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Hydrogenic impurities in GaAs–$Ga_{1-x}Al_xAs$ superlattices in an axial magnetic field

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Abstract. The binding energies of the ground state and the low-lying excited states of hydrogenic impurity in a GaAs–$Ga_{1-x}Al_xAs$ superlattice in a magnetic field have been calculated by applying the method of one-dimensionalization and the effective-mass approximation. In our calculations, the effects due to the different effective masses of electrons in different materials are included. Our results agree better with the experimental results than those of the calculation of a single quantum well.

1. Introduction

In recent years the hydrogenic impurity states relevant to semiconductor superlattices have become the subject of extensive experimental and theoretical investigations. Among these superlattices, GaAs–$Ga_{1-x}Al_xAs$ is regarded as the simplest and, consequently, has been the most extensively studied thus far. Bastard [1] was the first to treat the problem of a hydrogenic impurity state in a quantum well representing these systems but the horizontal stretch of his variational wavefunctions is larger than the real situation. Mailhiot *et al* [2, 3] and Greene and Bajaj [4] independently studied the binding energy of the hydrogenic impurity states in a well with realistic finite barriers, but their variational wavefunctions cannot give exact solutions for bulk $Ga_{1-x}Al_xAs$ and bulk GaAs when the well width $L \to 0$ and $L \to \infty$. Zhen-Peng Liu [5] calculated the hydrogenic impurity states in the infinite quantum well of GaAs–$Ga_{1-x}Al_xAs$ systems, which improved the results of [1]. He used the method of one-dimensionalization developed in [6]. Afterwards, Zhen-Peng Liu and Lin [7] calculated the hydrogenic impurity states in GaAs–$Ga_{1-x}Al_xAs$ finite quantum well structures by using the method of one-dimensionalization, which solved the problems appearing in [2–4]. However, there is no applied field in all the above-mentioned calculations.

Bajaj and co-workers [8, 9] calculated the binding energy of a hydrogenic impurity in a GaAs–$Ga_{1-x}Al_xAs$ symmetric quantum well in a magnetic field, which did not take into account the effects due to different effective electron masses in the GaAs and $Ga_{1-x}Al_xAs$ layers, and their results cannot give exact solutions of the bulk impurity states in the limiting case. Shu-Shen Li and Shan-Qing Jiao [10] have calculated the binding energies of the ground state and the low-lying excited states of a hydrogenic

impurity in a symmetric quantum well in a magnetic field, and they obtained the exact solutions which are well known for the limiting case.

In this paper we derive the one-dimensional equation of a hydrogenic impurity in superlattices in an applied magnetic field. In our calculation, we take into account the effects due to different effective electron masses in the GaAs and $Ga_{1-x}Al_xAs$ layers.

In section 2 we shall give the one-dimensional Schrödinger equation of a hydrogenic impurity in a GaAs–$Ga_{1-x}Al_xAs$ superlattice in a magnetic field. The main numerical results are in section 3. In section 4 we shall give a short summary and a discussion of our results.

2. Theoretical calculation

We consider the superlattice system of GaAs–$Ga_{1-x}Al_xAs$ structures; the superlattice structure forms many one-dimensional quantum wells for hydrogenic impurities, the layers of GaAs are wells and the layers of $Ga_{1-x}Al_xAs$ are barriers. This one-dimensional periodic potential can be obtained by the Kronig–Penney model. Let a, b and c be the period, the width of wells and the width of barriers; then $a = b + c$. The origin is chosen at the centre of the well. The z axis is along the superlattice axis, which is perpendicular to the layer planes. A magnetic field B is applied along the z axis. Then in the effective-mass approximation the corresponding Schrödinger equation and Hamiltonian of hydrogenic impurity are

$$\left\{\left[\sum_{n=-\infty}^{\infty}\theta(\tfrac{1}{2}b-|z-na|)\right]H_1+\left[\sum_{n=-\infty}^{\infty}\theta(\tfrac{1}{2}c-|z-(n+\tfrac{1}{2})a|)\right]H_2\right\}\psi=E\psi \tag{1a}$$

$$H_1=(1/2m_1^*)[-\hbar^2\nabla^2+(e^2B^2/4c^2)\rho^2+(eB/c)L_z]-e^2/\varepsilon_1 r \tag{1b}$$

