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Screening effect on polarizabilities of shallow donors and acceptors in infinite-barrier quantum wells

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Polarizabilities of shallow donors and acceptors in infinite-barrier $GaAs/Ga_{1-x}Al_xAs$ quantum wells have been calculated using the Hasse variational method within the effective mass approximation. The effect of spatially dependent screening on polarizabilities is taken into account with an r-dependent dielectric response. The effects of electric and magnetic fields are also presented.

1. Introduction

In the past few years, there had been considerable theoretical and experimental interest in the effect of confinement on shallow donor impurities in quantum well structures [1–3]. Bastard [4] was the first to treat this problem theoretically by considering a hydrogenic impurity in a quantum well with infinite-barrier height under the assumption of a parabolic conduction band.

In all of the above theoretical calculations, the Coulombic interaction energy has been scaled by a static dielectric constant ϵ_0. Csavinszky *et al.* [5] and Oliveira *et al.* [6] considered the dielectric response to the impurity in a quantum well of infinite depth with r-dependent dielectric function characteristic of bulk GaAs material.

The polarizability in low dimensional semiconducting systems, quantum well (QW), quantum well wire (QWW) and quantum Dot (QOD) have been calculated for shallow donors [7–12]. Recently, the effect of screening on the polarizability of shallow donors and acceptors in finite-barrier quantum wells has been studied [13].

In this work, the polarizabilities of shallow donors and acceptors in infinite-quantum wells have been calculated using Hasse variational method, where the spatially dependent screening effect on it is investigated, with different values of magnetic field. The effect of electric field on binding energy is also reported. Polarizability results for infinite and finite barrier quantum wells are compared.

In general, the calculation of polarizabilities of the acceptors in a quantum well is more complicated than that of the donors because of the more complex valence-band structure [14]. Therefore, a simple one-band model is used similar to that used for donors by [4,5,15] rather than the four valence-band model used in [14].

2. Theory

The Hamiltonian for a hydrogenic impurity located at the center of the well in the presence of weak applied electric field and magnetic field **B** in a single GaAs quantum well of infinite depth

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can be written, within the framework of an effective mass approximation, as

$$H=\frac{1}{2m^*}(\mathbf{P}+e\mathbf{A})^2-\frac{e^2}{\in(r)r}+V_B(z)+|e|\mathbf{F}\cdot\mathbf{z} \quad (1)$$

where curl $\mathbf{A}=\mathbf{B}$ is the magnetic field. Using the symmetric gauge $\mathbf{A}=(-B_y/2, B_x/2, 0)$, the Hamiltonian becomes

$$H=\frac{P^2}{2m^*}+\frac{1}{2}\hbar\omega_c L_z+\frac{1}{8}m^*\omega_c^2\rho^2-\frac{e^2}{\in(r)r}+V_B(z)+|e|\mathbf{F}\cdot\mathbf{z} \quad (2)$$

where $\omega_c=eB/m^*c$ is the cyclotron frequency and $\hbar L_z=(xP_y-yP_x)$.

The carrier effective mass and the GaAs spatially dependent screening are given by m^* and $\in(r)$ respectively. The spatially dependent dielectric screening used in the calculation is the one proposed by Hermanson [16].

$$\in^{-1}(r)=\in_0^{-1}+(1-\in_0^{-1})\exp(-r/\beta) \quad (3)$$

where $\in_0=13.1$ is the static dielectric constant, and $\beta=0.58$ Å is the characteristic value for the screening parameter, as assumed by Oliveira [6].

Introducing the effective Rydberg $Ry^*=m^*e^4/2\hbar^2\in^2$ as a unit of energy, and the effective Bohr radius $a_B^*=\hbar^2\in/m^*e^2$ as a unit of length, one obtains

$$H=-\nabla^2+\gamma L_z+\frac{1}{4}\gamma^2\rho^2-\frac{2}{r}[1+(\in_0-1)\exp(-r/\beta)]+V_B(z)+\eta z\ Ry^* \quad (4)$$

where $\eta=|e|a^*F$ is a measure of the electric field strength, and $\gamma=\hbar\omega_c/2\ Ry^*$. $V(z)$ in eqn (1) is the infinite-barrier potential which confines the carrier within the well of width L, is given by:

$$V(z)=\begin{cases}+\infty & |z|>L/2\\ 0, & |z|<L/2\end{cases} \quad (5)$$

The polarizability α is defined by:

$$E(B,\eta)=E(B,0)-\frac{1}{2}\alpha\eta^2, \quad (6)$$

i.e.

$$\alpha=2\lim_{\eta\to 0}\left[\frac{\mathrm{E}(B,0)-E(B,\eta)}{\eta^2}\right] \quad (7)$$

The trial wave function used in the Hasse variational method is

$$\Psi=\Psi_0(1+\lambda\hat{\varepsilon}\cdot\vec{r}) \quad (8)$$

where

$$\Psi_0=D\cos(\zeta z)\exp[-1/\mathbf{a}(\rho^2+z^2)^{1/2}] \quad (9)$$

with $\zeta=\pi/L$, and D is a normalization constant, where λ and $\mathbf{a}$ are used as variational parameters.

