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Excitons in a quantum wire subjected to a magnetic field

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We present variational calculations of the ground-state exciton binding energy and exciton radius in a quantum wire subjected to an external magnetic field. The magnetic field squeezes the exciton wave function, causing the binding energy to become very large and increase superlinearly with the field; at the same time, the exciton radius shrinks. The squeezing is more effective in wider wires, where the exciton wave function is "softer." These results are consistent with recently reported experimental observations.

I. INTRODUCTION

There is significant current interest in the exitonic properties of semiconductor quantum wires because of their role in optoelectronic applications. This interest stems from the observation that quantum wires exhibit large absorption and third-order nonlinear susceptibility as a result of quantum confinement of excitons. An external magnetic field further squeezes the exciton wave function, possibly leading to enhanced optical properties.

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 wave function to a size that is far below what can be achieved in quantum wells. This is very promising for potential optoelectronic applications.

In this paper, we present numerical calculations of the magnetic-field dependence of the exciton binding energy and the exciton radius in a GaAs quantum wire for different wire widths. In Sec. II, the theory of an exciton in a quantum wire subjected to a magnetic field is developed rigorously within the framework of a two-band model and perfect confinement of the exciton. Section III presents the result of variational calculations of the binding energy and exciton radius followed by a discussion of the excitonic properties. We also compare our results with the experimental observations of Ref. 1. Since Ref. 1 employed T-shaped edge quantum wires whose geometries are very different from ours, a direct quantitative comparison is not possible. Nonetheless, we find that our numerical results are within the same order of magnitude as theirs, and that their data are in excellent qualitative agreement with ours. Conclusions are given in Sec. IV.

II. THEORY

Let us consider a quantum wire where $L_z < a_B^*$ is the dimension along the thickness, L_y is the lateral dimension along the width, and a_B^* is the effective Bohr radius.

A magnetic field is applied along the z direction. Along that direction, we assume that confinement is complete and only one transverse subband is occupied. We choose the Landau gauge for the magnetic vector potential

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

where B is the z-directed magnetic flux density. For nondegenerate and isotropic bands, the Hamiltonian of the Wannier exciton subjected to a magnetic field is given by

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

where $m_{e,h}$, $\mathbf{r}_{e,h}$ $(= \mathbf{a}_x x_{e,h} + \mathbf{a}_y y_{e,h})$ are the effective masses and positions of electrons and holes, respectively, ϵ the dielectric constant, and $V_{\text{conf}}(y_e)$ and $V_{\text{conf}}(y_h)$ are the confinement potentials for electrons and holes along the y axis.

For convenience of numerical solution, we transfer to the center-of-mass and relative coordinate system along the x axis, but retain "old" coordinates of the electron and the hole along the y axis. This is accomplished by using a quantum-mechanical definition of momentum operators and taking into account that in a center-of-mass and relative coordinate system

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

$$\hat{p}_{x_{e,h}} = -\hbar^2 \left[\frac{m_{e,h}}{M}\right]^2 \pm 2\hbar^2 \frac{m_{e,h}}{M}\frac{\partial^2}{\partial X \partial x} - \hbar^2 \frac{\partial^2}{\partial x^2} ,$$

where

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

$$\mathbf{r} = \mathbf{r}_e - \mathbf{r}_h = \mathbf{a}_x x + \mathbf{a}_y y ,$$

$$\mathbf{R} = \mathbf{a}_x X + \mathbf{a}_y Y .$$

Simplifying, we obtain

$$\hat{H}=\frac{\hat{P}_X^2}{2M}+\frac{\hat{p}_x^2}{2\mu}+\frac{\hat{p}_{y_e}^2}{2m_e}+\frac{\hat{p}_{y_h}^2}{2m_h}+\frac{eB(y_e-y_h)}{M}\hat{P}_x$$
$$+eB(y_e/m_e+y_h/m_h)\hat{p}_x+\frac{e^2B^2}{2}(y_e^2/m_e+y_h^2/m_h)$$
$$-\frac{e^2}{4\pi\epsilon[x^2+(y_e-y_h)^2]^{1/2}}$$
$$+V_{\text{conf}}(y_e)+V_{\text{conf}}(y_h)\ , \qquad (2)$$

where $\hat{P}_X$ is the center-of-mass momentum and μ and M are the reduced and weighted total electron-hole masses. We have tacitly neglected any image force effect.

