Binding energy of a donor in a quantum-well heterostructure

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The binding energy of a hydrogenic donor in a quantum well is calculated as a function of well width, taking into account the nonparabolicity of the conduction band. The nonparabolicity causes an increase in the binding energy much greater than reported earlier. This increase, which is more pronounced for a deeper well, is attributed to the change in the quantum-well wave function outside the well due to the nonparabolicity. The nonparabolicity effectively increases the well depth, and this increase is larger for larger well depths.

The binding energy of a hydrogenic donor in a quantum-well structure has been recently calculated by a number of workers. A typical system considered by many is a layer of GaAs grown between thick layers of $Ga_{1-x}Al_xAs$. The band-gap discontinuity gives rise to a one-dimensional potential well. Bastard[1] has calculated the binding energy of a hydrogenic donor assuming an infinite potential at the surfaces and found a monotonic increase in the binding energy with decreasing well size, with the two-dimensional limit reached as the well thickness goes to zero. Mailhiot, Chang, and McGill[2] and Greene and Bajaj[3] obtained the binding energies for the ground state and a few low-lying excited states assuming a finite potential at the surfaces. The ground-state binding energy increases as the well thickness is reduced until a maximum is reached, and then decreases to the bulk value at zero well thickness. Chaudhuri[4] has considered a hydrogenic impurity in a multiple quantum-well structure. More recently, Chaudhuri and Bajaj[5] included the effect of nonparabolicity on the energy levels of hydrogenic donors in GaAs-$Ga_{1-x}Al_xAs$ quantum-well structures, and found that inclusion of nonparabolic effects leads to more binding. It seems that in Ref. 5, the effect of nonparabolicity on the wave function has been ignored. In all the above variational calculations the donor electron is assumed to see a potential $e^2/\epsilon_0 r$, where ϵ_0 is the static dielectric constant, in addition to the one-dimensional well. Chaudhuri and Bajaj[6] have also extended the work with parabolic bands to the problem of a donor in a quantum well in a magnetic field.

In our present work we examine the effect of nonparabolicity of the conduction band on the donor ground state in a quantum well, taking into account the change in the wave function due to the nonparabolic effect.

In the effective-mass approximation, the Hamiltonian for an electron in a hydrogenic donor located at the center of the well is given by

$$H=\frac{p^2}{2m^*}+\frac{e^2}{\epsilon_0 r}+V_B(z) \ , \tag{1}$$

where $V_B(z)$ is a one-dimensional, symmetrical well of width L and height V_0, and ϵ_0 is the static dielectric constant of GaAs. The nonparabolicity of the conduction band is included through an energy-dependent effective mass m^*, given by[5]

$$\frac{m^*}{m}=\gamma=1+\frac{\Gamma(E)}{0.0665} \ , \tag{2}$$

where

$$\Gamma(E)=0.0436E+0.236E^2-0.147E^3 \ , \tag{3}$$

with E expressed in eV. m is the conduction-band effective mass at the $\mathbf{K}=0$ point.

For a given V_0 and L, the subband energies (eigenstates of H without the Coulomb term) can be computed by solving the transcendental equation

$$\left[\frac{E}{V_0}\right]^{1/2}=\cos\left[(\gamma E)^{1/2}\frac{L}{2}\right] \ . \tag{4}$$

The lowest solution of Eq. (4) gives the lowest subband energy. We use the units of energy and length as in Ref. 5.

For a variational estimate of the lowest energy for the Hamiltonian in Eq. (1), we use a trial function[5] of the form

$$\psi(\mathbf{r})=f(z)g(\rho,z,\phi) \ , \tag{5}$$

where $f(z)$ is the exact solution to the finite-well problem:

$$f(z)=\begin{cases}\cos(\alpha z), & |z|<L/2 \ , \\ Be^{-\beta|z|}, & |z|>L/2 \ ,\end{cases} \tag{6}$$

where $\alpha=\sqrt{\gamma E}$, $\beta=\sqrt{\gamma(V_0-E)}$, and $B=\cos(\alpha L/2)e^{\beta L/2}$. The effect of nonparabolicity of the conduction band is reflected in the wave function $f(z)$ through the factor γ. With a trial function of the form

