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Effect of nonparabolicity on the energy levels of hydrogenic donors in GaAs-$Ga_{1-x}Al_xAs$ quantum-well structures

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Binding energies of the ground state and of a few low-lying excited states of a hydrogenic donor in a quantum-well structure consisting of a single layer of GaAs sandwiched between two-semi-infinite layers of $Ga_{1-x}Al_xAs$ are calculated, including the effect of nonparabolicity of the conduction band and following a variational approach. The effect of nonparabolicity of the conduction band is included by using an expression for the energy-dependent effective mass based on the $\vec{k}\cdot\vec{p}$ approximation. The variations of the binding energies of these states as a function of the size of the GaAs quantum well for different values of the potential barrier (or equivalently for different values of Al concentration x) are calculated. These results are compared with those obtained with the use of a parabolic conduction band.

INTRODUCTION

The behavior of a hydrogenic impurity center located in a quantum-well structure consisting of a single layer of GaAs sandwiched between two semi-infinite (greater than 200 Å) layers of $Ga_{1-x}Al_xAs$ has been a topic of considerable interest in the past couple of years.[1-3] Bastard,[1] for instance, has calculated the binding energy of the ground state of a hydrogenic donor associated with the lowest electron subband level, as a function of GaAs quantum-well size (L) and the position of the impurity ion, assuming infinite potential at the interfaces, with the use of a variational approach. Mailhiot *et al.*[2] and Greene *et al.*[3] have independently calculated the binding energies of the ground state and of several low-lying excited states of a hydrogenic donor as a function of L for finite values of the potential barriers. Both of these groups use variational techniques and find essentially the same results. For example, for an impurity ion located at the center of the well, they find that the value of the binding energy of the ground state, E_B, increases as L is reduced until it reaches a maximum value and then decreases to its bulk value in $Ga_{1-x}Al_xAs$ at $L=0$. For infinite barriers, however, E_B increases monotonically from its bulk value as the well size is reduced and approaches the well-known two-dimensional value (i.e., 4 times the value in bulk) at $L=0$. All these calculations use effective-mass approximation assuming a simple parabolic conduction band. For small values of L (<100 Å) and for large values of the potential barrier, the energy of the first electron subband can be quite significant. As was pointed out by Greene *et al.*[3] this should require including the contributions due to nonparabolicity of the conduction band. The larger the energy of the first subband, the more important this contribution becomes.

In this paper we report a first calculation of the binding energies of the ground state and of the first four excited states of a hydrogenic donor associated with the first subband in a GaAs-$Ga_{1-x}Al_xAs$ quantum well as a function of the potential barrier (or equivalently the x value) and the size of the quantum well, taking into account the effect of nonparabolicity of the conduction band. We follow a variational approach and include this effect by using a recently proposed[4] expression for the energy-dependent conduction-electron effective mass based on the $\vec{k}\cdot\vec{p}$ approximation, which has been used to explain emission spectra in thin quantum-well structures. We assume, for the sake of illustration, that the positive ion is located at the center of the well. The results thus obtained are compared with those calculated with the use of a parabolic conduction band. We find that inclusion of nonparabolic effects leads to more binding for all values of L.

THEORY

The Hamiltonian of a hydrogenic donor located in a GaAs quantum well can be written as

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

where the barrier potential $V_B(z)$ is taken to be square well of height V_0 and width L,

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

Here we have assumed, for the sake of illustration, that the positive ion of the donor impurity is located at the center of the well. The position of the electron is denoted by $\vec{r}$ where $r=(\rho^2+z^2)^{1/2}$, ρ being the distance in the x-y plane. The values of the effective mass m^* and the static dielectric constant ϵ_0 are assumed to be the same across the interface between the two semiconductors. This is a good approximation as seen by comparing the results of Mailhiot *et al.*[2] with those of Greene *et al.*[3] for parabolic bands. The former calculation takes into account the different effective masses and dielectric constants for GaAs and $Ga_{1-x}Al_xAs$ regions. The latter calculation, however, uses the same values for the effective mass and the dielectric constant for the two semiconductors. As mentioned earlier, these two calculations yield essentially the same results for values of x considered in these papers ($x \leq 0.4$), thus justifying our use of the same values for these two parameters.

