Polarizabilities of shallow donors in finite-barrier quantum wells

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Polarizabilities of shallow donors in finite-barrier GaAs/$Al_xGa_{1-x}As$ quantum wells are calculated with use of the Hasse variational method within the effective-mass approximation. The magnetic field dependence of polarizabilities is also studied.

I. INTRODUCTION

In recent years, there has been considerable theoretical and experimental interest in shallow donors in GaAs/$Al_xGa_{1-x}As$ quantum-well (QW) structures.[1-8] Far-infrared magnetospectroscopy experiments have provided detailed results, for QW's with the magnetic field along the growth direction, which are in good agreement with variational calculations.[5-8] Good agreement is also obtained for low magnetic fields in the case of an applied magnetic field in the plane of the quantum wells.[9] To the best of our knowledge, the polarizabilities of shallow donors in QW's are not yet reported. The earlier calculations of polarizabilities concentrated on the rather complicated case of bulk Si, where complications arise mainly from the many-valley structure.[10,11] Recently, we have calculated the polarizabilities of shallow donors in infinite-barrier QW's.[12]

In this work, we extend the Hasse variational approach[13] to the case of impurities in finite-barrier QW's.

II. DONOR POLARIZABILITIES

In the presence of weak applied electric field and magnetic field along the z direction, which is taken to be the growth direction of the QW, the Hamiltonian for the donor electron becomes

$$H=-\nabla^2-\frac{2}{r}+\eta z+V_B(z)+\gamma L_z+\tfrac{1}{4}\gamma^2\rho^2 . \tag{1}$$

Here, we use the quantities $a^*=\hbar^2\kappa_0/m^*e^2$, $\mathcal{R}^*=m^*e^4/2\hbar^2\kappa_0^2$, and $\gamma=\hbar\omega_c/2\mathcal{R}^*$, with $\omega_c=eB/m^*c$ as the units of length, energy, and magnetic field, respectively, and κ_0 is the static dielectric constant of GaAs. $\gamma=1$ is the magnetic field at which the diamagnetic energy is equal in magnitude to the Coulomb energy.

The electric field term is $\eta z=|e|a^*Fz|\mathcal{R}^*$, where η is a measure of the electric field strength. $V_B(z)$ in Eq. (2) is the barrier potential which is taken to be finite:

$$V_B(z)=\begin{cases}0, & |z|<L/2\\ V_0, & |z|>L/2 .\end{cases} \tag{2}$$

The polarizability α is defined by

$$E(B,\eta)=E(B,0)-\tfrac{1}{2}\alpha\eta^2 \tag{3}$$

i.e.,

$$\alpha=2\lim_{\eta\to 0}\left[\frac{E(B,0)-E(B,\eta)}{\eta^2}\right] . \tag{4}$$

The trial wave function used in the Hasse variational method is

$$\Psi=\Psi_0(1+\lambda\hat{\varepsilon}\cdot\mathbf{r}) , \tag{5}$$

where

$$\Psi_0=\begin{cases}C\exp(kz)\exp[-1/a(\rho^2+z^2)^{1/2}], & |z|>L/2\\ B\cos(\zeta z)\exp[-1/a(\rho^2+z^2)^{1/2}], & |z|<L/2\end{cases} \tag{6}$$

with $\zeta=(2m^*E_0)^{1/2}/\hbar$ and $k=[2m^*(V_0-E_0)]^{1/2}/\hbar$. The constants B,C and the subband energy E_0 is found by matching at the boundaries the logarithmic derivatives of the wave function, which yields

$$\frac{C}{B}=\cos(\zeta L/2)\exp(kL/2) , \tag{7}$$

$$\left[\frac{E_0}{V_0}\right]^{1/2}=\cos\left[\left[\frac{m^*E_0}{2\hbar^2}\right]^{1/2}L\right] . \tag{8}$$

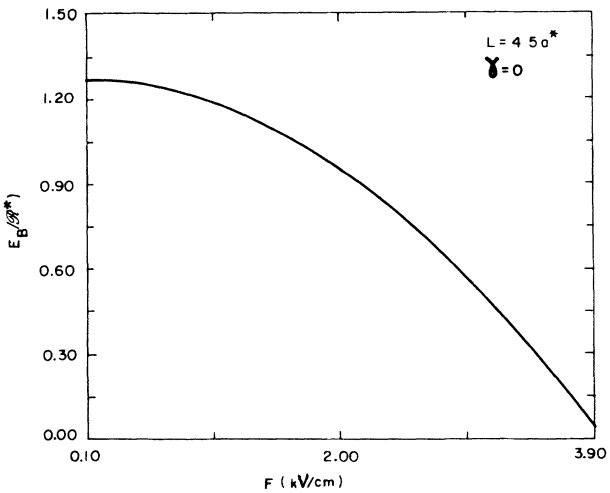

FIG. 1. The variation of impurity binding energy E_B as a function of electric field F.