With the trial function eqn (8), the energy expectation for donors and acceptors becomes,

$$\langle E\rangle=\frac{T_1+T_3\lambda\eta+T_2\lambda^2}{N_1+N_2\lambda^2}, \quad (10)$$

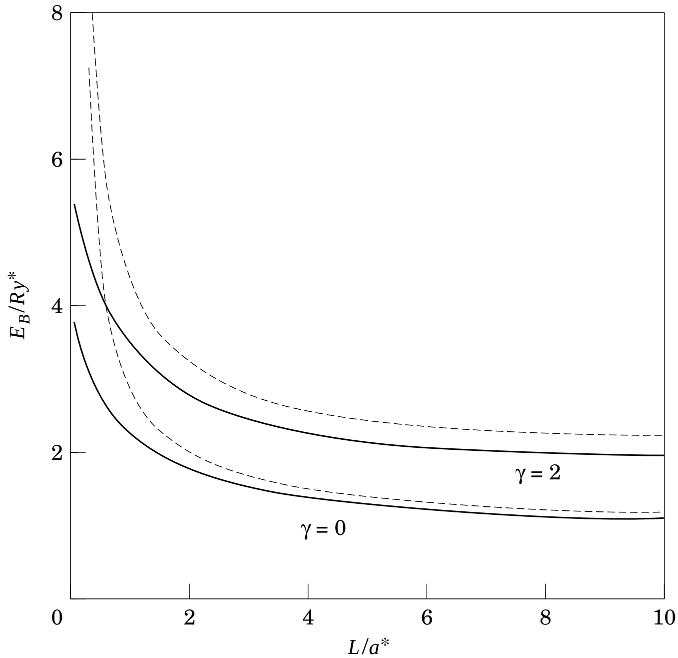

Fig. 1. Impurity binding energy E_B for acceptor as a function of well width L for $\gamma=0$ and $\gamma=2$. The dashed curve is for a spatially dependent $\in=\in(r)$; the solid curve is for constant $\in=\in_0$.

where

$$T_1=\langle\Psi_0|-\nabla^2+V_B(Z)-\frac{2}{r}[1+(\in_0-1)\exp(-r/\beta)]|\Psi_0\rangle, \tag{11}$$

$$T_2=\langle\hat{\varepsilon}\cdot\vec{r}\,\Psi_0|-\nabla^2+V_B(z)-\frac{2}{r}[1+(\in_0-1)\exp(-r/\beta)]|\hat{\varepsilon}\cdot\vec{r}\,\Psi_0\rangle, \tag{12}$$

$$T_3=\langle\hat{\varepsilon}\cdot\vec{r}\,\Psi_0|z|\Psi_0\rangle, \tag{13}$$

$$N_1=\langle\Psi_0|\Psi_0\rangle, \tag{14}$$

$$N_2=\langle\hat{\varepsilon}\cdot\vec{r}\,\Psi_0|\hat{\varepsilon}\cdot\vec{r}\,\Psi_0\rangle, \tag{15}$$

The value of λ that minimizes the energy expression $\langle E\rangle$ is obtained as:

$$\lambda=-\frac{N_2T_1-N_1T_2}{N_2T_3\eta}\left\{1-\sqrt{1+\frac{N_1N_2T_3^2\eta^2}{(N_2T_1-N_1T_2)^2}}\right\} \tag{16}$$

Substituting this value of λ into eqn (10), and expanding $\langle E\rangle$ binomially in powers of η, one gets for the polarizability,

