Effect of nonparabolicity on the binding energy of a hydrogenic donor in a quantum well with a magnetic field

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A hydrogenic donor in a quantum well in the presence of a magnetic field perpendicular to the barrier is considered in the effective-mass approximation. The nonparabolicity of the subband is included in the Hamiltonian by an energy-dependent effective mass. The donor binding energy is calculated variationally for different well widths and the effect of nonparabolicity is discussed in the light of recent experimental results.

I. INTRODUCTION

Many papers have appeared during the last few years on hydrogenic donors in a quantum well formed by a layer of GaAs between $Ga_{1-x}Al_xAs$ barriers.[1] Due to technological developments in the preparation and characterization of the samples, experimental results are also now forthcoming. For example, Jarosik *et al.*[2] have reported far-infrared magnetospectroscopic measurements on shallow donors in the central region of a GaAs quantum well. Greene and Bajaj[3] and Chaudhuri and Bajaj[4] have calculated the binding energies of the ground state and some of the low-lying excited states by donors in a quantum well in the presence of a magnetic field along the growth axis. The experimental results in Ref. 2 are in good agreement with the theoretical calculations.

Chaudhuri and Bajaj[5] in an earlier paper have reported their results on the effect of nonparabolicity on the energy levels of a hydrogenic donor in a quantum well. They have found pronounced effects on the binding energy for small well widths. In the light of new experiments, such as those in Ref. 2, it would be of interest to see the effect of nonparabolicity on the donor binding in the presence of a magnetic field. In the present work, we report our results, based on variational calculations, of the donor binding energy when a magnetic field is present, taking into account the nonparabolicity of the subband.

II. THEORY

The effective-mass Hamiltonian for a hydrogenic donor in a GaAs quantum well with a magnetic field **B** along the growth axis which will be taken as the z axis is given (with origin at the impurity at the center of the well) by

$$H=\frac{1}{\chi(E)}\left(-\nabla^2+\tfrac{1}{4}\gamma^2\rho^2+\gamma L_z\right)-\frac{2}{r}+V_B(z)\ , \tag{1}$$

where we have used the effective Bohr radius $a_B=\hbar^2\epsilon_0/m^*e^2$ as the unit of length and the effective Rydberg $R=m^*e^4/2\epsilon_0^2\hbar^2$ as the unit of energy. Using the numerical values of the static dielectric constant ϵ_0 and the electron effective mass m^* for GaAs, one has $a_B=98.7$ Å and $R=5.83$ meV. γ in Eq. (1) is a dimensionless parameter given by

$$\gamma=e\hbar B/2m^*cR\ . \tag{2}$$

L_z is the z component of the angular momentum and $\chi(E)$ is the nonparabolicity correction through an energy-dependent effective mass. $\chi(E)$ is given by[5]

$$\chi(E)=1+(0.0436E+0.236E^2-0.147E^3)/0.0665\ , \tag{3}$$

where E is in electron volts. $V_B(z)$ in Eq. (1) is the potential energy due to a symmetrical well of width L and height V_0.

We choose the variational trial function of the form[4]

$$\psi(\rho,\phi,z)=Ne^{-(a_1r+b_1\rho+c_1z^2)}f(z)\ , \tag{4}$$

where $f(z)$ is the exact ground-state wave function for the particle in the one-dimensional well $V_B(z)$. The lowest-energy eigenvalue for this problem gives the first electron subband energy E_{sb} which is the solution of the equation

$$\left[\frac{E}{V_0}\right]^{1/2}=\cos\left[[\chi(E)E]^{1/2}\frac{L}{2}\right]\ . \tag{5}$$

a_1, b_1, and c_1 in Eq. (4) are the variational parameters. In the expectation value of H with the wave function as in Eq. (4), the integrations with respect to ϕ and ρ are performed analytically, and the remaining integration with respect to z is done numerically. The minimum of the expectation value of H with respect to the parameter a_1, b_1, and c_1 is obtained. The donor ground-state binding energy E_B is given by

$$E_B=E_{sb}+\gamma-\langle H\rangle_{\min}\ . \tag{6}$$

The results are presented in the next section.

III. RESULTS AND DISCUSSION

The donor binding energy as a function of well width is presented in Fig. 1 for two values of γ. Table I shows the numerical values of the different terms in the expectation value of the Hamiltonian. Just as in the zero-field case

TABLE I. Variation of different terms in the expectation value of H with well width L for two different magnetic-field parameters γ. Quantities in parenthesis are for the parabolic case [with $\chi(E)=1.0$].