We will calculate the ground-state exciton binding energy by a standard variational procedure.[2,3] To facilitate calculations, we assume perfect confinement of electrons and holes along the y axis, such that the y components of the wave function obey

$$\phi_e(y_e=-L_y/2)=\phi_e(y_e=L_y/2)=0\ ,$$
$$\phi_h(y_h=-L_y/2)=\phi_h(y_h=L_y/2)=0\ .$$

Since the Hamiltonian does not depend on X (the coordinate of the center of mass along the wire axis), P_X is a good quantum number. Dropping the term associated with P_X, we take the following trial wave function:

$$\psi(x,y_e,y_h)=g_t(x,\eta)\phi_e(y_e)\phi_h(y_h)\ , \qquad (3)$$

where $g_t(x,\eta)$ is chosen to be the Gaussian-type "orbital" function:[4]

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

in which η is a variational parameter, and $\phi_e(y_e)$ and $\phi_h(y_h)$ are normalized electron and hole wave functions along the width to be calculated numerically when a magnetic field is present.

It is important to note here that one should separate two different cases of exciton quantization: as a whole particle, and as independently confined electron and hole. According to Ref. 5, the criterion for this separation is $L_y=3a_B^*$, where the effective Bohr radius a_B^* is that in the bulk. The trial wave function (3) assumes the electron and hole to be quantized independently, which corresponds to the case

$$L_y<3a_B^*\ . \qquad (4)$$

Minimizing the expectation value of the Hamiltonian in Eq. (2) (with given trial wave functions) with respect to the variational parameter η, one can find exciton binding energies and radii for different values of magnetic field and the wire width. The functional to be minimized can be written as follows:

$$\langle\psi|\hat{H}|\psi\rangle=\frac{\hbar^2}{2\mu\eta^2}+\frac{\hbar^2}{2m_e}\int_{-L_y/2}^{L_y/2}(\phi_e')^2dy_e+\frac{\hbar^2}{2m_h}\int_{-L_y/2}^{L_y/2}(\phi_h')^2dy_h$$
$$+\frac{e^2B^2}{2m_e}\int_{-L_y/2}^{L_y/2}(\phi_e y_e)^2dy_e+\frac{e^2B^2}{2m_h}\int_{-L_y/2}^{L_y/2}(\phi_h y_h)^2dy_h$$
$$-\frac{e^2}{4\pi\epsilon}\int_{-L_y/2}^{L_y/2}\int_{-L_y/2}^{L_y/2}\int_{-\infty}^{+\infty}\frac{g_t^2(x,\eta)\phi_e^2\phi_h^2}{[x^2+(y_e-y_h)^2]^{1/2}}dx\,dy_e dy_h\ , \qquad (5)$$

where the prime denotes a derivative with respect to the y coordinate and integration of the last (Coulomb) term is carried out over an infinite interval along the x direction. To obtain (5), we have used boundary conditions on functions ϕ_e and ϕ_h, which allowed us to integrate some of the terms analytically using integration by parts.

The evaluation of the integrals in the Coulomb term is not straightforward due to the $1/r$ singularity. The fact that the wave function ψ is variable-separable is of no consequence here, because the Coulomb term couples all the variables. Moreover, since we use exact wave functions ϕ_e and ϕ_h calculated numerically by the method described in Ref. 6, we cannot partially integrate this term analytically to avoid dealing with the singularity. Because of this, we applied a simple regularization of the Coulomb term in a way similar to Ref. 7, and made sure that the result did not depend on the regularization parameter used. Changing the parameter over five orders of magnitude resulted only in a 10% charge in the binding energy.

