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Magnetic field effect on the binding energy of a hydrogenic impurity in GaAs-$Ga_{1-x}Al_xAs$ superlattice

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Abstract. The binding energy of shallow hydrogenic impurity in GaAs-$Ga_{1-x}Al_xAs$ superlattices, under the influence of magnetic field, is theoretically studied following a variational procedure within the effective-mass approximation and the new analytic wave function of superlattice. The binding energy is calculed and analyzed for various applied magnetic field, different impurity position and superlattice with different widths. The result show that the impurity binding energy depends strongly on the impurity position and magnetic field. It is also found that for impurities located at the center of the quantum wells of superlattices the binding energy always increases with the applied magnetic field.

Keywords: semiconductor superlattice, impurity, binding energy, magnetic field.

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1. Introduction

With the development of several techniques, such as molecular beam epitaxy, metal organic chemical-vapor deposition and electron beam lithography combined with reverse mesa etching, it has been possible to realize the low dimensional quantum nanostructures. Such as quantum well (QW), quantum well wires (QWW), quantum dot (QD) and superlattice (SL), with very precisely controlled sizes and sharp interfaces. The physical properties of superlattices such as optical and electronic transport characteristics [1-8] differ from those of the bulk semiconductor constituents because the transition symmetry is broken. It is expected that these characteristics will be more pronounced as the electronic confinement increases with further reduction of dimensions [9-10]. Because they are presently utilized in ultrafast electronic devices, many theoretical and experimental works have been devoted to them [11-16].

The study of hydrogenic impurities is of the main problems in semiconductor superlattice [17, 18], because the presence of the impurity states in these nanostructures influences greatly both the electronic mobility [19] and their optical properties [20]. In various papers investigated were the hydrogenic impurity states in GaAs-$Ga_{1-x}Al_xAs$ quantum wells using both the infinite and finite potentials at the interface. Bastard [21] reported the first calculation for binding energies of hydrogenic impurities in quantum wells with an infinite potential in barriers. Chaudhuri and Bajaj include the effect of the band nonparabolicity in their calculations, where the effective mass of electron was only associated with the lowest subband of the quantum wells. Chaudhuri [22] extended the variational calculations of the ground-state energy of the donor electron in quantum wells to the situation of multiple–well structure.

The problem of the energy levels of an impurity in the presence of magnetic fields has become of increasing interest in semiconductor physics where typical values of the effective mass m^* and the dielectric constant ε make the effective Rydberg $\mathrm{Ry}^* = m^* e^4/(2\varepsilon^2\hbar^2)$. The magnetic field effect on impurity states can be measured by the dimensionless parameter $\gamma = \hbar\omega_c/(2R^*)$, where $\omega_c = eB/m^*$ is the cyclotron frequency of the carrier in the field *B*. For magnetic field such $\gamma << 1$, where the low-field perturbation method become applicable, the coulombic potential governs the magnetic field effect. Whereas for $\gamma >> 1$, the magnetic force on the electron is much greater than the Coulomb force, so the electron is tightly bound in the plane perpendicular to the magnetic field and comparatively weakly bound in the field direction.

The purpose of this paper is to study the magnetic field and the impurity position dependences of the

binding energy of hydrogenic impurity in superlattice. We employ the variational scheme. In the absence of the impurity, the wave function is the product of the new exact analytic eigenfunction of the superlattice. Hamiltonian along the *z*-axis and in the (x – y) plane without any restriction on the magnetic field. The remaining part of this paper is organized as follows. In Section 2, we present our approach to the problem of shallow donor impurities in the superlattice in the presence of the magnetic field using the new analytic waves of the superlattice [23]. The discussion of the results and the conclusion are given in Section 3.

2. Theoretical framework

We consider an in-plane magnetic field along the y direction, with a gauge choice for the vector potential such that $\vec{A} = zB\vec{i}$. The Hamiltonian for the carrier in the conduction miniband, within the effective mass approximation and using a parabolic-band model is

$$H_0 = \frac{1}{2m^*}\left(P_x + eBz\right)^2 + \frac{1}{2m^*}P_y^2 + \frac{1}{2m^*}P_z^2 + V(z), \qquad (1)$$

where $-e$ is the electron charge, $m^*(z)$ is the effective mass of the conduction electron. V(z) is the superlattice potential which is zero at the well and V_b in the barrier. V_b is about 60 of the bandgap difference $\Delta E_g = 1.247x$ between $Ga_{1-x}Al_xAs$ and GaAs for the conduction. The eigenstates $|\xi\rangle$ and eigenvalues ε_ξ of Eq. (1) are:

$$|\xi\rangle = \left|N,\ k_y\right\rangle \otimes \left|n_i, i, k_z\right\rangle = \\ = \Phi_N(z - I^2 k_z)(e^{ik_y y}\sqrt{y}) \otimes \left|n_i, i, k_z\right\rangle, \qquad (2)$$

$$\varepsilon_\xi = \varepsilon_{N,i,k_z} = (N + \frac{1}{2})\hbar\omega_0 + \varepsilon_j(k_z), \qquad (3)$$