The effect of nonparabolicity of the conduction band on the energy levels of our system is taken into account by assuming that the effective mass m^* is a function of energy (E). Recently Kolbas[4] has proposed the following expression for m^* in GaAs, i.e.,

$$m^*/m_0=(0.0665+0.0436E+0.236E^2-0.147E^3)\ , \tag{3}$$

where m_0 is the free-electron mass and energy E is expressed in terms of electron volts. The value of the effective mass at the Γ point, m, is taken to be $0.0665m_0$. This expression is obtained from the following relation first derived by Kane[5] using the $\vec{k}\cdot\vec{p}$ perturbation technique,

$$\frac{1}{m^*}=\frac{1}{m}\left[1-\frac{5k_BT}{3}\left[\frac{2}{E_g}+\frac{1}{E_g+\Delta}\right]\left[1-\frac{m}{m_0}\right]^2\frac{F_{3/2}}{F_{1/2}}\right]\ , \tag{4}$$

by fitting it to a third-order polynomial in E using a least-squares method. Here k_B is Boltzmann's constant, T is the absolute temperature, E_g is the energy gap of GaAs, Δ is the spin-orbit splitting, and $F_{1/2}$ and $F_{3/2}$ are the standard Fermi integrals as defined in Ref. 6. Although Eq. (3) was deduced from Eq. (4) at $T=77^\circ$ K, it is assumed to be applicable at liquid-helium temperatures as the variation of the effective mass with temperature in this range is very small. In addition, Eq. (3) is assumed to be valid for values of $E \lesssim 300$ meV.[4] The value of the potential barrier height V_0 is determined from the Al concentration in $Ga_{1-x}Al_xAs$ using the following expression[7] for the total energy-band-gap discontinuity:

$$\Delta E_g = 1.155x+0.37x^2\ , \tag{5}$$

in eV. It has been shown,[8] on the basis of fairly detailed optical-absorption measurements, that V_0 is about 85% of the band-gap difference between the two semiconductors.

It is convenient to express the Hamiltonian in dimensionless form. We have chosen to use the effective Bohr radius $a_B=\hbar^2\epsilon_0/me^2$ as our unit of length and the effective Rydberg $R=e^2/2\epsilon_0 a_B$ as the unit of energy. For GaAs ($m=0.0665m_0$ and $\epsilon_0=12.5$) these quantities are $a_B=99.4$ Å and $R=5.8$ meV.

An exact analytical solution of the Schrödinger equation corresponding to the donor Hamiltonian [Eq. (1)] is clearly not possible. We therefore follow a variational approach and write the trial wave function in the following form:

$$\psi=f(z)g(\rho,z,\phi)\ , \tag{6}$$

where $f(z)$ is the exact (unnormalized) solution[9] to the square-well problem,

$$f(z)=\begin{cases}\cos(\eta z), & |z|<L/2\\ Be^{-\kappa|z|}, & |z|>L/2.\end{cases} \tag{7}$$

The parameter η is determined from the energy of the first electron subband and B and κ are obtained from η by requiring continuity of f and its first derivative at the interface. The wave functions $g(\rho,z,\phi)$ where ϕ is the azimuthal angle, describe the bound states of the donor.

To calculate the binding energy of the ground state, E_B, of a donor in GaAs quantum well we proceed as follows. For a given value of V_0 and L we first determine the energy of the first electron subband (no Coulomb interaction) by solving the following transcendental equation,[9]

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

using Eq. (3) for the effective mass m, in a self-consistent manner. Note that m is the conduction-band-edge effective mass and m^* is the energy-dependent effective mass. The starting value of m^* in Eq. (8) is, of course, m. The value of m^* thus obtained is then used in Eq. (1) to solve for its eigenvalues. For the 1s level, we choose the following expression for the trial wave function g:

$$g(\rho,z,\phi)=N_1e^{-\alpha_1 r}\ , \tag{9}$$

where α_1 is a variational parameter and N_1 is the normalization constant. We then evaluate the expectation value of H, i.e.,

$$E_{1s}=\frac{\int\int\int \psi^*H\psi\rho\, d\rho\, dz\, d\phi}{\int\int\int \psi^*\psi\rho\, d\rho\, dz\, d\phi}\ , \tag{10}$$

and minimize this expression as a function of α_1. The value of E_B is now obtained by subtracting E_{1s} from the first subband energy E. This procedure results in our variational binding energies E_B being rigorous upper bounds for the true binding energies including the nonparabolicity effect.