III. RESULTS AND DISCUSSION

We numerically evaluated the remaining integrals in the expectation value of the functional [see Eq. (5)] and plotted $\langle\psi|\hat{H}|\psi\rangle$ as a function of the variational parameter η. The minima of $\langle\psi|\hat{H}|\psi\rangle$ give us values of the variational parameter η to be used in computing binding energies for a particular magnetic-flux density B. Figure 1 shows the dependence of $\langle\psi|\hat{H}|\psi\rangle$ on the variational parameter η for two different values of magnetic field and wire width. One can notice that the functional always has one well-resolved minimum. The physical parameters used for the calculations correspond to a GaAs quantum wire with $\epsilon=12.9\epsilon_0$, $m_e=0.067m_0$, and $m_h=0.5m_0$,

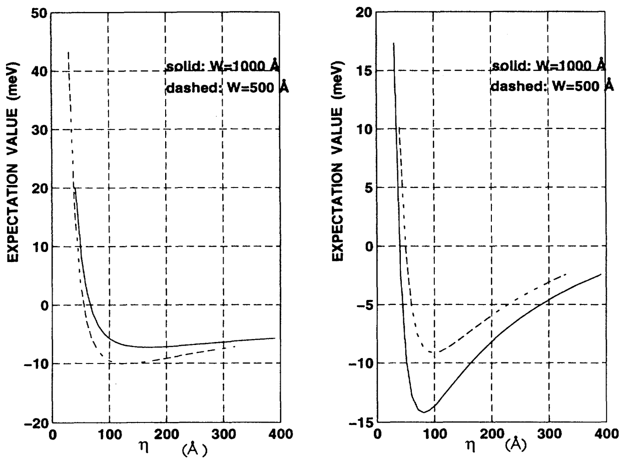

FIG. 1. Expectation value of the Hamiltonian as a function of the variational parameter η. The left panel corresponds to a magnetic-flux density of 1 T, the right panel to a flux density of 10 T.

where m_0 is the free-electron mass and ϵ_0 the electrical permittivity of the free space. The wire widths we used $W(=L_y)$ were within the limit of quantization condition (4).

Ground-state exciton binding energies E_B were found using the relation

$$E_B = E_{e1} + E_{\mathrm{hh1}} - \min\langle\psi|\hat{H}|\psi\rangle ,$$

where E_{e1} and E_{hh1} are the lowest electron and the highest heavy-hole magnetoelectric subband bottom energies in a quantum wire measured from the bottom of the bulk conduction band and the top of the bulk valence band.

In addition to the binding energies, we calculated the radius (or more correctly the length) of the exciton along the x axis given analytically as $\sqrt{\langle x^2\rangle} = \eta/2^{1/4}$ for different values of a magnetic field. Figure 2 shows both the exciton binding energy and the exciton radius as a function of the magnetic field. The binding energy increases with the magnetic field for all wire widths, which is in qualitative agreement with the results obtained for two-dimensional systems,[8,9] except that while the increase is sublinear in two-dimensional systems, it is superlinear in one-dimensional systems.

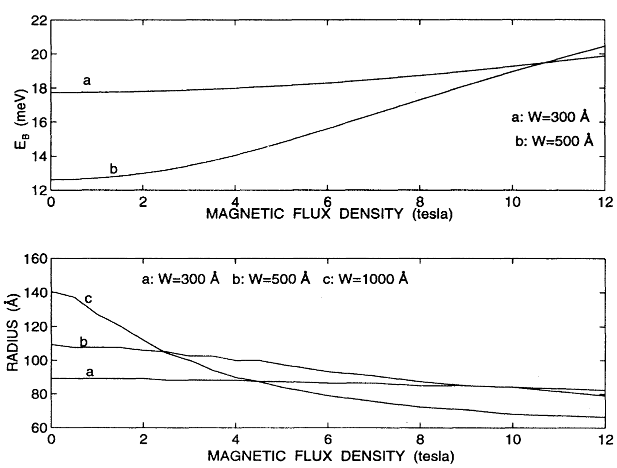

FIG. 2. Magnetic-field dependence of the exciton binding energy in a GaAs quantum wire (upper panel) and exciton radius (lower panel). The results are shown for different wire widths W.