$N = 0, 1, \ldots, i = 1, 2, \ldots$.

where $\omega_0 = |e|B/m^*$ is the cyclotron frequency, $I = \left(\hbar / m_w^* \omega_0\right)^{\frac{1}{2}}$ is the radius of the cyclotron orbit, m_w^* is the effective mass in the quantum wells of superlattice. Further Φ_N represents the harmonic oscillator wave function centred at $z = I^2 k_{x,N}$, with the Landau level index N and $\left|n_i, i, k_z\right\rangle$ wave function in the z-direction with eigenvalue $\varepsilon_j(k_z)$, j being the miniband index.

$$\left\langle z \middle| n, i, k_z \right\rangle = \psi(z - nl) = \frac{e^{ik_z l}}{\sqrt{S}}\varphi(z - nl), \qquad (4)$$

where

$$\varphi(z - nl) = \frac{e^{-ik\frac{1}{2}}e^{ink_z l}}{\sqrt{N}}$$

$$\begin{cases} \{p^* \cosh[\rho(z - nL + L_w/2)] + \\ q^* \sinh[\rho(z - nL + L_w/2)]\}; & -b - L_w \le z - nL \le -L_w/2 \\ b_2 \exp ik(z - nL) + \\ + \beta \exp -ik(z - nL); & -L_w/2 \le z - nL \le L_w/2 \\ \{p \cosh[\rho(z - nL - L_w/2)] + \\ q \sinh[\rho(z - nL - L_w/2)]\}; & L_w/2 \le z - nL \le b + L_w/2 \end{cases} \qquad (5)$$

with

$\hbar^2 k^2 = 2m_w^* E$, $\hbar^2 \rho^2 = 2m_b^*(V_b - E)$, $\lambda = m_w^*/m_b^*$,

$L = L_b + L_w$, $x = k L_w$, $y = \rho L_w L$,

$$\beta^- = \sin(x)\cosh(x) - \\ - K^- \cos(x)\sinh(y) - \sin(k_z l),$$

$$p = b_2 e^{(ix/2)} + \beta^- e^{-(ix/2)},$$

$$q = \frac{ik}{\lambda\rho}\left(e^{(ix/2)} - \beta^- e^{-(ix/2)}\right),$$

$$k^\pm = \frac{1}{2}\left(\frac{\lambda\rho}{k} \pm \frac{k}{\lambda\rho}\right),\ b_2 = K^+ \sinh(y),$$

$$N = A'\left(b_2^2 + \left(\beta^-\right)^2\right) + B'\beta^-,$$

$$\Pi^\mp = \left(\frac{2K}{\lambda\rho}\right)K^\pm$$

$$A' = L_w + \left(L_b\left[\frac{\Pi^-}{2} + \Pi^- \frac{\sinh(2y)}{4y}\right]\cos x + \right. \\ \left. + \left[\frac{1}{k} - \frac{k}{\lambda\rho}\frac{\cosh(2y) - 1}{2\rho}\right]\sin(x)\right),$$

$$B' = 2b_2\{L_b[\Pi^+/2 + \\ + \Pi^-(\sinh(2L_b\rho)/4L_b\rho)]\cos(kL_w) + \\ + [(1 - \cosh(2L_b\rho)2\lambda\rho)k + 1/k]\sin(kL_w), \qquad (6)$$

$$\varepsilon_j(k_z) = E_1^* - (-1)^j \frac{\Delta_j}{2}\cos(k_z l),$$

Δ_j is the miniband width and k_x, k_y, k_z are the wavevectors in the x-, y-, z-direction, respectively.

In the presence of a shallow donor impurity, the Hamiltonian of one electron is

$$H_1 = H_0 - \frac{e^2}{\varepsilon_0\sqrt{(z - z_i)^2 + r_\perp^2}}, \qquad (7)$$

where $\varepsilon_0 = 12.35$ is the dielectric constant of GaAs, $r = \sqrt{r_\perp^2 + (z - z_i)^2}$ is the electron position relatively to the impurity, where z_i is the position of the impurity along the growth direction. The trial wave function considered is:

$$\psi_\alpha = A\psi(z - nL)\exp(\frac{1}{\alpha}\sqrt{r_\perp^2 + (z - z_i)^2}) \qquad (8)$$

with α being a variational parameter obtained by minimizing the impurity energy [24-26] and A constant being the normalization factor. The binding energy of the impurity is given by

$$E_b(z_i) = \varepsilon_\xi - \min_\alpha \langle \Psi_\alpha | H_1 | \Psi_\alpha \rangle . \qquad (9)$$

3. Numerical results and discussion

For numerical computations, we have chosen the GaAs-$Ga_{1-x}Al_xAs$ as a superlattice. The parameters pertaining to the system are: $x = 0.1$, $V_b = 18\text{Ry}^*$, barrier size $L_b = 0.50a^*$, $a^* = 98.88$ Å, $\text{Ry}^* = 5.53$ meV, $m_w^* = 0.067m_0$, $m_b^* = 0.092m_0$, m_0 is the free electron mass, Ry^* is the donor effective Rydberg and a^* is the effective Bohr radius.