$$\alpha=\frac{T_3^2}{2(N_2T_1-N_1T_2)}. \tag{17}$$

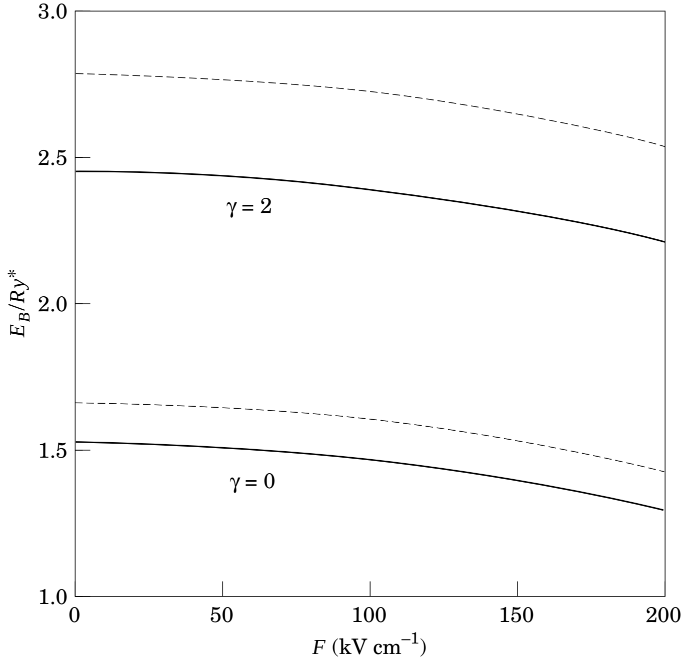

Fig. 2. Impurity binding energy E_B for acceptor as a function of electric field F for $\gamma = 0$ and $\gamma = 2$. The dashed curve is for a spatially dependent $\epsilon = \epsilon(r)$; the solid curve is for constant $\epsilon = \epsilon_0$.

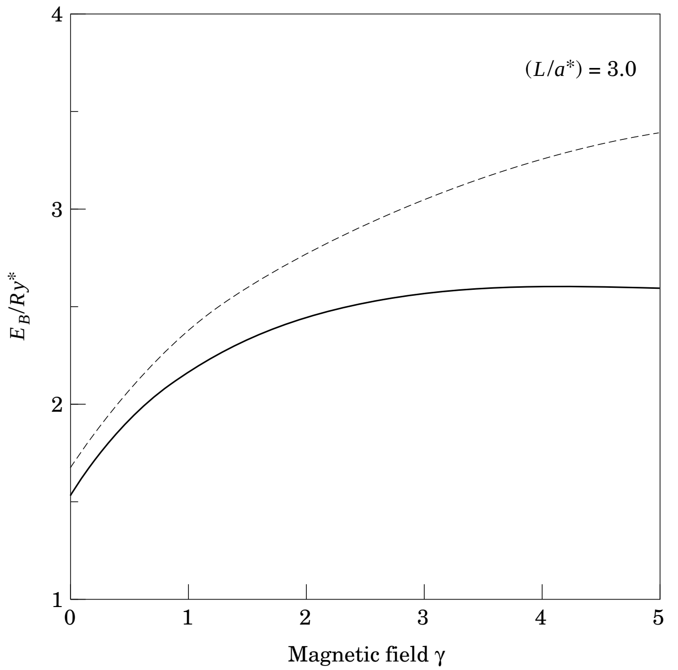

Fig. 3. Impurity binding energy E_B for acceptor as a function of magnetic field γ. The dashed curve is for a spatially dependent $\epsilon = \epsilon(r)$; the solid curve is for constant $\epsilon = \epsilon_0$.

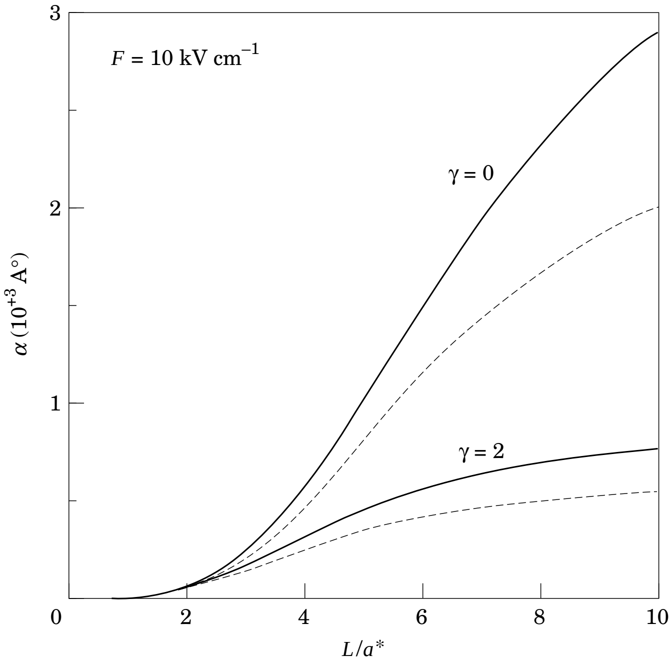

Fig. 4. Polarizability values α for acceptor as a function of well width L for $\gamma=0$ and $\gamma=2$. The dashed curve is for a spatially dependent $\epsilon=\epsilon(r)$; the solid curve is for constant $\epsilon=\epsilon_0$.