It is interesting to note that the effect of the magnetic field is much more pronounced for the wider wire $W=500$ Å than for the narrower wire $W=300$ Å. This can be explained in two different ways. A magnetic field squeezes the electron and hole wave functions along all directions (see Figs. 3 and 4) causing these states to condense into cyclotron (Landau) orbits whose radii shrink with increasing magnetic fields. As long as the wire width W is smaller than the magnetic length or the lowest cyclotron radius $l(=\sqrt{\hbar/eB})$, the effect of the magnetic field is not very pronounced and the geometric confinement predominates. It is only when $W>l$ that the effect of the magnetic field becomes predominant. Therefore, a wider wire will show a stronger magnetic-

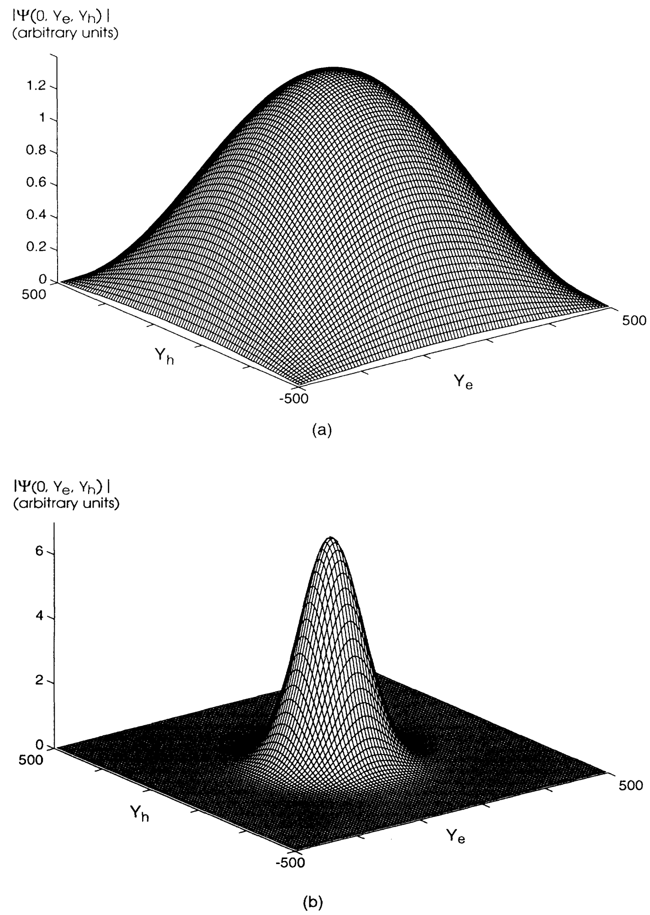

FIG. 3. The exciton wave function $\psi(0,y_e,y_h)$ vs coordinates y_e, y_h. (a) At a magnetic flux density of 1 T. (b) At a magnetic-flux density of 10 T.

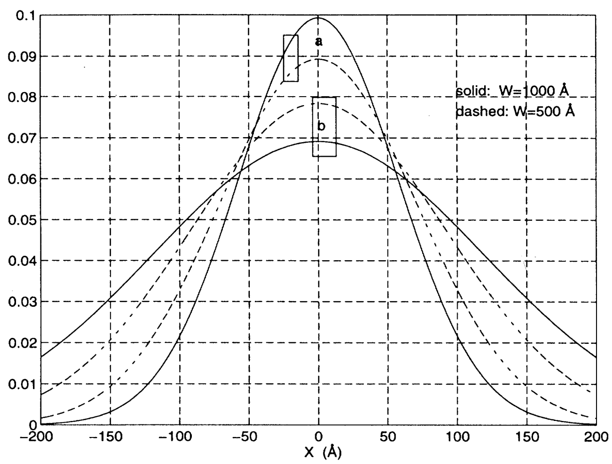

FIG. 4. The x component of the exciton wave function $g_t(x,\eta_{\rm opt}(B))$. The two curves grouped as a correspond to a magnetic-flux density of 10 T, while those grouped as b correspond to 0 T. These wave functions are Gaussian-type orbital functions.

