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Quasi one-dimensional excitons in a quantum wire subjected to a magnetic field

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We have calculated the binding energy and 'length' of a quasi one-dimensional exciton in a semiconductor quantum wire subjected to a magnetic field. The magnetic field causes these quantities to have *non-monotonic* dependences on wire width. Below a critical width, the binding energy decreases with increasing wire width as usual, but above this critical width the opposite behavior is observed. This gives rise to a pronounced minimum in the binding energy. A similar behavior gives rise to a pronounced maximum in the exciton length. These features are explained by invoking the complementary roles of the electrostatic and magnetostatic confinement of the exciton.

1. Introduction

Quasi one-dimensional excitons and biexcitons in quantum wires are dirctly responsible for the giant third order non-linear susceptibility $\chi^{(3)}$ in these systems. The large magnitude of $\chi^{(3)}$ is caused by the increased binding energy of excitonic complexes due to one-dimensional confinement. A magnetic field can further enhance the confinement, leading possibly to improved performance in non-linear optics, specifically in low power and high density systems. Additionally, the field can act as an agent to modulate the non-linear absorption/gain in quantum wires which opens up the possibility of realizing *externally tunable* couplers, limiters, phase shifters, switches, etc.

Recently, Someya, Akiyama and Sakaki [1] reported the effect of an external magnetic field on the exciton binding energy and radius in a GaAs quantum wire by measuring the photoluminescence spectra and comparing them with those of quantum wells. They found that a magnetic field squeezes the exciton wavefunction to a size that is far below what can be achieved in quantum wells. This is consistent with our observation. We provide a detailed theoretical calculation which sheds light on this effect.

This paper is organized as follows. In Section 2, the theory of a quasi 1D exciton subjected to a magnetic field is developed rigorously within the framework of a two band model and perfect confinement. Section 3 presents the results of the variational calculations of the binding energy and exciton 'length' followed by a discussion of the excitonic properties. Conclusions are given in Section 4.

2. Theory

2.1 Exciton binding energy

Let us consider a quantum wire as shown in the inset of Fig. 1 with infinite potential barriers located at $y = \pm L_y/2$ and $z = \pm L_z/2$. A magnetic field of flux density B is applied along the z-direction.

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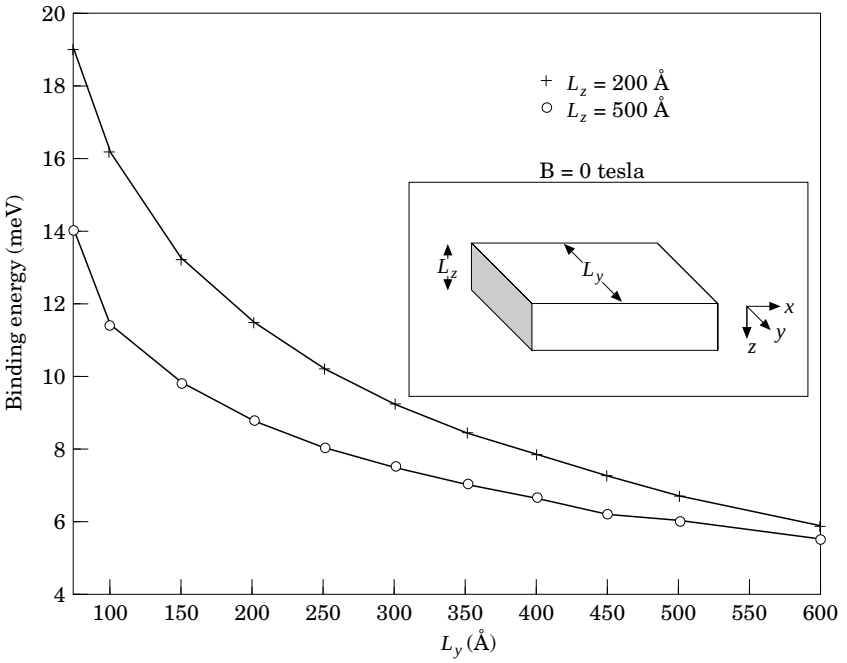

Fig. 1. Exciton binding energy in a GaAs quantum wire as a function of wire width L_y for two different values of wire thickness L_z. No magnetic field is present. The binding energy decreases with increasing wire width approaching the bulk value in sufficiently wide wires. The decrease is more rapid in the thicker wire because of the weaker confinement along the thickness. The inset shows a wire with the various coordinate directions defined.

