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HAL Id: jpa-00249401
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Submitted on 1 Jan 1995

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Excitonic Properties in GaAs Parabolic Quantum Dots

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(Received 14 April 1995, revised 19 June 1995, accepted 11 July 1995)

Abstract. — Certain classes of semiconductor quantum dots being actually fabricated exhibit a nearly parabolic confinement for both the electron and the hole. In undoped quantum dots, excitonic effects are important. In this work, first we present theoretical results on exciton properties in parabolic quantum dots: resonance energy, binding energy and oscillator strength. Then, we investigate the effects of external electric and magnetic fields on exciton in quantum dots.

1. Introduction

The development of high-quality layered semiconductor materials has motivated research in physics of systems with reduced dimensionality. Advances in the nanofabrication of semiconductors structures: Quantum Wells (QW), Quantum Well Wires (QWW) and Quantum Dots (QD) systems bring new phenomena in semiconductor physics and give rise to very promising application in optoelectronics and performance of the transistors and lasers. Excitons in these confined systems are important. Confinement of excitons in parabolic quantum dots nanostructures enhances their optical properties [1–3]. There has been considerable recent interest in the physics of excitons in semiconductors with reduced dimensionality in the absence or presence of a magnetic or electric field. Halonen et al. [6] investigated the properties of an exciton in a parabolic quantum dot in an external magnetic field. The results for the interplay between the competing spatial and magnetic effects for the ground state and low-lying excited states are presented. Effects of electric field on excitons in quantum wells have been of interest for many years. The calculations of electric-field-effects on the ground-state of the exciton in quantum wells have been performed by Bastard et al. [9].

In this contribution, we present a theoretical study of the optical properties of excitons in parabolic quantum dots. The quantum dots being fabricated now [1] have parabolic confinement potential. The effects of external electric or magnetic fields on excitons in parabolic quantum dots are analyzed.

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2. Formalism

Our calculation is based on the effective-mass approximation and ignores the valence bandstructure effects. For simplicity, we consider the GaAs quantum dot with the parabolic confinement for the electrons and holes having the same quantization energy $\hbar \Omega$ [3-5]. We present the total Hamiltonian for the exciton in a parabolic quantum dot in the presence of an electric $(F)$ and a magnetic $(B)$ fields applied in the same direction ($z$-axis), which can be expressed as:

$$H = H_e + H_h - \frac{e^2}{\epsilon r}$$

\(H_e = \frac{1}{2m_e}(p_e - \frac{e}{c}A_e)^2 + \frac{1}{2} m_e \Omega^2 r^2_e - e F z_e\)

\(H_h = \frac{1}{2m_h}(p_h + \frac{e}{c}A_h)^2 + \frac{1}{2} m_h \Omega^2 r^2_h + e F z_h\)

where \(H_e\) and \(m_e\) are the single-particle Hamiltonian and the effective-mass for the electron (hole). $\epsilon$ is the GaAs background dielectric constant. In order to solve this total Hamiltonian, we use the relative coordinate $r = (r_e - r_h)$ and the corresponding momenta $p$ with reduced mass $\mu$ and center-of-mass coordinate and the corresponding momenta $P$ with the total-mass $M$. For the magnetic vector potential, we consider the symmetric gauge vector potentials for the electron and hole as in reference [6]. According to references [4,6], the crossed term in the Hamiltonian $H$, which couples the center-of-mass and relative motions leads to a negligible perturbation of the ground exciton energy. Then it is neglected in the following (see also below). We can see that the exciton properties in the ground-state can be essentially determined by the relative Hamiltonian $H_r$. The relative Hamiltonian describing the exciton motion is:

$$H_r = \frac{p_{\perp}^2}{2\mu} + \left( \frac{1}{2} m\Omega^2 + \frac{1}{2} \mu \Omega^2 \right) \rho^2 + \frac{p_{\parallel}^2}{2\mu} + \frac{1}{2} m\Omega^2 z^2 - e F z - \frac{e^2}{\epsilon \sqrt{\rho^2 + z^2}}$$

where $p_{\perp}$ and $p_{\parallel}$ are the transverse and longitudinal electron-hole relative momenta respectively. To solve this hamiltonian, we add and subtract to the relative electron-hole hamiltonian $H_r$ a term $V(r)$ in order to split $H_r + V(r)$ into two parts [3,4]. The first one $H_0$ should be analytically solvable while the second one $H_1$, expected to be small, will be treated by first order perturbation calculus on the eingenstates of $H_0$. Then we choose [3-5]: $V(r) = \lambda(\frac{1}{2}\mu \Omega^2 r^2 - \hbar \Omega)$; where $\lambda$ is still an unknown parameter. In this case

\(H_0 = \frac{p_{\perp}^2}{2\mu} + \left( \frac{1}{2} \mu \Omega^2 + \frac{1}{2} \mu \Omega^2 \right) \rho^2 + \frac{p_{\parallel}^2}{2\mu} + \frac{1}{2} \mu \Omega^2 z^2 - \frac{e^2 F^2}{2\mu \Omega^2(1 + \lambda)} - \lambda \hbar \Omega\)