We also calculate the binding energies of the first four excited states following a procedure essentially similar to the one described for E_B. For convenience we label these states by their bulk hydrogenic limits, namely, 2s, $2p_\pm$, and $2p_0$. The presence of the potential barrier at the interfaces lifts the degeneracy of this $n=2$ state into these three distinct states. We use the following trial wave functions to calculate their binding energies:

$$g_{2p_\pm}=N_2\rho e^{\pm i\phi}e^{-\alpha_2 r}\ , \tag{11}$$

$$g_{2p_0}=N_3 z e^{-\alpha_3 r}\ , \tag{12}$$

and

$$g_{2s}=N_4(1-\delta r)e^{-\alpha_4 r}\ . \tag{13}$$

Here α_2, α_3, and α_4 are variational parameters, N_2, N_3, and N_4 are normalization constants, and δ is determined

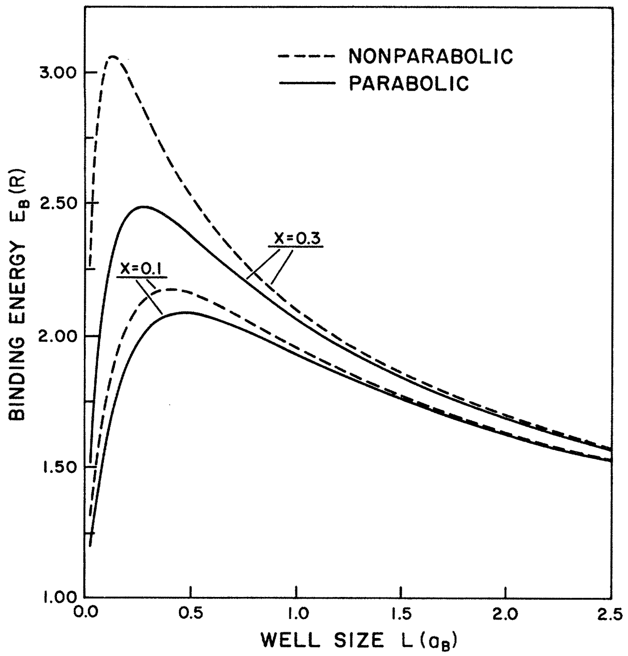

FIG. 1. Variation of the binding energy of the ground state, E_B, of a donor as a function of the GaAs well size (L) for Al concentrations $x=0.1$ and 0.3 using a parabolic conduction band (solid lines) and a nonparabolic conduction band (dashed lines). All energies are expressed in terms of an effective Rydberg (R) and all distances are expressed in terms of Bohr radius (a_B).

by requiring g_{2s} to be orthogonal to the 1s trial wave function g_{1s}.

RESULTS AND DISCUSSION

In Fig. 1 we display the variation of the binding energy of the ground state, E_B, of a donor as a function of GaAs well size L for $V_0=101$ and 322 meV corresponding to Al concentrations $x=0.1$ and 0.3, respectively, including the effects of nonparabolicity of the conduction band (dashed lines). For comparison, we also plot the variation of E_B as a function of L, assuming a simple parabolic band (solid lines). The latter results agree (within a few percent) with those of Greene *et al.*,[3] who use a much more general trial wave function. This suggests that the results obtained with the use of the present, rather simple trial wave function for the case of a nonparabolic conduction band should be quite accurate. We find, as expected, that the effect of nonparabolicity on E_B is negligible for $L > a_B$. For values of L smaller than a_B, this contribution can, however, be quite signficant. For $x=0.3$, for instance, the maximum value of E_B including nonparabolic effects is about 20% larger. In addition, the maximum in E_B is reached at a smaller value of L. Our results, however, should be less applicable for thin wells ($L < 25$ Å) as we have assumed the same values for the effective mass and the dielectric constant in the two semiconductors. For thin wells, a significant part of the donor wave function lies in the $Ga_{1-x}Al_xAs$ layers. This makes the above approximation less valid.