For nondegenerate and isotropic bands, the Hamiltonian of a free Wannier exciton in this system is given within the envelope-function approximation by

$$\hat{H}^X = \frac{1}{2m_e}(\hat{p}_{x_e} - eBy_e)^2 + \frac{1}{2m_h}(\hat{p}_{x_h} + eBy_h)^2 + \frac{\hat{p}_{y_e}^2 + \hat{p}_{z_e}^2}{2m_e} + \frac{\hat{p}_{y_h}^2 + \hat{p}_{z_h}^2}{2m_h}$$
$$- \frac{e^2}{4\pi\varepsilon[(x_e - x_h)^2 + (y_e - y_h)^2 + (z_e - z_h)^2]^{1/2}} + V_{conf}(y_e, y_h, z_e, z_h) \quad (1)$$

where we have chosen the Landau gauge for the magnetic vector potential:

$$\vec{A} = (-By, 0, 0).$$

The quantities $m_{e,h}$ and $x_{e,h}$, $y_{e,h}$, $z_{e,h}$ are the effective masses and coordinates of electrons and holes, respectively, ϵ is the dielectric constant, $V_{conf}(y_e, y_h, z_e, z_h)$ is the confinement potentials for electrons and holes along y and z directions.

For convenience, we replace $x_{e,h}$-coordinates by the center-of-mass (X) and relative coordinates (x). This is accomplished by using quantum mechanical definition of momentum operators and taking into account that in a center-of-mass and relative coordinate system

$$\hat{p}_{x_{e,h}} = -i\hbar \frac{m_{e,h}}{M} \frac{\partial}{\partial X} \mp i\hbar \frac{\partial}{\partial x},$$

$$\hat{p}^2_{x_{e,h}} = -\hbar^2 \left(\frac{m_{e,h}}{M}\right)^2 \frac{\partial^2}{\partial X^2} \mp 2\hbar^2 \frac{m_{e,h}}{M} \frac{\partial^2}{\partial X \partial x} - \hbar^2 \frac{\partial^2}{\partial x^2}.$$

Defining

$$\hat{P}x \equiv -i\hbar \frac{\partial}{\partial X}$$

$$\hat{p}_x \equiv -i\hbar \frac{\partial}{\partial x}$$

we obtain

$$\hat{H}^X = \frac{\hat{P}x^2}{2M} + \frac{\hat{p}_x^2}{2\mu} + \frac{\hat{p}_{ye}^2 + \hat{p}_{ze}^2}{2m_e} + \frac{\hat{p}_{yh}^2 + \hat{p}_{zh}^2}{2m_h} + \frac{eB(y_e - y_h)}{M} \hat{P}x + eB(y_e/m_e + y_h/m_h)\hat{p}_x$$
$$+ \frac{e^2B^2}{2}(y_e^2/m_e + y_h^2/m_h) + V_{conf}(y_e, y_h, z_e, z_h) - \frac{e^2}{4\pi\varepsilon(x^2 + (y_e - y_h)^2 + (z_e - z_h)^2)^{1/2}}, \tag{2}$$