$$H_2=(1/2m_2^*)[-\hbar^2\nabla^2+(e^2B^2/4c^2)\rho^2+(eB/c)L_z]-2e^2/(\varepsilon_1+\varepsilon_2)\gamma+V_0 \tag{1c}$$

where m_1^* and ε_1 are the effective mass and the dielectric constant of the bulk GaAs, and m_2^* and ε_2 refer to the interpolated values in $Ga_{1-x}Al_xAs$. z_0 is the coordinate of the impurity site. L_z is the angular momentum of the hydrogenic impurity along the z axis. θ is the step function.

If all the energies and distances are measured in units of the GaAs effective Rydberg constant $R_1^*(=m_1^*e^4/2\hbar^2\varepsilon_1^2)$ and the GaAs effective Bohr radius $a_1^*(=\hbar^2\varepsilon_1/m_1^*e^2)$, respectively, then the Hamiltonians (1b) and (1c) can be rewritten as

$$H_1=-\nabla^2+\tfrac{1}{4}\gamma^2\rho^2+\gamma L_z-2/r \tag{2b}$$

$$H_2=\alpha(-\nabla^2+\tfrac{1}{4}\gamma^2\rho^2+\gamma L_z)-2\beta/r+V_0 \tag{2c}$$

where

$$\alpha=m_1^*/m_2^* \qquad \beta=2\varepsilon_1/(\varepsilon_1+\varepsilon_2) \qquad \gamma=e\hbar B/2m_1^*cR_1^*. \tag{2d}$$

The wavefunction satisfies the following boundary conditions [11]:

$$\Psi_-=\Psi_+ \tag{3a}$$

$$(\partial\Psi/\partial z)|_-=\alpha(\partial\Psi/\partial z)|_+ \tag{3b}$$

where $\pm$ denote $|Z|\to na+\frac{1}{2}b+0^{\pm}$.

According to the procedure of one-dimensionalization [7], the wavefunction of equation (2) may be written as

$$\Psi = f_1^{-1/2} W(z) \Phi \exp(\lambda r). \tag{4}$$

We can obtain a one-dimensional Schrödinger equation:

$$\left\{\left[\sum_{n=-\infty}^{\infty} \theta(\tfrac{1}{2}b - |z - na|)\right]\tilde{H}_1 + \left[\sum_{n=-\infty}^{\infty} \theta(\tfrac{1}{2}c - |z - (n+\tfrac{1}{2})a|)\right]\tilde{H}_2\right\} W(z) = EW(z) \tag{5a}$$

$$\tilde{H}_1 = -\mathrm{d}^2/\mathrm{d}z^2 + U \tag{5b}$$

$$\tilde{H}_2 = -\alpha\, \mathrm{d}^2/\mathrm{d}z^2 + \bar{U}. \tag{5c}$$

The one-dimensional equivalent potentials are

$$U = -K/F_1 - \tfrac{1}{4}(F_1'/F_1)^2 + (\gamma^2/4)(F_4/F_1) + m\gamma \tag{5d}$$

$$\bar{U} = V_0 + \alpha U + 2(\alpha - \beta)F_2/F_1 \tag{5e}$$

with

$$K = \tfrac{1}{2}(\eta F_1' - F_1'') + \lambda[F_2 + \eta(F_1 - z_1 F_2) + z_1 F_2'] + F_3 \tag{5f}$$

and the boundary conditions

$$W_- = W_+ \tag{6a}$$

$$(\mathrm{d}W/\mathrm{d}z)|_- = \alpha(\mathrm{d}W/\mathrm{d}z)|_+. \tag{6b}$$

Hereafter the prime means a derivative of the function with respect to z. f_i ($i = 1, 2, 3, 4$) is

$$f_1 = \int \exp(2\lambda r)\, |\Phi|^2 \,\mathrm{d}x\,\mathrm{d}y = A \exp(-\eta z_1)\, F_1(z_1) \tag{7a}$$

$$f_2 = \int \exp(2\lambda r)\, |\Phi|^2 \frac{1}{r} \,\mathrm{d}x\,\mathrm{d}y = A \exp(-\eta z_1)\, F_2(z_1) \tag{7b}$$

$$f_3 = \int \exp(2\lambda r)\, \Phi\Omega^* \,\mathrm{d}x\,\mathrm{d}y = A \exp(-\eta z_1)\, F_3(z_1) \tag{7c}$$

$$f_4 = \int \exp(2\lambda r)\, |\Phi|^2 \rho^2 \,\mathrm{d}x\,\mathrm{d}y = A \exp(-\eta z_1)\, F_4(z_1). \tag{7d}$$

