\mathrm{c}_{(b)} + H^{\mathrm{e-ph}}_{(b)} + \widetilde{H}_{(b)} + H^\mathrm{B}_{(b)}\right) + H_\mathrm{ee} + H_\mathrm{ph}, \quad (10)$$

where $H^\mathrm{e}_{(b)}$, $H^\mathrm{c}_{(b)}$, H_ee, H_ph, $H^\mathrm{B}_{(b)}$ have been defined as before, and

$$H^{\mathrm{e-ph}}_{(b)} = \sum_{\nu j\mathbf{k}_\parallel}[\Gamma_{\nu jk_\parallel}(z_b)\mathrm{e}^{\mathrm{i}\mathbf{k}_\parallel\cdot\rho_b}a_{\nu j\mathbf{k}_\parallel} + \mathrm{h.c.}] + \sum_{i\mathbf{k}_\parallel}[\Gamma_{ik_\parallel}(z_b)\mathrm{e}^{\mathrm{i}\mathbf{k}_\parallel\cdot\rho_b}a_{i\mathbf{k}_\parallel} + \mathrm{h.c.}], \quad (11)$$

$$\widetilde{H}_{(b)} = \sum_j \frac{e^2}{\pi\varepsilon_\mathrm{f}T_w}\left(\frac{1}{\epsilon_{\infty w}} - \frac{1}{\epsilon_{0w}}\right) \times K_0(\rho_b q^j_w)\sin(q^j_w z_b)\sin(q^j_w z_\mathrm{d}) + \sum_{i\mathbf{k}_\parallel}\frac{1}{\hbar\omega_{ik_\parallel}}\Gamma_{ik_\parallel}(z_b)\Gamma^{(+)*}_{ik_\parallel}(z_\mathrm{d})\cos(\mathbf{k}_\parallel\cdot\rho_b), \quad (12)$$

where K_0 is the Bessel function of imaginary argument.

If the double donor center binds a single electron, then it is positive charged; for this ionized donor the only modifications of Hamiltonians in the above equations are removing H_ee and all the summation sign $\sum_{b=1}^{2}$ and all the subscript b, and finally multiply the coefficients in front of $\Gamma^{(+)}$ by 2 in equation (12).

We introduce the following variational trial wave function ψ in the case of ionized donor:

$$|\psi\rangle = U\Phi(\rho, z)|0\rangle, \quad (13)$$

$$\Phi(\rho, z) = N\mathrm{e}^{-\mu\sqrt{\rho^2+z^2}}\phi(z), \quad (14)$$

where N is the normalization constant.

$$\phi(z) = \begin{cases} A_l\mathrm{e}^{k_l z}, & z < 0, \\ A_w\sin(k_w z) + A_l\cos(k_w z), & 0 \le z \le L, \\ \mathrm{e}^{-k_r z}, & z > L, \end{cases} \quad (15)$$

with $k_\nu \equiv [2m_\nu(E_1)(V_\nu - E_1)]^{1/2}/\hbar$, $(\nu = l, r)$; and $k_w \equiv [2m_w(E_1)E_1]^{1/2}/\hbar$, where E_1 is the ground state eigenvalue of the electron Hamiltonian H^e. A_l and A_w are defined as

$$A_l = \mathrm{e}^{-k_r b}/[f_{wl}\sin(k_w b) + \cos(k_w b)], \\ A_w = A_l f_{wl}. \quad (16)$$

The subband energy equation in our QW potential $V(z)$ is obtained to be

$$(f_{wr}f_{wl} - 1)\sin(k_w b) + (f_{wr} + f_{wl})\cos(k_w b) = 0, \quad (17)$$

where

$$f_{wr} \equiv \frac{m_w(E_1)k_r}{k_w m_r(E_1)}, \qquad f_{wl} \equiv \frac{m_w(E_1)k_l}{k_w m_l(E_1)}. \quad (18)$$

