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LETTER TO THE EDITOR

Maximum binding energy of a shallow donor in GaAs–$Ga_{1-x}Al_xAs$ quantum wells

Jia-Lin Zhu

Centre of Theoretical Physics, CCAST (World Laboratory), Beijing, People's Republic of China and Department of Physics, Tsinghua University, Beijing, People's Republic of China

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Abstract. Using a novel trial function for the ground state of a shallow donor in GaAs–$Ga_{1-x}Al_xAs$ quantum wells, we have obtained a larger maximum of the binding energy than others. It shows that the coupling effect between the donor potential and the quantum wells is important.

Numerous studies have been devoted to various aspects of the electronic states associated with the GaAs–$Ga_{1-x}Al_xAs$ superlattice. From a theoretical point of view, Bastard (1981) was the first to treat the hydrogenic impurity states in the quantum well (QW) representing the superlattice. In his approach, the barrier height of the quantum well was assumed to be infinite. Mailhiot *et al* (1982), hereafter MCM, and Greene and Bajaj (1983), hereafter GB, have independently studied the energy levels of the hydrogenic impurity states in the superlattice system with a finite barrier height. Liu and Quinn (1985), hereafter LQ, have also studied the impurity states as a function of the well width, the impurity position within the well, and the potential barrier height. For a finite barrier height, MCM, GB and LQ have shown that the binding energy goes through a maximum as the well size is reduced instead of continuously increasing as is found in the infinite-barrier calculation. The maximum is dependent on the barrier height, i.e., the Al concentration.

In all of the above calculations it has been assumed that the GaAlAs layers are thick enough to confine the wavefunctions so that they do not spill over to adjacent GaAs quantum wells. Assuming that the wavefunctions spill over to the next-nearest-neighbour wells, with the one containing the impurity at the centre, Chaudhuri (1983) performed the calculation of the wavefunctions and binding energies with only one well on each side of the well under consideration. It was shown that the binding energies of the multiple wells are different to those of the single wells.

Because the transverse and longitudinal variables do not separate, the impurity states cannot be solved exactly, and approximation methods should be used. In this Letter we introduce a novel trial wavefunction for determining the binding energy of a shallow donor and its maximum in GaAs–$Ga_{1-x}Al_xAs$ quantum wells. It is different from the others. The coupling effect between the donor potential and the narrow quantum wells

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is correctly included to obtain a lower variational ground state and a larger maximum of the binding energy.

Let us consider a donor impurity atom at the centre of a quantum well of thickness $L = 2a$. With only one well on each side of the well under consideration, the potential due to the discontinuity of the band edges at the GaAs–$Ga_{1-x}Al_xAs$ interface is as follows:

$$V(Z) = \begin{cases} V_0 & \text{if } a < |Z| < a + b \quad \text{or} \quad 3a + b < |Z| \\ 0 & \text{if } |Z| < a \quad \text{or} \quad a + b < |Z| < 3a + b \end{cases} \tag{1}$$

where the Z axis is normal to the interface and b is the $Ga_{1-x}Al_xAs$ barrier thickness. The barrier height V_0 is obtained from a fixed ratio of the band gap discontinuity (Lee *et al* 1980). According to the hydrogenic-effective-mass theory (Pantelides 1978), the Hamiltonian for the donor at the centre of the quantum well is

$$H = -\nabla^2 - 2/r + V(Z). \tag{2}$$

It is written in a dimensionless form so that all energies are measured in units of the effective Rydberg R^* and all distances are measured in units of effective Bohr radius a^*. In order to compare with Chaudhuri's and LQ's results, the differences in the effective masses and dielectric constants of GaAs and $Ga_{1-x}Al_xAs$ have been neglected.

The novel trial function for the ground state of the full Hamiltonian H is

$$\psi = \psi_z \psi_{xy} \tag{3}$$

with

$$\psi_{xy} = (2/\lambda)(2/\pi)^{1/2} \exp(-2r_\perp/\lambda) \tag{4}$$

where λ is the variational parameter and $r_\perp$ is equal to $(x^2 + y^2)^{1/2}$ (Zaslow and Zandier 1967). ψ_z is the normalised ground-state eigenfunction of $H_z(\alpha, \beta)$ defined as follows:

$$H_z(\alpha, \beta) = -\mathrm{d}^2/\mathrm{d}Z^2 - \beta/(|Z| + \alpha) + V(Z) \tag{5}$$

that is,

$$H_z(\alpha, \beta)\psi_z = E_z(\alpha, \beta)\psi_z. \tag{6}$$

The α and β are variational parameters. Therefore, the variational ground-state energy E is given by

$$E = \min_{\alpha,\beta,\lambda} \langle \psi | H | \psi \rangle \tag{7}$$

where

$$\langle \psi | H | \psi \rangle = E_z(\alpha, \beta) - 4/\lambda^2 + E'(\alpha, \beta, \lambda). \tag{8}$$

The $E'(\alpha, \beta, \lambda)$ are given by

$$E'(\alpha, \beta, \lambda) = \langle \psi | H'(\alpha, \beta, \lambda) | \psi \rangle \tag{9}$$

where

$$H'(\alpha, \beta, \lambda) = \beta/(|Z| + \alpha) + 2/\lambda r_\perp - 2/r \tag{10}$$

and r is equal to $(x^2 + y^2 + z^2)^{1/2}$.