F_i ($i = 1, 2, 3, 4$) is a polynomial of z_1 and A is a common constant with respect to z_1 but depends on η, and

$$z_1 = |z - z_0| \qquad \eta = 2(1/n - \lambda)$$

where φ is the same as in [7].

The magnetic quantum number $m = 0$ for the ground state; choosing φ_{100} as the skeletal state and $\xi_r = 0$, one obtains

$$K = 1 + \lambda \qquad F_1 = z_1 + 1/[2(1-\lambda)]$$
$$F_2 = 1 \qquad F_3 = 0 \tag{8}$$
$$F_4 = [1/(1-\lambda)][z_1^2 + 3z_1/2(1-\lambda) + 3/4(1-\lambda)^2].$$

When the skeletal states are $2p_{xy}$, $\varphi_{n,l,m} = \varphi_{2,1,\pm 1}$ and $\xi_r = 0$, we obtain

$$K = (1+2\lambda)z_1 + (1+6\lambda)/2(1-2\lambda)$$
$$F_1 = z_1^2 + 3z_1/(1-2\lambda) + 3/(1-2\lambda)^2$$
$$F_2 = z_1 + 1/(1-2\lambda) \tag{9}$$
$$F_3 = 0$$
$$F_4 = [4/(1-2\lambda)][z_1^3 + 6z_1^2/(1-2\lambda) + 15z_1/(1-2\lambda)^2 + 15/(1-2\lambda)^3].$$

It is quite evident that the exact results can be obtained in the limiting case when γ^2-terms are omitted.

3. Numerical results

We adopt the material parameters in [2, 3, 12]:

$$V_0 = 0.85(1.155x + 0.37x^2)\ \text{eV}$$
$$m_1^* = 0.067m_0 \qquad m_2^* = (0.067 + 0.083x)m_0 \tag{10}$$
$$\varepsilon_1 = 13.1\varepsilon_0 \qquad \varepsilon_2 = [13.1(1-x) + 10.1x]\varepsilon_0.$$

Here m_0 and ε_0 are the free-electron mass and vacuum static dielectric constant, respectively. Let the aluminium concentration x be 0.3.

The ground-state energy E_0 of an electron in the superlattice without an impurity potential and magnetic field may be determined by numerically solving the transcendental equation

$$[(\alpha^2\xi^2 - \eta^2)/2\alpha\xi\eta]\sin(\eta b)\sinh(\xi c) + \cos(\eta b)\cosh(\xi c) = 1 \tag{11a}$$
$$\xi = [m_2(V_0 - E_0)/m_1]^{1/2} \qquad \eta = (E_0)^{1/2} \tag{11b}$$

for E_0.

Thus the impurity binding in a magnetic field is

$$E_b = E_0 + \gamma - E \tag{12}$$

where γ is the energy of the first Landau level [13].

Figure 1 shows the energy spectrum of the centre of the GaAs-well hydrogenic impurity ground state as a function of the slab thicknesses of GaAs and $Ga_{1-x}Al_xAs$ (let $b = c = L$). Comparing our results with those in [9, 10], we find that the peaks will appear in a wider well structure (L is approximately $0.7a_1^*$ in the superlattice but approximately $0.1a_1^*$ in a single quantum well) and the intensities of the peaks are

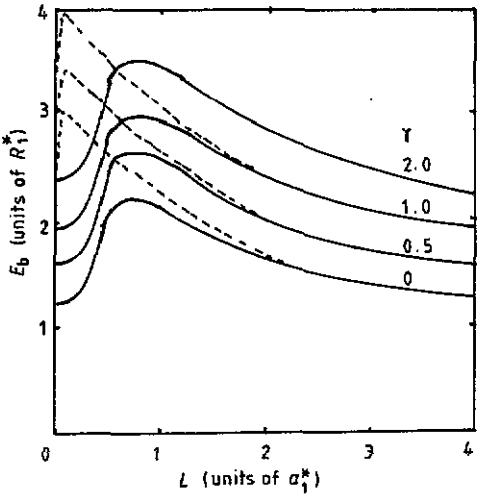

Figure 1. Variation in the binding energies of the ground state as a function of the slab thickness ($b = c = L$): ——, our results; – – –, results in [9, 10].