In Fig. 1, we display the variation of the binding energies as a function of the well width in the superlattice for fixed barrier L_b and different values of $k_z l$. As for the case of the finite square [27-30] and of the quantum-well wires [31], the binding energy increases as the size of the well is reduced, until it reaches a maximum value, for $L_w = 0.51a^*$ in our calculations, and then it starts decreasing. This behaviour is explained by the fact that, as the value of L_w is reduced, the particle becomes confined in a narrower region, which leads to increased binding.

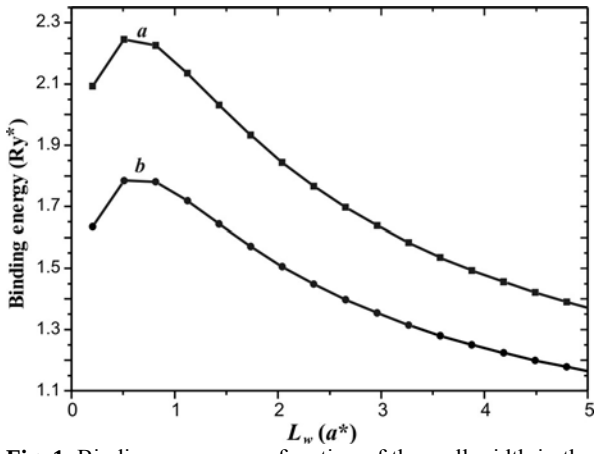

Fig. 1. Binding energy as a function of the well width in the superlattice: a) for $k_zL = \pi/L$ and b) for $k_zL = 0$.

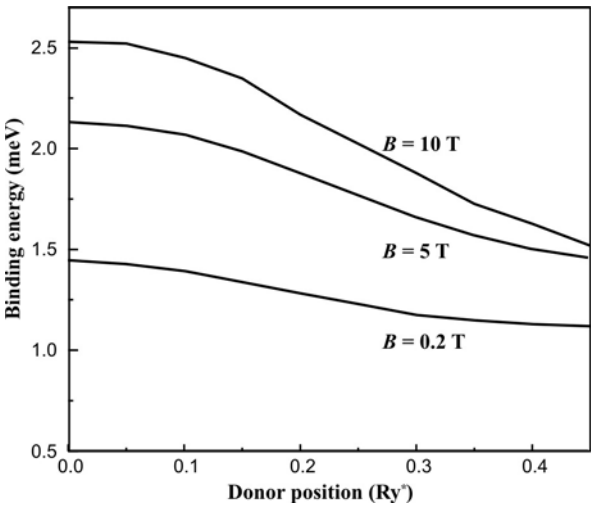

Fig. 2. Donor binding energy as a function of the impurity position for various values of the magnetic field.

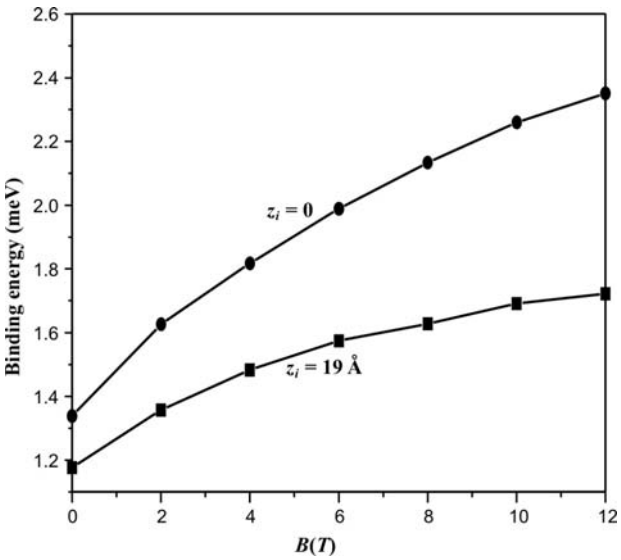

Fig. 3. Donor binding energy as a function of the magnetic field for various values of the impurity position z_i .

Fig. 2 shows that the binding energy is enhanced in proportion with an increase of the magnetic field for any impurity position. In Fig. 3, we display the variation of the binding energy as a function of the magnetic field in the superlattice for the donor position. We observed that for an impurity located at the centre of the well, the binding energy increases with the magnetic field, while for an impurity located next to the border of the wells, the binding energy decreases with the magnetic field because the electronic amplitude probability increases as the magnetic field is augmented.

In conclusion, we have studied in the effective-mass approximation and with the new analytic wave function associated to electron miniband conduction the properties of a hydrogenic donor impurity in the presence of the magnetic field. We have shown that the impurity binding energy depends strongly on the impurity position and magnetic field.

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