In equation (13), $|0\rangle$ is the phonon vacuum state, and the canonical transformation U is given by

$$\begin{aligned} &U = U_1 U_2, \\ &U_1 = \exp\{\sum_{\nu j \mathbf{k}_\parallel} [\gamma_{\nu j \mathbf{k}_\parallel}(\rho, z) a^+_{\nu j \mathbf{k}_\parallel} - \gamma^*_{\nu j \mathbf{k}_\parallel}(\rho, z) a_{\nu j \mathbf{k}_\parallel}]\}, \\ &U_2 = \exp\{\sum_{i \mathbf{k}_\parallel} [\gamma_{i \mathbf{k}_\parallel}(\rho) a^+_{i \mathbf{k}_\parallel} - \gamma^*_{i \mathbf{k}_\parallel}(\rho) a_{i \mathbf{k}_\parallel}]\}, \end{aligned} \tag{19}$$

with

$$\begin{aligned} &\gamma_{\nu j \mathbf{k}_\parallel}(\rho, z) = \alpha_{\nu j \mathbf{k}_\parallel} u(q^j_\nu, z) \mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel \cdot \rho}, \\ &\gamma_{i \mathbf{k}_\parallel}(\rho) = \beta_{i \mathbf{k}_\parallel} \mathrm{e}^{-\mathrm{i}\mathbf{k}_\parallel \cdot \rho}. \end{aligned} \tag{20}$$

In equation (19), there are three real variational parameters $\mu > 0$, $\alpha_{\nu j \mathbf{k}_\parallel}$ and $\beta_{i \mathbf{k}_\parallel}$ which will subsequently be determined by minimizing the energy of the system. Our approximation is particularly appropriate for a well width less than several effective Bohr radii (the effective Bohr radius is about 9.87 nm for GaAs). It covers the whole range of commonly used values of well width. Moreover, only in this range, can the polaronic effects including all phonon modes be important.

The binding energy in the case of ionized donor is obtained from

$$E_{\mathrm{B}}(\text{ionized}) = E_{\mathrm{sub}} + E_{\mathrm{L}} - \langle \psi \mid H_{\mathrm{ion}} \mid \psi \rangle_{\min}, \tag{21}$$

where E_{sub} is the lowest energy solution of equation (17); and

$$E_{\mathrm{L}} = \frac{eB\hbar}{2m}$$

is the ground-state Landau level, $\langle H_{\mathrm{ion}} \rangle_{\min}$ is the minimum of $\langle H_{\mathrm{ion}} \rangle$, the expectation value of the Hamiltonian of ionized donor system.

In the case of neutral donor center, the trial wave function of the double bound polaron is

$$|\Psi\rangle = \left(\prod_{b=1}^{2} U_{(b)} \Phi(\rho_b, z_b) \right) |0\rangle, \tag{22}$$

where $U_{(b)}$ and Φ are similar to those in the case of the single bound polaron.

The binding energy in the neutral donor case is obtained to be

$$\begin{aligned} E_{\mathrm{B}}(\text{neutral}) = E_{\mathrm{sub}} + E_{\mathrm{L}} - (&\langle \Psi \mid H_{\mathrm{neu}} \mid \Psi \rangle_{\min} \\ &- \langle \psi \mid H_{\mathrm{ion}} \mid \psi \rangle_{\min}), \end{aligned} \tag{23}$$

where the expectation value of the electron-electron interaction term is approximately evaluated as in reference [4]. We also treat the electron-electron interaction term as the only correlation term between these two electrons, *i.e.* we will disregard any other correlation of these two electrons *via* phonon field in our further approximate numerical evaluations.

3 Numerical results and discussion

As an example of the application of our theory we have calculated the binding energy of a single bound polaron and a double bound polaron for a helium-type impurity in $\mathrm{Al}_{x_l}\mathrm{Ga}_{1-x_l}\mathrm{As}/\mathrm{GaAs}/\mathrm{Al}_{x_r}\mathrm{Ga}_{1-x_r}\mathrm{As}$ symmetric QWs. The parameter $E_{\mathrm{g}\nu}$ is given as $E_{\mathrm{g}\nu} = 1424 + 1266x_\nu + 260x_\nu^2$ meV ($\nu = l, w, r$) and the other parameters are the same as in reference [6]. The minimization of $\langle H \rangle$ is carried out using the direct optimization techniques.