where

$$\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_h},$$

$$M\vec{R} = m_e\vec{r}_e + m_h\vec{r}_h,$$

$$\vec{r} = \vec{r}_e - \vec{r}_h,$$

$$\vec{R} = \hat{x}X + \hat{y}Y + \hat{z}Z,$$

Even for this relatively simple Hamiltonian of eqn (2), no exact analytical solution of the exciton wave function is possible. Therefore we adopt the standard variational approach [2–4]. Since the Hamiltonian does not depend on X, P_X is a good quantum number. Dropping the term associated with P_X we take the following trial wave function:

$$\psi \equiv \psi(x, y_e, y_h, z_e, z_h) = g_t(x, \eta)\phi_e(y_e)\phi_h(y_h)\chi_e(z_e)\chi_h(z_h), \tag{3}$$

where $g_t(x,\eta)$ is chosen to be the Gaussian-type 'orbital' function [6–8]:

$$g_t(x, \eta) = \frac{1}{\eta^{1/2}} \left(\frac{2}{\pi}\right)^{1/4} e^{-(x/\eta)^2} \tag{4}$$

in which η is a variational parameter. The variables $X_{e,h}(Z_{e,h})$ are the z-components of the wave functions which are not affected by the magnetic field. They are given by particle-in-a-box states

$$\chi_{e,h}(z_{e,h}) = \sqrt{\frac{2}{L_z}} \cos\left(\pi \frac{z_{e,h}}{L_z}\right). \tag{5}$$

The electron and hole wave functions along the y direction, $\phi_{e,h}(y_{e,h})$, are to be calculated numerically when a magnetic field is present. This is done by solving the Schrödinger equation directly following the prescription given in Ref. [11].

It is important to note that there are really two different cases of exciton quantization: (i) an electron-hole droplet whereby the exciton is considered to be a particle by itself, and (ii) an entity consisting of independently confined electron and hole. According to Ref. [9,10], the criterion for this separation is L_y, $L_z = 3a_B^*$, where a_B^* is the effective Bohr radius in the bulk. The trial wave function (3) implicitly assumes the electron and the hole are independently confined along the y- and z-directions, which corresponds to the case

$$L_y, L_z < 3a_B^*.$$

The wave function (3) is probably the simplest that can be chosen while still preserving the principal features of the actual wave function. The results obtained with this trial function can be checked '*a posteriori*' by evaluating the zero-field binding energy and comparing it with binding energy calculated by other methods or extracted from experimental data.

The wave function (3) involves the variational parameter η which is evaluated by minimizing the expectation value of the Hamiltonian in Equation (2) (based on given trial wave functions) with respect to η. Once this is accomplished, one can find the exciton binding energies and the exciton length for different values of magnetic field and the wire width. The functional to be minimized can be written as follows

$$\langle\psi|\hat{H}^X|\psi\rangle = \frac{\hbar^2}{2\mu\eta^2} + \frac{\hbar^2}{2\mu W^2} + \frac{\hbar^2}{2m_e}\int_{-L/2}^{L/2}(\phi_e')^2 dy_e + \frac{\hbar^2}{2m_h}\int_{-L/2}^{L/2}(\phi_h')^2 dy_h + \frac{e^2B^2}{2m_e}\int_{-L/2}^{L/2}(\phi_e y_e)^2 dy_e$$
$$+ \frac{e^2B^2}{2m_h}\int_{-L/2}^{L/2}(\phi_h y_h)^2 dy_h - \frac{e^2}{4\pi\varepsilon}\int_{\Omega}\frac{g_t^2(x,\eta)\phi_e^2\phi_h^2\chi_e^2\chi_h^2}{[x^2+(y_e-y_h)^2+(z_e-z_h)^2]^{1/2}}\,d\zeta, \tag{6}$$

where $d\zeta = dx dy_e dy_h dz_e dz_h$. The integration of the last (Coulomb) term is carried out over a hyperrectangle Ω which has an infinite interval along the x direction and limited by $\pm L_y/2$ and $\pm L_z/2$ along y and z directions respectively. To obtain (6), we have made use of the boundary conditions $\phi_{e,h}(\pm L_y) = 0$ which allowed us to integrate some of the terms analytically using integration by parts. Note that the expectation value of the non-Hermitean operator $eB(y_e/m_e + y_h/m_h)\hat{p}_x$ (which arises in the presence of a magnetic field) is identically zero for the chosen trial wave function which makes the expectation value in (6) strictly real and shows that the trial wave function space is admissible.