\(H_1 = -\frac{e^2}{\epsilon \sqrt{\rho^2 + (z + z_1)^2}} - \lambda \left[ \frac{1}{2} \mu \Omega^2 r^2 - \hbar \Omega + \frac{1}{2} \mu \Omega^2 z_1(z_1 + 2z) \right] \)

where $z_1 = eF/\mu \Omega^2(1 + \lambda)$. The perturbed term $H_1$ restores the character of the Coulomb interaction. The unknown parameter $\lambda$ in equations (3) is determined by requiring that the first order energy shift $<\Psi_\lambda|H_1|\Psi_\lambda>$ vanishes, where the $\Psi_\lambda$ is the ground state of $H_0$. The zero$^{th}$ order wavefunction and energy of the ground state of $H_0$ are determined exactly. This
is possible because the unperturbed eingentfunctions are separable and analytically expressed as:

$$\chi(R, r, B, \lambda) = \Phi(R)\psi(\rho, B, \lambda)\theta(z, \lambda)$$
$$= \Phi(R)\left(\frac{1}{R_B\sqrt{\pi}}\right)\left(\frac{1}{R_r\sqrt{\rho}}\right)^{1/2}e^{-\rho^2/2R_r^2}e^{-z^2/2R_B^2}$$

(4)

with the total energy:

$$E_T(F, B) = \frac{3}{2}h\Omega + \frac{1}{2}h\Omega_r + h\Omega_B - \frac{e^2F^2}{2\mu\Omega^2(1 + \lambda)} - \lambda h\Omega$$

(5)

$$R = \sqrt{\frac{h}{\mu\Omega}}, R_r = \frac{R}{\sqrt{1 + \lambda}},$$
$$R_B = \sqrt{\frac{h}{\mu\Omega_B}}, \Omega_B = \sqrt{\omega^2 + \Omega^2(1 + \lambda)}, \Omega_r = \Omega(1 + \lambda)$$

where the first term in equation (4) is the exciton center-of-mass wavefunction for a harmonic oscillator and the last terms correspond to the exciton relative motion: $\psi(\rho, \lambda)$ is the two-dimensional compression and $\theta(z, \lambda)$ the one-dimensional distortion of the exciton wavefunctions.

In equations (4,5) we have introduced the center-of-mass contribution.

Note that the crossed term $H_{\text{coup}} = i\hbar e \frac{\mathbf{B}}{M_c} \mathbf{r} \times \nabla \mathbf{R}$ couples only states of different relative and center-of-mass motions. Thus, the lowest order correction to the ground exciton energy equation (5) vanishes exactly.

We calculate the exciton binding energy defined by:

$$E_b(F, B) = E_e(F, B) + E_h(F, B) - E_T(F, B)$$

(6)

where $E_{e,h}$ is the ground state energy of non interacting electron-hole.

We calculate the oscillator strength of the exciton in the ground state in the dot normalized to that of a free exciton in a bulk material with volume $V = \frac{4}{3}\pi R^3$. The normalized oscillator strength is given by [2,7,8]:

$$f/f_{\text{ex}} = \frac{E_{\text{ex}}\pi a_{3D}^2D}{E_T(F, B)V}\left|\Psi_\lambda(R, z_1, F, B, \lambda)\right|^2$$

(7)

where $E_{\text{ex}}$ and $E_T(F, B)$ are the total exciton energies in the bulk and quantum dot respectively, and $a_{3D}$ is the bulk effective Bohr radius.

3. Excitons in Parabolic Quantum Dot ($F = 0, B = 0$)

We present detailed calculation for exciton referring to GaAs parabolic quantum dot with the parameter values: dielectric constant $\varepsilon = 13.1$, effective-masses for the electron ($e$), heavy hole (hh) and the light hole (lh), $m_e = 0.067 m_0$, $m_{hh} = 0.377 m_0$ and $m_{lh} = 0.09 m_0$ ($m_0$ is the free-electron mass). In the absence of the electric and magnetic fields we plot in Figure 1 the ground state energy and the binding energy, in Figure 2 and Figure 3 the relative
Fig. 1. — The exciton energy of GaAs parabolic quantum dot as a function of the effective confinement radius of the quantum dot $R$. The right ordinate indicates the (e-hh) exciton binding energy.

Fig. 2. — The normalized oscillator strength of the exciton in GaAs parabolic quantum dot as a function of the effective confinement radius of the quantum dot $R$.

