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Exciton binding energy in quantum-well wires

Marcos H. Degani and Oscar Hipólito
Departamento de Física e Ciência dos Materiais, Instituto de Física e Química de São Carlos, Universidade de São Paulo, Caixa Postal 369, 13560 São Carlos, São Paulo, Brazil

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The binding energies of excitons in quantum-well wires of GaAs surrounded by $Ga_{1-x}Al_xAs$ are calculated with the use of variational solutions to the effective-mass equation. The results we obtained show that the energies are dramatically dependent on the sizes of the wire, and also that their magnitudes are greater than those in comparable quasi-two-dimensional quantum-well structures.

With the recent advances in the technique of molecular-beam epitaxy, it has been possible to confine electrons in extremely thin semiconducting wires, namely, quantum-well wires, with submicron dimensions. In these quasi-one-dimensional structures the electron motion along the length of the wire is free but it is quantized in the two dimensions perpendicular to the wire. A great deal of theoretical and experimental interest has been devoted to the study of the electronic properties of these one-dimensional semiconductor systems. Sakaki[1] first investigated the electron transport of ultrathin GaAs-$Ga_{1-x}Al_xAs$ quantum wires and showed that a high-mobility effect would be expected. Petroff, Gossard, Logan, and Wiegmann[2] fabricated and studied some of the optical properties of GaAs quantum wires. They have observed cathodoluminescence which was attributed to transitions involving exciton states. The emission line was observed to be two to three times broader than that of the two-dimensional quantum wells and occurred at 6–10 meV higher binding energy. More recently several authors have reported calculations of the mobility of electrons scattered by ionized donors and also by optical and acoustic phonons.[3-5] The optical absorption due to direct intersubband transitions as well as the free-carrier absorption in quasi-one-dimensional semiconducting structures for the case where the electrons are scattered by acoustic phonons have also been investigated.[6,7] The binding energies for the bound states of hydrogenic impurity placed in a quantum-well wire of GaAs surrounded by $Ga_{1-x}Al_xAs$ have been calculated and the results are 2 to 3 times greater than those in comparable two-dimensional wells.[8]

One of the important features of these new one-dimensional structures already observed but not addressed by any theoretical calculations until now is the presence of excitons which play a fundamental role in the cathodoluminescence spectra of these systems. Because of the energy-band discontinuity at the interface between the two semiconductors the degeneracy of the valence band of GaAs is removed enough that these may be treated as isolated bands, leading as a consequence to two-exciton systems, namely, a heavy-hole exciton and a light-hole exciton.

The purpose of this paper is to report a first calculation of the exciton binding energies associated with the lowest electron and hole subbands in a quantum-well wire of GaAs surrounded by $Ga_{1-x}Al_xAs$. We have also calculated the effects of the electron- and hole-optical-phonon interaction on the exciton binding energies and showed that the corrections are quite significant. For the phonon system we have used the so-called bulk-phonon approximation instead of the confined phonon modes as discussed by Babiker[9] and Babiker and Ridley[10] for the cases of quantum wells and superlattices. Inclusion of the confined phonons would certainly alter the binding-energy values in comparison with that of the bulk-phonon model. The calculation is performed following a variational approach by retaining only the diagonal term of the Luttinger-Kohn Hamiltonian. We find that the binding energies of two excitons as a function of the size of the GaAs wires show the same qualitative behavior as those in comparable two-dimensional wells but with much higher magnitudes.

In the effective-mass approximation the Hamiltonian of an exciton associated with either the heavy-hole band or the light-hole band in a GaAs quantum-well wire surrounded by $Ga_{1-x}Al_xAs$ and interacting with the optical phonons of the GaAs can be written in the following form:

$$H=E_G+\frac{p_{xe}^2+p_{ye}^2}{2m_e}+\frac{p_{xh}^2+p_{yh}^2}{2m_h}+\frac{P_Z^2}{2M_\pm}+\frac{p_z^2}{2\mu_\pm}-\frac{e^2}{\epsilon_\infty[(x_e-x_h)^2+(y_e-y_h)^2+z^2]^{1/2}}+V(x,y)$$
$$+\sum_{\mathbf{q}}\hbar\omega_0 a_{\mathbf{q}}^\dagger a_{\mathbf{q}}+\sum_{\mathbf{q}}[\Gamma_{\mathbf{q}}e^{iq_zZ}(e^{i\mathbf{Q}\cdot\mathbf{R}_e}e^{i\beta_h q_z z}-e^{i\mathbf{Q}\cdot\mathbf{R}_h}e^{-i\beta_e q_z z})a_{\mathbf{q}}^\dagger+\text{H.c.}]\ , \quad (1)$$

where E_G is the GaAs band gap; m_e and m_h are the band masses of the electron and the hole, respectively; $\mathbf{R}_i=(x_i,y_i)$ and $\mathbf{p}_i=(p_{xi},p_{yi})$, $i=e,h$ are the in-plane projection of the electron and hole coordinates and momenta; Z,P_Z are the center-of-mass coordinate and momentum; z,p_z are the electron-hole relative position and momentum; $M_\pm=m_e+m_{h\pm}$ is the total mass along the z direction; and $\mu_\pm$ are the heavy-hole (+) and light-hole (−) reduced masses for the z motion. $V(x,y)$ is the confined potential well for the electron and hole and will be taken to be $V(x,y)=0$ for $|x|<L_x$ and $|y|<L_y$ and $V(x,y)=+\infty$ otherwise. $a_{\mathbf{q}}^\dagger$ is the creation operator

for the optical phonons of wave vector $\mathbf{q}=(\mathbf{Q},q_z)$ and frequency ω_0. $\Gamma_{\mathbf{q}}$ is the Fourier coefficient of the electron- and hole-phonon interaction given by

$$\Gamma_{\mathbf{q}}=\frac{-i\hbar\omega_0}{q}\left[\frac{2\pi}{\Omega}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\frac{e^2}{\hbar\omega_0}\right]^{1/2}, \tag{2}$$