γ	L	$\langle -\nabla^2/\chi(E)\rangle$	$\langle \gamma^2\rho^2/4\chi(E)\rangle$	$\left\langle -\frac{2}{r}\right\rangle$	$\langle V_B(z)\rangle$
0.2	0.1	9.938	0.0030	−5.203	38.961
		(7.814)	(0.0075)	(−3.865)	(42.683)
	0.3	14.582	0.0042	−5.042	13.199
		(14.459)	(0.0064)	(−4.432)	(14.983)
	0.5	11.592	0.0054	−4.513	5.566
		(11.769)	(0.0067)	(−4.244)	(6.072)
	1.0	6.219	0.0076	−3.699	1.228
		(6.268)	(0.0082)	(−3.626)	(1.273)
1.0	0.1	10.186	0.068	−5.395	38.904
		(8.204)	(0.162)	(−4.087)	(42.527)
	0.3	14.621	0.095	−5.230	13.385
		(14.676)	(0.141)	(−4.629)	(14.973)
	0.5	11.796	0.122	−4.705	5.565
		(12.017)	(0.148)	(−4.460)	(6.050)
	1.0	6.436	0.162	−3.903	1.233
		(6.493)	(0.172)	(−3.847)	(1.285)

presented in Ref. 4 (see also Ref. 6) the nonparabolic effects are important, as can be seen from Fig. 1, even in the presence of a magnetic field when the well widths are small. For small well widths, the electron wave function is more localized in real space, and hence more delocalized in k space, thus making is necessary to sample larger k values in the band. For $L \rightarrow 0$, the limiting values for the binding energy are different for the parabolic and nonparabolic cases. It is easy to see that E_B (nonparabolic)/E_B (parabolic) has the limiting value (as $L \rightarrow 0$ $\chi(E_{sb})$, where $E_{sb}=V_0$ when $L=0$. Figure 1 also shows that the nonparabolicity effects are significant when L is large. In the experiments of Jarosik *et al.*[2] the sample had $L = 210$ Å $\approx 2a_B$, and thus nonparabolicity effects are negligible. Also, experimentally one sees the transition from $1s \rightarrow 2p_+$ states, and hence to some extent there will be cancellation of the nonparabolicity effects. However, since the excited states are more extended than the ground state, the nonparabolicity effects may be less pronounced for the excited states compared to the ground state. To some extent this is seen in the results for the zero-magnetic-field case reported in Ref. 5.

From Table I one can see that the nonparabolicity affects not only the kinetic energy terms but also the potential-energy terms through the wave function, especially for small well widths. In conclusion, we can say that nonparabolicity effects are quite pronounced for small well widths, and magnetospectroscopic measurements performed with suitable samples should reveal this.

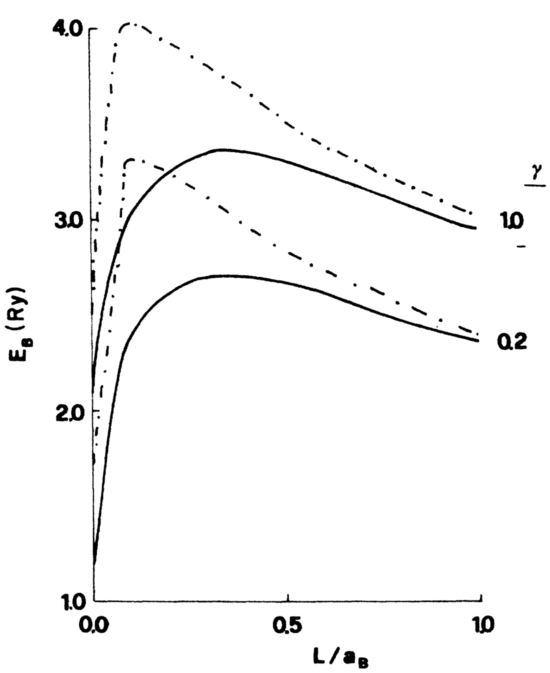

FIG. 1. Variation of the binding energy of the ground state of a donor (E_B) as a function of well width (L) for two different values of the magnetic-field parameter γ ($\gamma=1.0$ corresponds to $B=67.4$ kG and $\gamma=0.2$ corresponds to $B=13.48$ kG) for Al concentration $x=0.3$ which corresponds to $V_0=55.37$ Ry. —— represents the parabolic case; —·—·— represents the nonparabolic case.

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