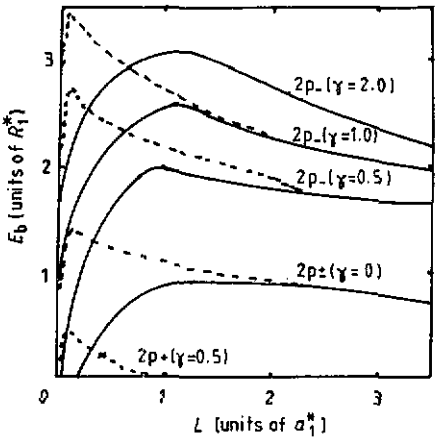

Figure 2. The binding energies of the 2p state as a function of the slab thickness ($b = c = L$): ——, our results; – – –, results in [9, 10].

smaller than those of a single quantum well. This is because the hydrogenic impurity has a smaller binding energy in a superlattice than in a single quantum well.

Figure 2 shows the binding energy of 2p states for a donor at the centre of a GaAs quantum well as a function of the well size (let $b = c = L$). From this figure it can be seen that the peaks also appear in a wider well structure in a superlattice; L is about $0.9a_1^*$. This value is larger than that in a single quantum well (about $0.05a_1^*$). The intensities of the peaks are smaller than those of a single quantum well. When $L > 2.0a_1^*$, the results for a superlattice are approximately equal to those of a single quantum well.

4. Summary and discussion

In theoretical calculations it is necessary to take into account the multilayer effect of the superlattice since experimental samples are almost all multilayer structures and a single quantum well is not a good approximation unless the width of the GaAs slab is sufficiently large. To our knowledge, it is the first time that the binding energy of a hydrogenic impurity in a GaAs–$Ga_{1-x}Al_xAs$ superlattice in a magnetic field has been calculated. In comparing our calculation with a single-well model, we find broadened and lower peaks.

Recently, Jarosik *et al* [14] have measured the energy transition value of a hydrogenic impurity in a GaAs–$Ga_{1-x}Al_xAs$ quantum well structure in a magnetic field. They studied the energy transition values of $1s \rightarrow 2p_+$ and $1s \rightarrow 2p_-$ for a hydrogenic impurity at the centre of a GaAs quantum well as a function of magnetic field. The differences

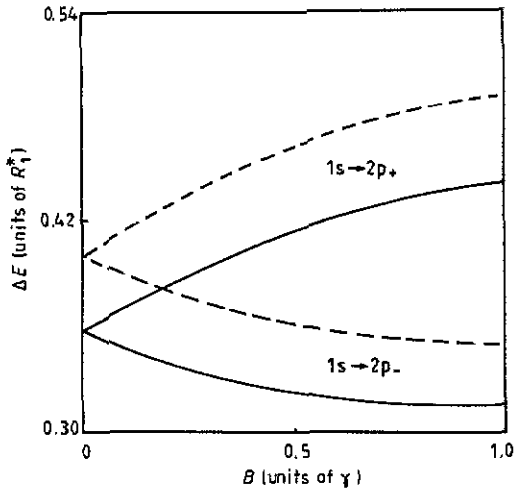

Figure 3. The differences between the theoretical and experimental results: ——, our results; – –, results in [9, 10].

between the theoretical calculation and the experimental results are shown in figure 3. Our results are closer to the results of Jarosik *et al* than to those in [9, 10], although our improvement is not very important. The thickness of slab, L, in [14] is equal to $1.5a_1^*$. From figures 1 and 2 it can be seen that this value is too large for the multilayer effect to be significant, which will become more important as L becomes smaller.

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