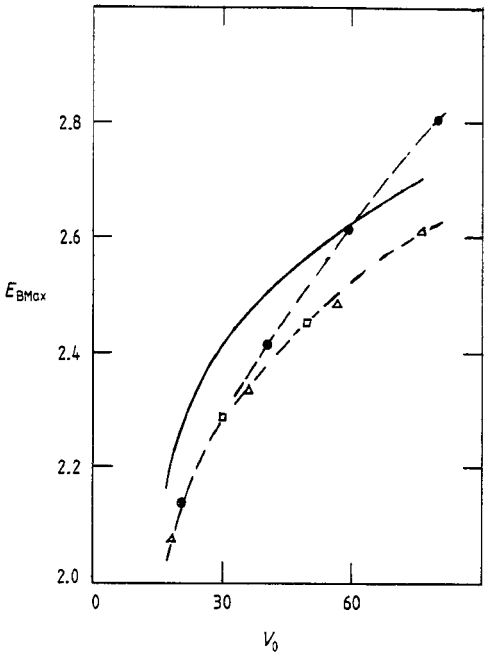

Figure 1. Maximum binding energy E_{BMax} for the hydrogenic-donor ground state in the single well as a function of the barrier height V_0. The full curve is our result. Full circles, open triangles and squares represent data from MCM, LQ and Chaudhuri, respectively. The broken curves are empirical. All energies are expressed in terms of the effective Rydberg (R^*).

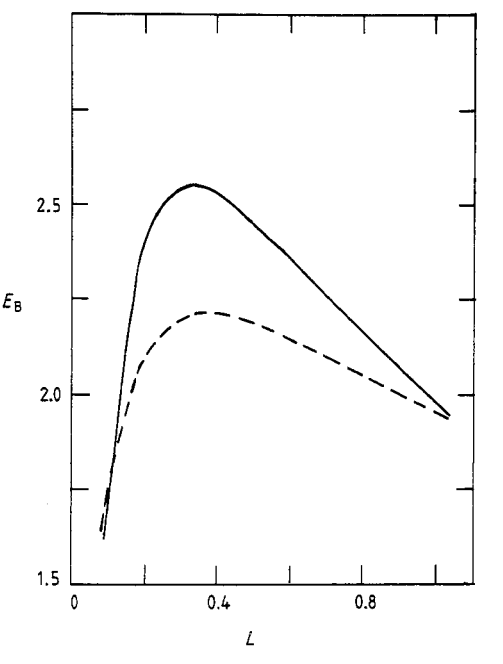

Figure 2. Binding energies for hydrogenic-donor ground states in MQW with $V_0 = 76\,R^*$ and $b = a^*$ (see the text) as a function of the GaAs layer thickness L. The full and broken curves represent the theoretical predictions of the text and Chaudhuri, respectively. The effective atomic units are used.

Using the method of series expansion we solve (6) in different regions to obtain the part ψ_z of the trial function ψ in (3). It is worthwhile pointing out that in the region $3a + b < |Z|$, infinity is an irregular singular point of (6) and there is a normal solution (Erdélyi 1956). It approaches zero at the infinite point. Based on the calculation of ψ_z, the $E'(\alpha, \beta, \lambda)$ of (9) can be integrated partly analytically and partly numerically. When $\beta = 0$, the smallest eigenenergy of $H_z(\alpha, \beta)$ gives the lowest sub-band energy E_{zg}. Therefore, the binding energy of the variational ground state is given by

$$E_B = E_{zg} - E \tag{11}$$

where E is obtained from (7).

We have performed a numerical calculation for the single-quantum-well (SQW) structure, which has infinite $Ga_{1-x}Al_xAs$ layer thickness, and the multiple-quantum-well (MQW) structure, which has finite $Ga_{1-x}Al_xAs$ layer thickness and is defined in (1). In figure 1 it is seen that the maximum E_{BMax} of the binding energy in the SQW is increased when the barrier height V_0 is increased from 17 to 80 R^*. Our calculated results of the maximum are larger than those of Chaudhuri and LQ. The difference is from 0.1 to 0.15 R^*. Including the effect of the differences in the effective masses and dielectric constants of GaAs and $Ga_{1-x}Al_xAs$, the maximum E_{BMax} obtained by MCM are also shown by full circles in figure 1. As is seen, ours are larger than MCM's when V_0 is smaller than 60 R^*. Based on the comparisons above, it is concluded that our trial function is

more reasonable than others in narrow SQWs. From the comparison with MCM's results, it is known that the coupling effect on the maximum binding energy is as important as the differences in the effective masses and dielectric constants.

In order to compare with Chaudhuri's results in MQWs, we have calculated the binding energy in the MQW with $V_0 = 76\,R^*$ and $b = a^*$, which has been plotted in figure 2. The value of the binding energy of the MQW is smaller than that of the SQW because of the spread of the wavefunction in the MQW mentioned above. It is readily seen that the difference between Chaudhuri's results and ours is increased when the binding energy approaches the maximum. The maximum difference is equal to $0.35\,R^*$ which is much larger than that in the SQW. It means that the coupling effect is more important in the MQW than in the SQW.

In conclusion, we have used the novel trial function and obtained larger binding energies and their maxima not only in SQWs but also in MQWs. It shows that our trial function is excellent for the ground state of a shallow donor in narrow GaAs–$Ga_{1-x}Al_xAs$ QWs and that the coupling effect is stronger in MQWs than in SQWs. Finally, it is worthwhile to point out that the concept of the coupling is important not only in shallow impurity states of QWs but also in exciton states of QWs. It is, therefore, interesting to extend the present work to the calculation of the maximum of exciton binding energy in QWs and other kinds of calculations, for example, the exciton-tunnelling-lifetime enhancement by the coupling in a QW with a perpendicular field (Wu *et al* 1988).

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