Fig. 3. — The normalized exciton extension in GaAs parabolic quantum dot.

position and the normalized oscillator strength for the heavy hole exciton (e-hh) and the light hole exciton (e-lh) respectively, as function of the size quantum dot $R$. The heavy- and light-hole exciton energies are shown in Figure 1, the energy decreases rapidly with increasing radius. For smaller $R$, the exciton energy is sensitive to the quantum dot radius. For narrower dots, the effect of the parabolic confinement is more pronounced, leading to increasing exciton energies. For larger quantum-dot radius the exciton’s confinement becomes too weak, the exciton behavior begins to resemble that of the bulk. The Coulomb potential confines the
electron-hole pair via the quadratic and interaction potential \( V(r) \). In the bulk limit, the energies converge to the respective bulk-Rydberg of the heavy- and light-hole exciton. In Figure 1 we can see the decrease of the binding energy of the heavy-hole exciton confined in quantum dot with increasing dot size, and is found to be almost 2-3 times that of the one confined in quantum well [9] with the same size. The enhancement of the energy of the light-hole exciton is larger than that of heavy-hole for the same quantum dot radius, as expected from the lighter carrier mass, the quantum confinement effect appears more for (e-hl) than (e-hh) exciton. Figure 2 shows the electron-hole separation of the heavy- and light-hole exciton in the ground state, for narrower dots, the curve is linear and the normalised electron-hole position \( < r > / R \) approaches the unity [2,3,8]. The electron-hole separation becomes insensitive to the wide quantum dots and converges to the bulk value separation. The size dependence of the normalized oscillator strength (Fig. 3) is determined essentially by the integral in equation (7), while the energy-dependent term displays negligible variations [2,8]. As the quantum dot size is increased the envelope function becomes more and more flat, the integral term decreases rapidly and converges to a constant. This point has already been noticed in references [2,7,8]. This result should be generally independent of the confining and interaction potentials.

4. Stark Effect on Excitons in Parabolic Quantum Dot \((F_0 \neq 0, B = 0)\)

In the Hamiltonian \( H_r \) subjected to an applied electric field, the field term added to the \( z \)-direction confinement describes a displaced harmonic oscillator centred in \( -z_0 = eF/\mu \Omega^2 \) with the frequency \( \Omega_r < \Omega \), due to combined effects of the electric field and Coulombic potential. The exciton is bound only in \( x-y \) plane. The electron-hole pair is correlated in the transverse layer-plane by the Coulomb attraction. In Figure 4 we plot the calculated heavy-hole exciton resonance energy shift \( \Delta E \) versus the electric field strength for several quantum-dot radius: 50 Å, 80 Å, 120 Å and 200 Å. The variation of the exciton energy from 10 to 200 meV is found about the same as that in parabolic quantum-well [9,10]. The shift of the exciton in the wider quantum-dot presents a rapid decrease even at relatively low fields. In large quantum-dot size, the confinement is reduced and the exciton has the bulk behavior and cannot stand high fields. We can see that the energy decreases as the field strength increases. This result can be
explained easily: the electric field increased the distance between the electron and the hole so the exciton binding energy decreases. This indicates that the parabolic confinement work well in this range of quantum-dot size.

We see in Figure 5 that the polarization increases with the quantum-dot size. For a given quantum-dot, we see that the increase of the polarization with the increase of the electric field too. On the other hand, the electric field forces the carriers towards the walls. We notice for the box $R = 100 \text{ Å}$, the normalized polarization becomes greater than the unity for the range of strength field $F \geq 100 \text{ kV/cm}$. At high field the particles are pushed towards the limit of the dot. The wall of the dot (parabolic-confinement) prevents the particles from escaping from the dot.
Fig. 7. — Exciton binding energy in GaAs parabolic quantum dot as a function of magnetic and electric fields for two effective confinement radii of the quantum dot.

5. Magneto-Excitons in Parabolic Quantum Dot ($F_0 \neq 0, B_0 \neq 0$)

Numerical results of the exciton properties in the presence of an applied magnetic field in Figure 6 and 7. The set of curves in Figure 6 show the diamagnetic shift of exciton in the ground-state for different parabolic quantum dot radii, as a function of increasing magnetic field. The diamagnetic split increases as the magnetic field increases. The split is largest for wider quantum dots (weak confinement). The influence of the magnetic field on the exciton resonance energy is smaller than the electric field effect. Figure 7 shows the ground-state exciton binding energy as a function of magnetic field for two quantum dot sizes $R = 50$ Å and $R = 120$ Å. We see that the binding energy increases slowly for narrower quantum dots ($R = 50$ Å) in comparison with the wider one ($R = 120$ Å). The reason is that the exciton behaviour is more dominated by the influence of the confinement potential than that of the magnetic field effects. In the wider dots, diamagnetic split (Fig. 6,7) and binding energy are more affected by the increase of the magnetic field than the confinement potential. The application of the electric field induces a spatial separation of the carriers leading to a decrease in the binding energy. The application of the magnetic field leads to additional confinement, which induces an enhancement in the exciton binding energy. In the case of narrower dots, we have found that the binding energy is little affected by the electric and magnetic fields. The influence of the external fields is greater on exciton binding energy for wider quantum dots ($R > 100$ Å).
Acknowledgments

The authors would like to thank Gérald Bastard and Robson Ferreira for their fruitful discussions and help.

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