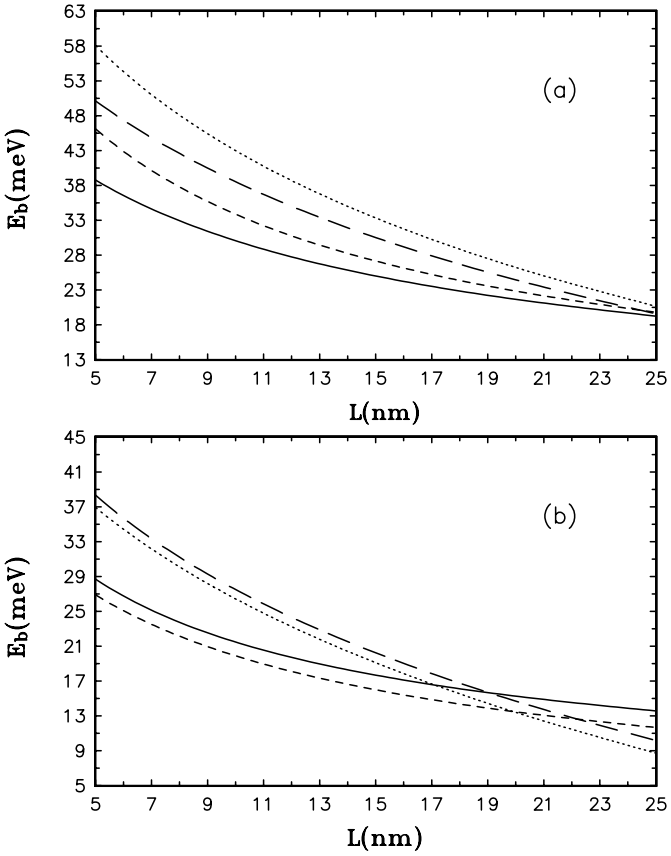

Fig. 1. Binding energy as a function of the well width L for $\mathrm{Al}_{0.3}\mathrm{Ga}_{0.7}\mathrm{As}/\mathrm{GaAs}/\mathrm{Al}_{0.3}\mathrm{Ga}_{0.7}\mathrm{As}$ symmetric single QWs: (a) for a single bound polaron in the case of ionized donor; (b) for the double bound polaron in the case of neutral donor. The solid line (for $B = 0$) and the long dashed line (for $B = 20$) correspond to the total binding energy including the interaction of the electron and impurity with phonons in the case of the donor impurity localized at the center of the well ($z_{\mathrm{d}} = L/2$). The dashed line (for $B = 0$) and the dot line (for $B = 20$) is obtained by neglecting the presence of phonons.

Figure 1 shows the binding energy E_{B} as a function of the well width L for $\mathrm{Al}_{0.3}\mathrm{Ga}_{0.7}\mathrm{As}/\mathrm{GaAs}/\mathrm{Al}_{0.3}\mathrm{Ga}_{0.7}\mathrm{As}$ symmetric QWs; Figure 1a is for the case of ionized donor and Figure 1b is for the case of neutral donor. Figure 1 indicates that in the case of ionized donor when the well width $L < 15$ nm, we should take into account the effect of the phonon field in order to get the correct value of the binding energy of the polaron. In the case of neutral donor, the polaronic effect is not very important, however, the magnetic field significantly modifies the binding energy of the double donor. Figure 1b shows that the magnetic field steepen the curves of binding energy for neutral donor. When the magnetic field intensity and well width