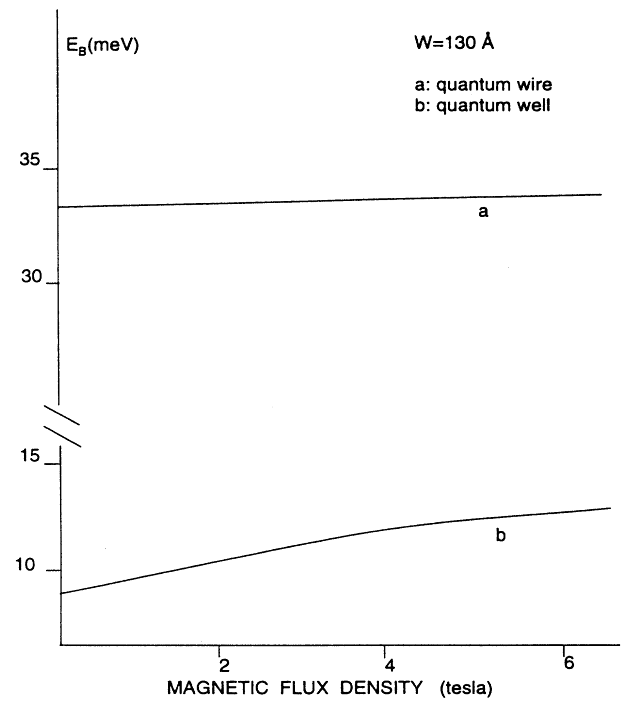

FIG. 5. Comparison of the magnetic-field dependence of the exciton binding energy in a quantum well and quantum wire of the same width (13 nm). The quantum-well results are reproduced from Ref. 9.

field-induced effect. Another way of explaining the same wire-width dependence 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

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

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

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

it is easy to see that the correction decreases with decreasing wire width. Since it is this correction 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-induced 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.[10]

The exciton radius decreases with magnetic field for all wire widths and is in the range of 70–140 Å. Figure 3 shows the exciton wave function (3) for relative coordinate $x=0$ for two different values of a magnetic field. To elucidate the effect of a magnetic field on the exciton radius, we considered a relatively wide wire of width 1000 Å, so that the squeezing induced by the magnetic field was large. One can clearly see from these figures that a magnetic field localizes the exciton wave function at the center of the wire. Another interesting thing to note is that both wave functions are symmetric: a magnetic field does not skew them toward one or the other edge of the wire. This is due to the fact that we have used the wave functions $\phi_e(y_e)$ and $\phi_h(y_h)$ of states at the subband extrema. These states have a zero translational velocity and therefore experience no Lorentz force[10] to skew the wave functions.

The effect of localization can also be observed along the x direction. Figure 4 shows the x component of the exciton wave function $g_t(x,\eta_{\rm opt}(B))$ for two different wire widths, with and without a magnetic field [$\eta_{\rm opt}$ is the value of η that minimizes the functional in Eq. (5) at a given magnetic-flux density]. Again, the effect produced by the field is stronger for the wider wire.

Finally, Fig. 5 provides a direct comparison of the behavior of the exciton binding energy in a quantum wire with that in a quantum well of the same width. The quantum-well data are reproduced from Ref. 9. It is worth noting that the binding energy of quasi-one-dimensional excitons lies well above that of two-dimensional excitons, obviously as a result of the additional degree of quantum confinement. For the chosen width of 13 nm, the effect of the magnetic field is not pronounced in the quantum wire since the geometric confinement is the dominant squeezing agent which completely overshadows the magnetic-field-induced squeezing. The effect of the magnetic field will of course be more pronounced in wider wires, where the exciton wave function is softer and more squeezable.

IV. CONCLUSION

We found that the ground-state exciton binding energy in a GaAs quantum wire increases superlinearly with increasing magnetic field. The increase is due to the compression of the exciton wave function by the field. It was also found that the effect of a magnetic field is stronger in wider wires, which has been explained in terms of the time-independent perturbation theory.

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