$$g(\rho,z,\phi)=N\exp[-(\rho^2+z^2)^{1/2}/\lambda] \ , \tag{7}$$

where λ is the variational parameter, the expectation value of H is minimized with respect to λ, and the donor binding energy is obtained as

$$E_B=E-\langle H\rangle_{\min} \ . \tag{8}$$

The normalization constant N and the expectation values of the operators of H are given by[4,7]

$$N=\left[\frac{2}{\pi\lambda^3}\right]^{1/2}\left\{1+\frac{1}{(1+\alpha^2\lambda^2)^2}-e^{-L/\lambda}\left[1+\frac{L}{2\lambda}+\frac{\cos(\alpha L)}{1+\alpha^2\lambda^2}\left(\frac{L}{2\lambda}+\frac{1}{1+\alpha^2\lambda^2}\right)\right.\right.$$
$$\left.\left.-\frac{\alpha\lambda\sin(\alpha L)}{2(1+\alpha^2\lambda^2)}\left(1+\frac{L}{\lambda}+\frac{2}{1+\alpha^2\lambda^2}\right)-\frac{\cos^2(\alpha L/2)}{1+\beta\lambda}\left(1+\frac{L}{\lambda}+\frac{1}{1+\beta\lambda}\right)\right]\right\}^{1/2} \ , \tag{9}$$

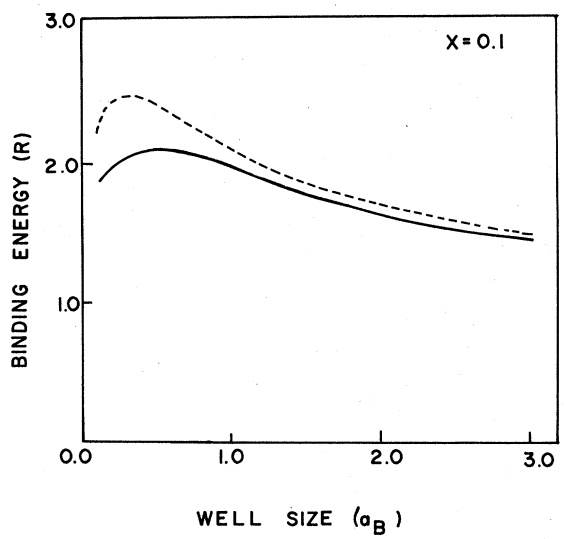

FIG. 1. Binding energy (in units of effective rydberg R) as a function of well size (in units of Bohr radius a_B) for $x=0.1$. ——, parabolic band model. — — —, nonparabolicity included.

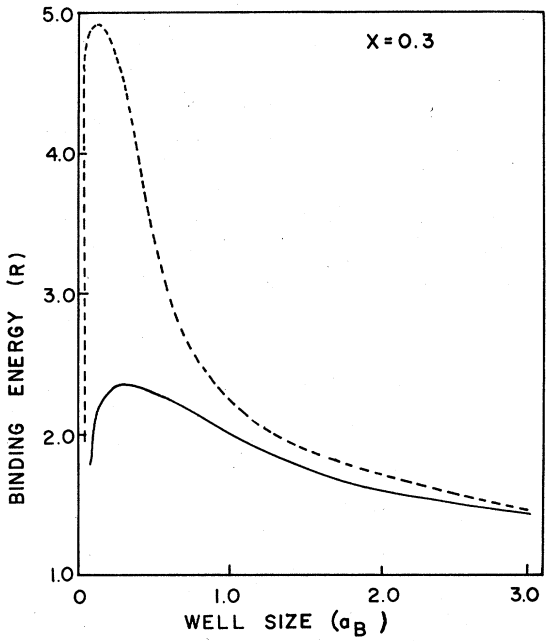

FIG. 2. Binding energy as a function of well size for $x=0.3$. ——, parabolic band model. — — —, nonparabolicity included.