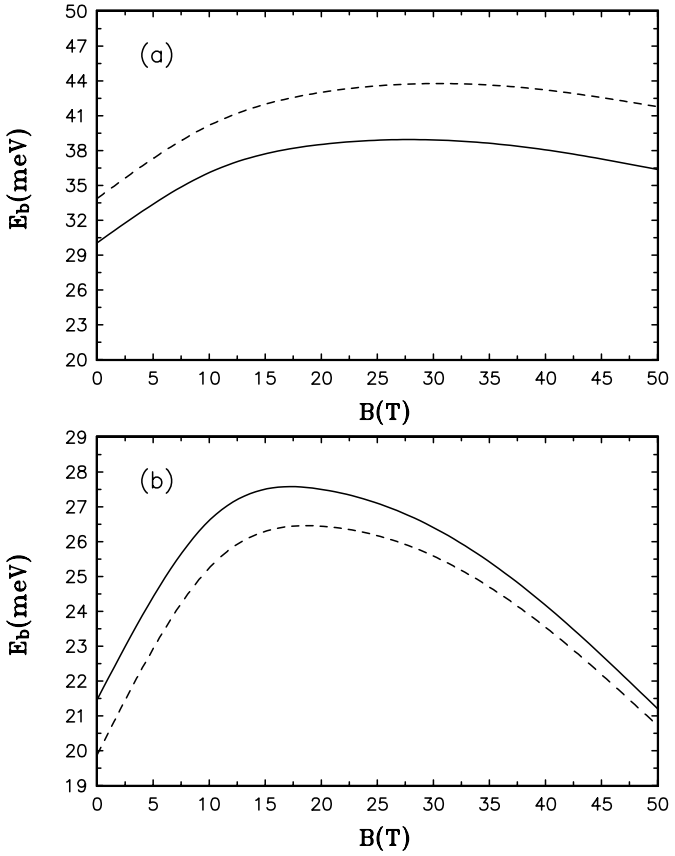

Fig. 2. Binding energy as a function of the magnetic field B for $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ symmetric single QWs: (a) for a single bound polaron in the case of ionized donor; (b) for the double bound polaron in the case of neutral donor. The solid line corresponds to total binding energy including the interaction of the electron and impurity with phonons in the case of the donor impurity localized at the center of the well ($z_d = L/2, L = 10$ nm). The dashed line is obtained by neglecting the presence of phonons.

are enough large, the binding energy of double donor will be very small. In this case the double donor easy loses one of its electrons and becomes ionized donor.

We can observe from Figure 2 that the polaronic effect for binding energy is also obvious in the case of ionized donor. In the case of neutral donor, the binding energy increases at first when the magnetic field B is increased, after B reaches a certain value, the binding energy will decrease when B is increased. When well width is 10 nm the contribution of the polaronic effect is less than 10% of the double donor binding energy for all the values of magnetic fields studied. It shows again that for large magnetic field the binding energy of double donor can be very small and the neutral donor is easy to ionized.

Another difference is the polaronic effect raise the binding energy in the ionized donor case and lower the binding energy in the neutral donor case.

In Table 1 the binding energy in two cases are listed when the position of impurity center located at (0,0,0) in $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ symmetric QW with

Table 1. Binding energy of single and double bound polaron in a QW.

B	E_b(single)/meV				E_b(double)/meV			
Tesla	$z_d = 0$		$z_d = 5$ nm		$z_d = 0$		$z_d = 5$ nm	
0	22.2	26.4[a]	30.1	33.8[a]	16.3	13.2[a]	21.5	19.9[a]
50	31.5	40.8[a]	36.4	41.8[a]	20.9	18.1[a]	21.2	20.7[a]

[a] Binding energy without phonon field.

fixed well width $b = 10$ nm. We can find that the binding energy when the impurity center is at the edge of the well is smaller than that when the impurity center is at the center of the well.

In summary, for a helium-type impurity in symmetric or asymmetric QWs in the presence of a magnetic field, the Hamiltonian of a single and double bound polarons is proposed, in which the interactions of the electron and the impurity with the phonon field are included. We have calculated the binding energy of the single and double bound polarons in QWs including all the polaronic contributions due to (i) electron-confined bulk-like LO phonon coupling, (ii) electron-half-space LO phonon coupling, (iii) electron-interfacial phonon coupling, as well as the coupling between the positive charge of impurity ion and the above various phonon modes. We have considered the impurity ion which is located at an arbitrary position in the well. In addition, the effects of the subband nonparabolicity and the finiteness of barrier height are all taken into account at the same time. In numerical calculation we find that the interaction between the point positive charge of impurity and the phonons has a significant contribution to the binding energy of the bound polarons in QWs. The cumulative polaronic effect is also significant in the case of ionized donor for thin well. When the magnetic field intensity is enough large and well width beyond a certain value, the neutral donor is easy to become an ionized donor by lose one of its electrons.

Analysis and numerical results presented here may be of interest for further theoretical investigation and device applications.

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