Equation (6) allows us to treat the Coulomb interaction term exactly in its full 3D form throughout the calculation, which is physically more realistic than the approach employed in our previous (2D) exciton binding energy calculation [12].

Ground state exciton binding energies E_B^X can now be found using the relation

$$E_B^X = E_{conf}^{e1} + E_{conf}^{hh1} - min\langle\psi|\hat{H}^X|\psi\rangle, \tag{7}$$

where E_{conf}^{e1}, E_{conf}^{hh1} are the lowest electron and the highest heavy hole magneto-electric subband bottom energies in a quantum wire measured from the bottom of the bulk conduction band and the top of the bulk valence band. At the same time, the exciton length is simply $\eta_{opt}/2^{1/4}$ where η_{opt} is the value of η that minimizes the expectation value in eqn (6).

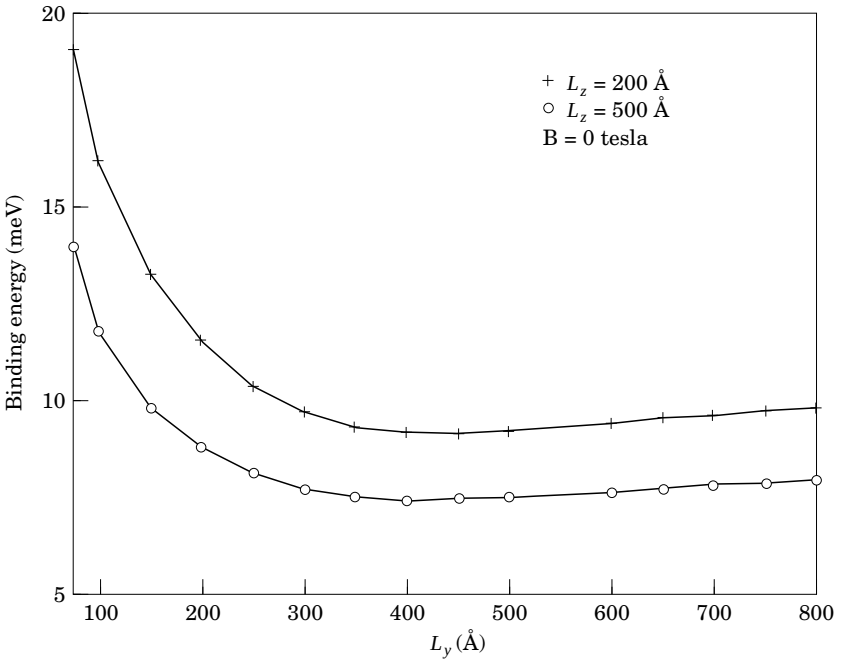

Fig. 2. The same results as in Fig. 2 in the present of a magnetic flux density of 10 tesla. There are pronounced minima around a wire width of 400 Å. The magnetic length in this case is 96 Å.

3. Results and Discussion

In Fig. 1 we present the exciton binding energy as a function of L_y (wire dimension along y direction) for two values of L_z (wire dimension along z direction) when no magnetic field is present. With increasing values of L_y, the binding energy rapidly decreases and begins to approach the bulk value (about 5.5 meV for GaAs). The binding energy does not approach the 2D limit because confinement along the z direction is not strong enough. In Fig. 2 we display the same results when a magnetic flux density of 10 tesla is present. It is interesting to note that when a magnetic field is present, the binding energy curves have a clearly resolved *minima* at $L \approx 400$ Å. An explanation for this somewhat surprising behavior is provided later. Figure 3 show the exciton length as a function of wire width. Pronounced maxima at $L \approx 400$ Å are seen corresponding to the minima in the binding energy.