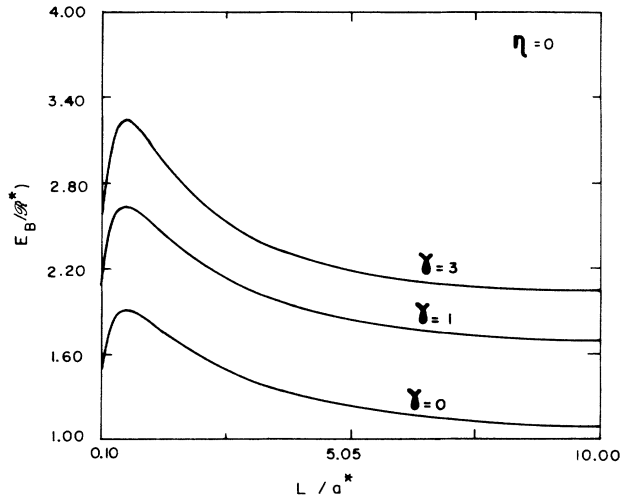

FIG. 2. The variation of impurity binding energy E_B as a function of well width L and magnetic field γ.

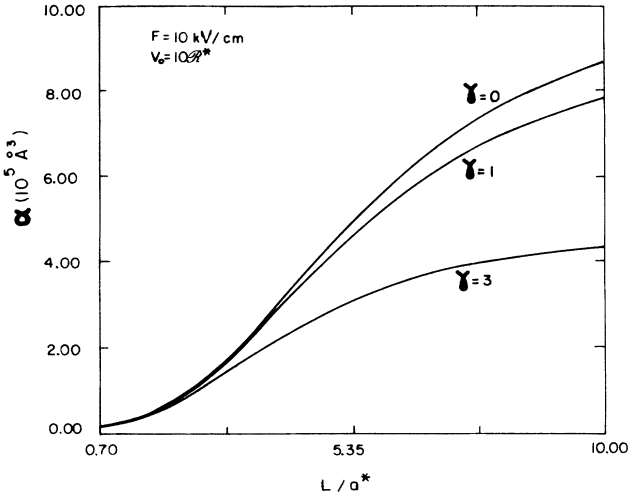

FIG. 3. The impurity polarizability values α as a function of well width L and magnetic field γ.

In Eq. (5), λ is used as a variational parameter.

With the trial function (5), the donor electron energy expectation becomes

$$\langle E \rangle = \frac{T_1 + T_3\lambda\eta + T_2\lambda^2}{N_1 + N_2\lambda^2} , \tag{9}$$

where

$$T_1 = \langle \Psi_0 | [-\nabla^2 + V_B(Z) - 2/r] | \Psi_0 \rangle , \tag{10}$$

$$T_2 = \langle \hat{\varepsilon}\cdot\mathbf{r}\Psi_0 | [-\nabla^2 + V_B(z) - 2/r] | \hat{\varepsilon}\cdot\mathbf{r}\Psi_0 \rangle , \tag{11}$$

$$T_3 = \langle \hat{\varepsilon}\cdot\mathbf{r}\Psi_0 | z | \Psi_0 \rangle , \tag{12}$$

$$N_1 = \langle \Psi_0 | \Psi_0 \rangle , \tag{13}$$

$$N_2 = \langle \hat{\varepsilon}\cdot\mathbf{r}\Psi_0 | \hat{\varepsilon}\cdot\mathbf{r}\Psi_0 \rangle . \tag{14}$$

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

$$\lambda = -\frac{N_2T_1 - N_1T_2}{N_2T_3\eta}\left[1 - \left[1 + \frac{N_1N_2T_3^2\eta^2}{(N_2T_1 - N_1T_2)^2}\right]^{1/2}\right] . \tag{15}$$

Substituting this value of λ into Eq. (9) and expanding $\langle E \rangle$ binominally in powers of η, one gets for the polarizability

$$\alpha = \frac{T_3^2}{2(N_2T_1 - N_1T_2)} . \tag{16}$$

III. RESULTS AND CONCLUSIONS

Polarizability values with and without the magnetic field are calculated using the following input parameters: $m^* = 0.067m_e$ and $\kappa_0 = 12.5$ suitable for quantum wells made out of GaAs. The effective rydberg $\mathcal{R}^* = 5.83$ meV and the effective Bohr radius $a^* = 98.7$ Å define the relevant energy and length scale.