3. Results and conclusions

The results in reduced atomic units (a.u.*) are presented, which correspond to a length unit of an effective Bohr radius a^*, and an energy unit of an effective Rydberg Ry^*. For GaAs these units are $a^*=103.5$ Å and $Ry^*=5.31$ meV for donors (electrons), and $a^*=20.4$ Å and $Ry^*=26.9$ meV for acceptors (hole). The effective mass $m^*=0.067\,m_0$ and $m^*=0.34\,m_0$ for both donors (electrons) and acceptors (hole), respectively are used. The effect of electric field on the impurity binding energy $E_B=E_0-\langle H\rangle_{min}$ is used, by first calculating E_B variationally without the electric and magnetic field terms and with wavefunction eqn (8) taking $\lambda=0$, where $E_0=(\pi/L)^2$ is the subband energy for the ground state. In this calculation, **a** appearing in Ψ_0 is treated as a variational parameter. The calculation with full Ψ is repeated to calculate E_B including the electric field term. The impurity binding energy as a function of well width is shown in Fig. 1, for $\gamma=0$ and $\gamma=2$, where $\gamma=1$ corresponds to a magnetic field of 67.4 kG. The calculated binding energy E_B as a function of electric field F is shown in Fig. 2, for $\gamma=0$ and $\gamma=2$, taking into account the shift in subband energy ΔE_0 introduced by Bastard *et al.* [17], using the second-order perturbation theory approach. Figure 3 shows the binding energy as a function of magnetic field γ. Figs 1, 2 and 3 show that the binding energy increases as the magnetic field increases, as a result of increasing confinement, whereas Fig. 2 shows that the electric field reduces the binding energy effectively as a consequence of the displacement of the electronic charge with respect to the impurity position. As also seen from the figures, the effect of spatially dependent $\epsilon(r)$ dielectric function which, as opposed to a dielectric constant ϵ_0, leads to an increase in the binding energy of the impurity.

As a result, the effect of spatially dependent screening is negligible for shallow donors, because of the large (electron) effective Bohr radius ($a^*=103.5$ Å), whereas its effect is quite important for acceptors due to the relatively small (hole) effective Bohr radius ($a^*=20.4$ Å).

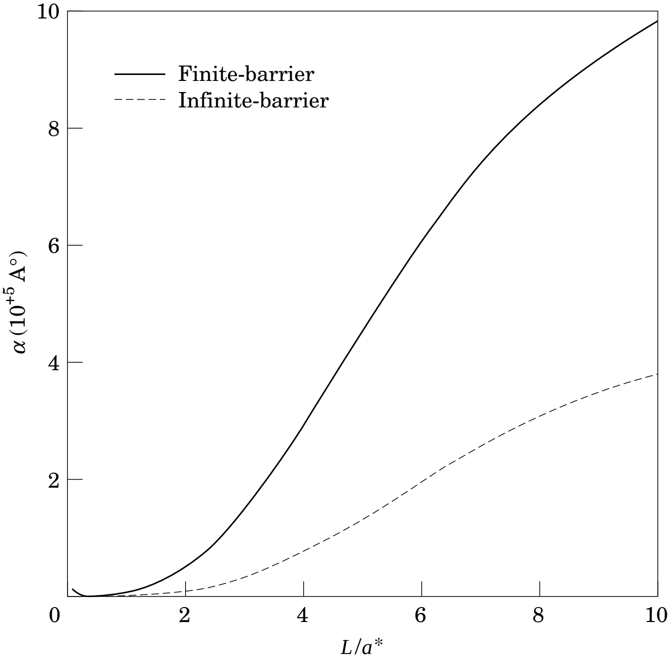

Fig. 5. Polarizability values α for donor as a function of well width L for finite and infinite barrier well.

In Fig. 4, the values of polarizability α for acceptor as a function of well width for $\gamma=0$ and $\gamma=2$, are presented. The calculated polarizability values have reasonable magnitudes and reflect correctly the effect of a magnetic field which confines the electron more and reduces the polarizability. The effect of spatially dependent screening function $\epsilon=\epsilon(r)$ on polarizability values (dashed curves) are clearly shown, which reduces the polarizability values.

The polarizability values for the finite- and infinite-barrier quantum wells, as a function of well width L are presented in Fig. 5, the confinement effect for the infinite case are clearly shown, which reduces the polarizability values as expected.

It should be noted that as the r-dependent dielectric function used in this paper possesses spherical symmetry, the neglected two-dimensional effect may have some important contributions to the binding energy of the screening impurity.

The best way to treat screening effects is through a first-principles calculation, which unfortunately lacks the simplicity of the present calculation.

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