Unfortunately, we cannot examine the behavior of the binding energy or the exciton length in the limit $L \to \infty$ because our model does not contain any provision to make the transverse components of the wavefunction to deform into atomic Slater orbitals. However, a direct comparison of our results for zero magnetic field with those in Refs [6,13] shows excellent agreement.

Figure 4A and B shows the exciton binding energy as a function of the magnetic field for different values of L_y and L_z. Binding energy increases with the magnetic field for all wire widths, which is in qualitative agreement with the results obtained for 2D systems [14,15], except that while the increase is sublinear in 2D systems, it is *superlinear* in 1D systems. This can be explained in two different ways. A magnetic field squeezes the electron and hole wavefunctions along all directions causing these states to condense into cyclotron (Landau) orbits whose radii shrink with increasing magnetic fields. As long as the wire width W is comparable to the magnetic length or the lowest cyclotron radius l $(=\sqrt{\hbar/eB})$, the additioal confinement induced by the magnetic field is not very important and the geometric (i.e. the electrostatic confinement of the walls) confinement predomi-

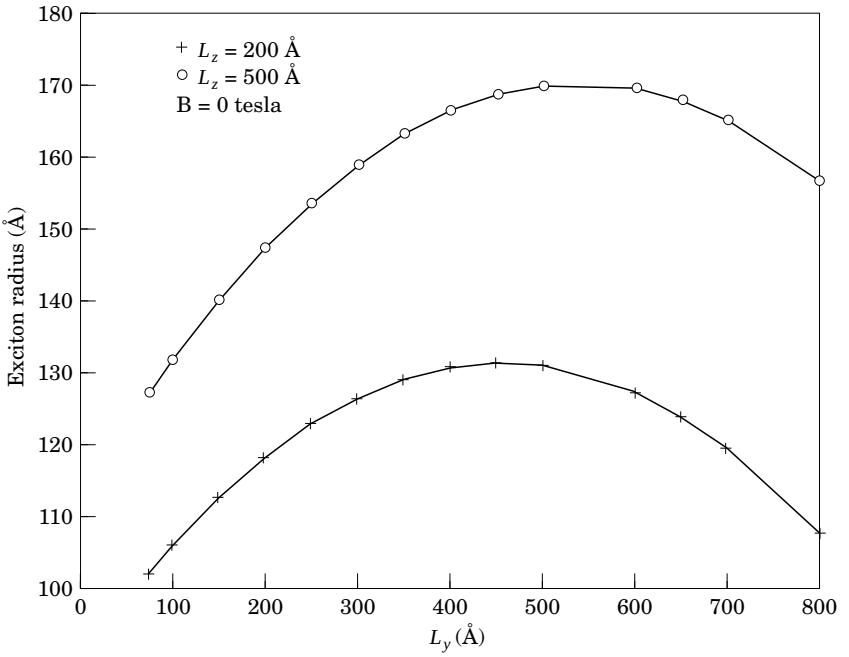

Fig. 3. Exciton length versus wire width at a magnetic flux density of 10 tesla. There are maxima around a wire width of 400 Å corresponding to the minima in the binding energy shown in Fig. 2.

nates. It is only when $W > l$ that the effect of the magnetic field becomes predominant. Therefore, a wider wire will show a stronger dependence of the binding energies on the magnetic field. Another way to explain the relation between the wire width and the sensitivity to the magnetic field is in terms of the standard time-independent perturbation picture. The magnetic field perturbs the quantum wire states, and the first order correction to the wave functions that correspond to the perturbed states is given by the formula

$$\psi_n^{(1)} = \sum_{m \neq n}^{\infty} \frac{|H'_{mn}|}{E_n^{(0)} - E_m^{(0)}} \psi_m^{(0)}, \tag{8}$$