We study first the effect of electric field on the impurity binding energy $E_B = E_{SB} - \langle H \rangle_{min}$, where E_{SB} is the subband energy, by first calculating E_B variationally without the electric and magnetic field terms and with wave function (5) taking $\lambda = 0$. In this calculation, a appearing in Ψ_0 is treated as a variational parameter. We then repeat the calculation with full Ψ to calculate E_B including the electric field term. The calculated E_B values are shown in Fig. 1, for a well width of $L = 4.5a^*$. The electric field reduces the binding energy effectively.

We study next the effect of the magnetic field, by omitting the electric field term in the Hamiltonian and the λ term in the trial wave function (5). The donor binding energy E_B is then calculated, taking into account the shift in subband energy in a perturbation theory approach, as a function of well width L and the magnetic field. The results are shown in Fig. 2. The binding energy increases as the magnetic field increases, as a result of increasing confinement. As also seen from the figure, the difference between the results for the finite- and infinite-barrier quantum wells becomes important for smaller well widths.

The impurity binding energies calculated in this work, without the magnetic and electric fields, are almost exactly the same as those found by Liu and Quinn,[14] who used the same V_0 value. The binding energies with magnetic field compare rather well with those calculated by Green and Bajaj,[5] who used a different V_0 value. The values for polarizability α are shown in Fig. 3 for $\gamma = 0, 1, 3$, where $\gamma = 1$ corresponds to a magnetic field of 67.4 kG. 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.

There are, certainly, several points in this calculation that could be improved. Firstly, the form of variational wave function Eq. (6) could be further modified to take into account the presence of the magnetic field better.

This will also improve the calculation of subband energy shift as a function of magnetic field. No effort is made here for a better handling of the screening effects. This could be done in a variational manner by using the r-dependent dielectric function $\kappa_0(r)$ instead of the constant κ_0 in Eq. (1), as done, for example, by Oliveira and Falicov[15] for the bulk case. The best way to treat screening effects is through a first-principles calculation, which unfortunately lacks the simplicity of the present calculation. Another questionable point is to use the effective-mass approximation for quantum wells with small L value where the potential seen by the impurity electron changes rather rapidly. The numerical results for this limit should be taken with caution.

[1]G. Bastard, Phys. Rev. B **24**, 4714 (1981).
[2]C. Mailhot, Y. C. Chang, and T. C. McGill, Phys. Rev. B **26**, 4449 (1982).
[3]R. L. Greene and K. K. Bajaj, Solid State Commun. **45**, 825 (1983).
[4]G. Bastard, E. E. Mendez, L. L. Chang, and L. Esaki, Phys. Rev. B **28**, 3241 (1983).
[5]R. L. Greene and K. K. Bajaj, Phys. Rev. B **31**, 913 (1985).
[6]B. V. Shanabrook and J. Comas, Surf. Sci. **142**, 504 (1984), and references therein.
[7]N. V. Jarosik, B. D. McCombe, B. V. Shanabrook, J. Comas, J. Ralston, and G. Wicks, Phys. Rev. Lett. **54**, 183 (1985).
[8]G. Brozak, B. D. McCombe, and D. M. Larsen, Phys. Rev. B **40**, 1265 (1989), and references therein.
[9]M. Cahay and E. Kartheuser, Solid State Commun. **48**, 781 (1983).
[10]E. Kartheuser, J. Schmit, and T. Szwacka, Solid State Commun. **53**, 551 (1985).
[11]K. Manimahali and E. Palaiyandi, J. Phys. Chem. Solids **46**, 831 (1985).
[12]M. El-Said and M. Tomak, Phys. Rev. B (to be published).
[13]H. R. Hasse, Proc. Cambridge Philos. Soc. **26**, 542 (1930).
[14]Wen-ming Liu and J. J. Quinn, Phys. Rev. B **31**, 2348 (1985).
[15]L. E. Oliveira and L. M. Falicov, Phys. Rev. B **34**, 8676 (1986).