In Fig. 2 we display the variations of the binding ener-

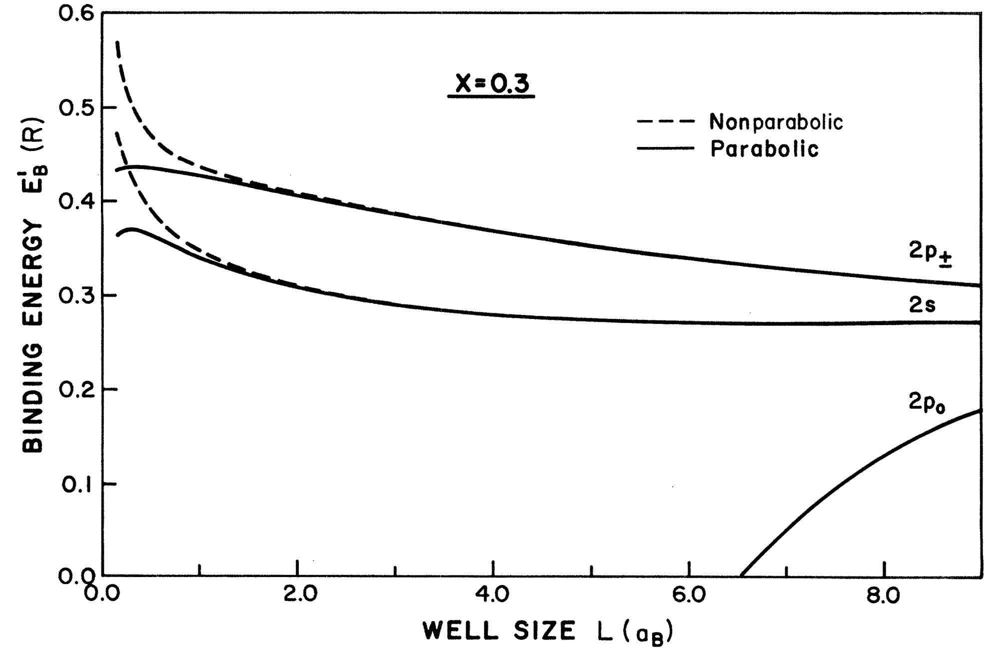

FIG. 2. Variation of the binding energies (E_B') of $2p_\pm$-, 2s-, and $2p_0$-like states of a donor as a function of the GaAs well size (L) for Al concentration $x=0.3$ using a parabolic conduction band (solid lines) and a nonparabolic conduction band (dashed lines). All energies are expressed in terms of an effective Rydberg (R) and all distances are expressed in terms of Bohr radius (a_B).

gies of $2s$, $2p_{\pm}$, and $2p_0$ states as a function of the GaAs quantum-well size L for Al concentration $x=0.3$. The contribution of nonparabolicity to the binding energy of $2p_0$ state is negligible as it becomes unbound at $L=650$ Å. The effect of nonparabolicity on the binding energies of $2s$ and $2p_{\pm}$ states, however, is very similar to that on the ground state. Both $2s$ and $2p_{\pm}$ states show a maximum in binding energy (not shown in Fig. 2) for values of L smaller than the corresponding values for the parabolic band.

It is difficult to know how accurate the present approach is in taking into account the effect of nonparabolicity on the energy levels of a hydrogenic donor in quantum-well structures. We know that in the absence of the Coulomb term in the Hamiltonian, the conduction-electron dispersion relation can be described fairly accurately by Kane's $\vec{k}\cdot\vec{p}$ expression. In the presence of the Coulomb term, however, one needs to take into account the contributions from other bands. Thus a calculation using an impurity wave function composed of contributions from several different bands is expected to give better results. It is still possible, however, to use an energy-dependent effective mass to calculate the effect of nonparabolicity on the energy levels of a hydrogenic donor as long as this effect is rather small. We believe our approach is fairly reliable to calculate the change in the binding energy of the ground state, E_B, for small values of Al concentration x (approximately less than 0.1), where for $x=0.1$, for instance, the maximum change in E_B is only about 6%. For larger values of x and for smaller values of L our calculations become less valid. For example, for $x=0.3$, the maximum change in E_B can be as large as 20%. It is clear that for $x=0.3$ our calculations will be valid only for large L (greater than $0.5a_B$) values where the changes in E_B are rather small. For values of L smaller than $0.5a_B$ our results should be viewed as no more than indicating the trend. However, our results should be applicable to most practical quantum-well structures which often have well sizes larger than $0.5a_B$. It should be pointed out that the contribution of nonparabolicity of the conduction band to the binding energy of the ground state of a donor in bulk GaAs, as obtained by Eq. (3) (here m^* is calculted for $E=R=5.80$ meV), is about 0.022 meV, which is very close to that obtained by Stillman *et al.*[10] using a multiband approach.

CONCLUDING REMARKS

We have calculated the binding energies of the ground state and of $2s$-, $2p_{\pm}$-, and $2p_0$-like states of a hydrogenic donor in a GaAs-$\text{Ga}_{1-x}\text{Al}_x\text{As}$ quantum-well structure including the effects of nonparabolicity of the conduction band following a variational approach. The effect of nonparabolicity on the energy levels is taken into account by using an expression for the energy-dependent effective mass based on the $\vec{k}\cdot\vec{p}$ approximation. The variations of the binding energies of these states as a function of the GaAs quantum-well size for different values of Al concentration are calculated. These results are compared with those obtained with the use of a parabolic conduction band. We find that inclusion of nonparabolic effects leads to more binding for all values of L.

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