where $E_m^{(0)}$, $\psi_m^{(0)}$ are the unperturbed energy eigenvalue and eigenfunction of the mth subband respectively, $|H'_{mn}|$ is a perturbation matrix element due to the magnetic field. Since in the case of perfect confinement

$$E_n^{(0)} = \frac{\pi^2 \hbar^2 n^2}{2 m_{e,h} L_y^2}, \tag{9}$$

it is easy to see that the perturbation decreases with decreasing wire width. Since it is this perturbation that squeezes the exciton wave function, we see clearly that the squeezing is more effective in wider wires. In other words, the wave function is softer and more 'squeezable' in wider wires which causes the magnetic field effect to be more dominant in those wires. A very similar physics causes the hole wave function to be perturbed more than the electron wave function in a quantum wire [12].

We can now revisit the pronounced minima in Fig. 2 and try to explain their physical origin.

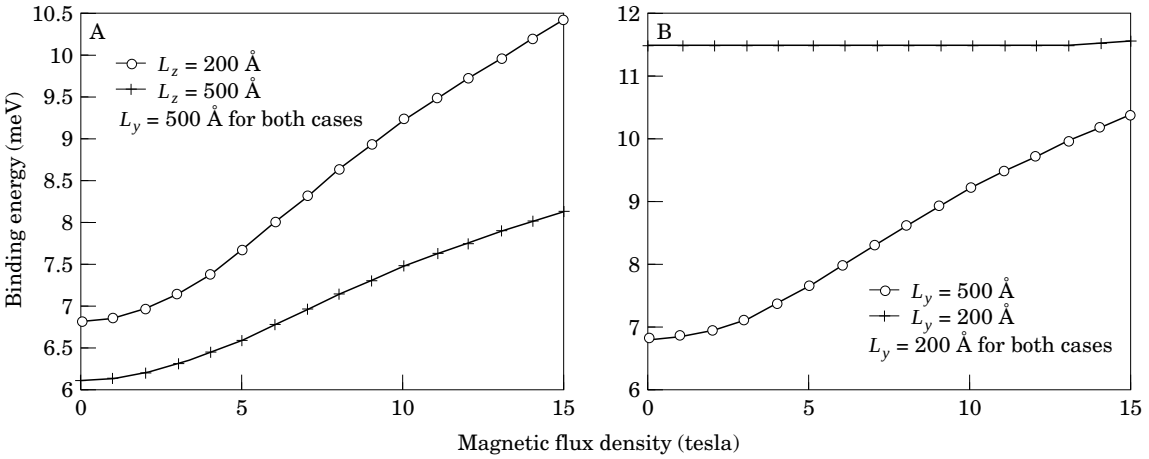

Fig. 4. Binding energy versus magnetic field for A, two different wire thicknesses and a fixed wire width, and B, two different wire widths and a fixed wire thickness.

At small values of L_y, the magnetic field is not very effective in squeezing the exciton wave function since the geometric confinement predominates. Consequently, the binding energy decreases with decreasing geometric confinement or increasing wire width. At large values of L_y, the geometric confinement becomes weak and yields the predominant role to the magnetic field induced confinement. With increasing wire width, the magneto-static confinement becomes stronger since the wave function becomes 'softer' and more squeezable. This causes the binding energy to reverse trend and increase with increasing wire width resulting in the occurrence of a minimum. The same physics explains the magnetic field dependence of the exciton radius as well.

4. Conclusion

In this paper, we have calculated the magnetic field dependence of the ground state exciton binding energy and exciton radius in a GaAs quantum wire. Two important observations are that: (i) the binding increases superlinearly with increasing magnetic field unlike in a quantum well where the increase is sub-linear [15], and (ii) there are pronounced mimima in the binding energy (and corresponding pronounced maxima in exciton length) as a function of wire width when a magnetic field is present. To our knowledge, the existence of these extrema was never shown before. Occurrence of these extrema has been explained in terms of the time-independent perturbation theory.

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