$$\langle\psi|(-\nabla^2)|\psi\rangle=\left\{\frac{1}{\lambda^2}+\alpha^2-\frac{\pi N^2\alpha\lambda^2}{2}e^{-L/\lambda}\left[1+\frac{L}{\lambda}\right]\sin(\alpha L)\right.$$
$$\left.+\frac{\pi N^2\lambda}{2}\cos^2\left[\frac{\alpha L}{2}\right]e^{-L/\lambda}\left[1+\left[\beta+\frac{1}{\lambda}\right]L+\frac{\beta^2-\alpha^2}{\beta\lambda+1}\lambda^2-\frac{1+\alpha^2\lambda^2}{(1+\beta\lambda)^2}-\frac{(1+\alpha^2\lambda^2)}{1+\beta\lambda}\frac{L}{\lambda}\right]\right\}\Big/\gamma\ , \tag{10}$$

$$\langle\psi|(-2/r)|\psi\rangle=-\pi N^2\lambda^2\left[1+\frac{1}{1+\alpha^2\lambda^2}-e^{-L/\lambda}\left[1+\frac{\cos(\alpha L)}{1+\alpha^2\lambda^2}-\frac{\alpha\lambda\sin(\alpha L)}{(1+\alpha^2\lambda^2)}\right]+\frac{2B^2}{1+\beta\lambda}e^{-(\beta+1/\lambda)L}\right]\ , \tag{11}$$

$$\langle\psi|V(z)|\psi\rangle=\frac{\pi N^2\lambda^3\cos^2(\alpha L/2)}{2(\beta\lambda+1)}e^{-L/\lambda}V_0\left[1+\frac{L}{\lambda}+\frac{1}{1+\beta\lambda}\right]\ , \tag{12}$$

when $\Gamma(E)\to 0$, Eq. (4) reduces to the parabolic subband energy.

Figure 1 shows the variation of binding energy E_B of the ground state as a function of well thickness L for composition $x=0.1$, which corresponds to well height $V_0\sim 17R$, where R is the effective rydberg, including the nonparabolicity of the conduction band. Figure 2 gives the result for $x=0.3$ and $V_0\sim 56R$. The binding energy shows a large increase for $L<a_B$ when compared to the parabolic case (a_B is the effective Bohr radius). At the peak position the binding energy is almost doubled for the composition $x=0.3$ while for $x=0.1$ the increase is about 15%. The model, of course, is less applicable for $L<25$ Å, as remarked by Chaudhuri and Bajaj.[5]

Chaudhuri and Bajaj[5] have reported a maximum increase in the binding energy of only about 20% even for $x=0.3$ due to nonparabolic effect. When we run our computer program with values of α and β in the wave function the same as in the parabolic case, while the nonparabolicity is included in the kinetic energy term, the results of Chaudhuri and Bajaj could be reproduced. Thus it appears that Chaudhuri and Bajaj have neglected the change in the quantum-well wave function due to the nonparabolic effect and when these are included, the binding energy further increases. This change in the quantum-well wave function may be seen to be appreciable for the part of the wave function outside the well and this change is also more for larger V_0. The nonparabolicity effectively increases V_0 by a factor γ and this modification is larger for larger V_0.

Note added in proof. The increase in the binding energy of a hydrogenic donor in a quantum well due to nonparabolicity reported by us as much more pronounced when compared to the results of Chaudhuri and Bajaj[5] is now regrettably noted as due to a program error. The results of Ref. 5 stand within the variational procedure adopted.

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[1]G. Bastard, Phys. Rev. B **24**, 4714 (1981).
[2]C. Mailhiot, 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]S. Chaudhuri, Phys. Rev. B **28**, 4480 (1983).
[5]S. Chaudhuri and K. K. Bajaj, Phys. Rev. B **29**, 1803 (1984).
[6]S. Chaudhuri and K. K. Bajaj, Solid State Commun. **52**, 967 (1984).
[7]Two printing errors in Ref. 4 have been corrected in the expression for the expectation of the potential energy (our L is Chaudhuri's $2a$).