Ω is the volume of the system, and

$$\beta_e=m_e/M_\pm,\ \beta_h=m_{h\pm}/M_\pm .$$

In order to calculate the exciton binding energy, we first eliminate the coordinate Z of the center of mass from the Hamiltonian H, through the canonical transformation

$$H'=U_1^{-1}HU_1 ,$$

where

$$U_1=\exp\left(-i\sum_{\mathbf{q}}q_zZa_{\mathbf{q}}^\dagger a_{\mathbf{q}}\right) .$$

Then, the binding energy of the exciton formed between the ground electron subband and the ground heavy- or light-hole subband will be obtained by choosing the simplest approximation for the trial wave function that is a product ansatz state,

$$\psi(\mathbf{r}_e,\mathbf{r}_h)=\left(\frac{4}{L_xL_y}\right)\cos\left(\frac{\pi x_e}{L_x}\right)\cos\left(\frac{\pi y_e}{L_y}\right)\times\cos\left(\frac{\pi x_h}{L_x}\right)\cos\left(\frac{\pi y_h}{L_y}\right)\phi(z)U_2|0\rangle , \tag{3}$$

where $\phi(z)$ is a variational wave function depending on the electron-hole relative coordinate which we will choose to be hydrogenic,

$$\phi(z)=(\lambda/2)^{1/2}\exp(-\lambda|z|/2) , \tag{4}$$

U_2 is a unitary transformation which displaces the phonon coordinates,

$$U_2=\exp\left(\sum_{\mathbf{q}}(f_{\mathbf{q}}a_{\mathbf{q}}^\dagger-f_{\mathbf{q}}^*a_{\mathbf{q}})\right) , \tag{5}$$

and $|0\rangle$ is the phonon vacuum state. The variational parameter λ and the function $f_{\mathbf{q}}$ are to be determined by minimizing the expectation value of the Hamiltonian, that is, $E=\langle\psi|H'|\psi\rangle$. We then obtain the energy of the exciton in the following form:

$$E=E_G+E_{\rm kin}+E_{\rm Coul}+E_{\rm pol} , \tag{6}$$

in which $E_{\rm pol}$ is the polaronic contribution to the binding energy and can be easily obtained in a standard way and is given by

$$E_{\rm pol}=\frac{-e^2\hbar\omega_0}{\pi}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\int dQ\frac{F(Q)}{\hbar\omega_0+(\hbar^2Q^2/2M_\pm)}\left(\frac{1}{1+(\beta_hQ/\lambda)^2}-\frac{1}{1+(\beta_eQ/\lambda)^2}\right)^2 \tag{7}$$

and

$$E_{\rm Coul}=\frac{-2\lambda^2e^2}{\pi\epsilon_\infty}\int dQ\frac{F(Q)}{\lambda^2+Q^2} , \tag{8}$$

where $F(Q)$ is the form factor for the quasi-one-dimensional system which is given by

$$F(Q)=\int dK\frac{G(K)H(Q,K)}{(Q^2+K^2)^{1/2}} , \tag{9}$$

where

$$G(K)=\left(\frac{2}{L_xK}\right)^2\frac{\sin^2(L_xK/2)}{[1-(L_xK/2\pi)^2]^2} \tag{10}$$

and[11]

$$H(Q,K)=\frac{2(u^2+8\pi^2)}{(u^2+4\pi^2)^2}(1-e^{-u})+\frac{u}{u^2+4\pi^2}+\frac{2}{u}\left[1-\frac{1}{u}(1-e^{-u})\right] , \tag{11}$$

with $u=L_y\sqrt{Q^2+K^2}$. $E_{\rm kin}$ is the kinetic energy.

It is interesting to stress that this result for the energy, Eq. (6), represents the interaction of an electron with a hole in a quantum-well wire through a Coulomb potential which is screened by the optical dielectric constant, while each of them is interacting with the optical phonons of the GaAs. In this sense, this result is a generalization of the exciton, polaron, and impurity-bound polaron energies. In the limit of $m_h\to\infty$, that is, $\beta_e\to 0$ and $\beta_h\to 1$, we obtain the impurity-bound polaron problem in the same way we have recently worked out for the case of a two-dimensional quantum well.[11] In this limit the effect of the canonical transformation is to eliminate the electron coordinate from the Hamiltonian and to replace $1/\epsilon_\infty$ by $1/\epsilon_0$ in the Coulomb term.[12]

The minimization of the energy given by Eq. (6) with respect to the variational parameter λ gives the ground-state energy of the exciton. Then, the exciton binding energy is obtained as the difference between the total ground-state energy of the electron and the hole and this minimized value of E. We have then numerically minimized the energy expression given by Eq. (6) with and without the presence of the electron- and hole-optical-phonon interactions for several values of the size of the quantum-well wire. In the present calculations we have used the following physical parameters: $\epsilon_0=12.5$, $m_e=0.067m_0$, $m_{h+}=0.45m_0$, $m_{h-}=0.08m_0$, and $\hbar\omega_0=35.2$ meV, where m_0 is the free-electron mass.

We have calculated the heavy-hole and the light-hole exciton binding energies as a function of the length of one side L_x of the GaAs quantum-well wire for several values of the length of the other side L_y. The results we obtained are plotted in Fig. 1 for the heavy-hole exciton and in Fig. 2 for the light-hole exciton. As we can see from these figures, the exciton binding energies decrease monotoni-

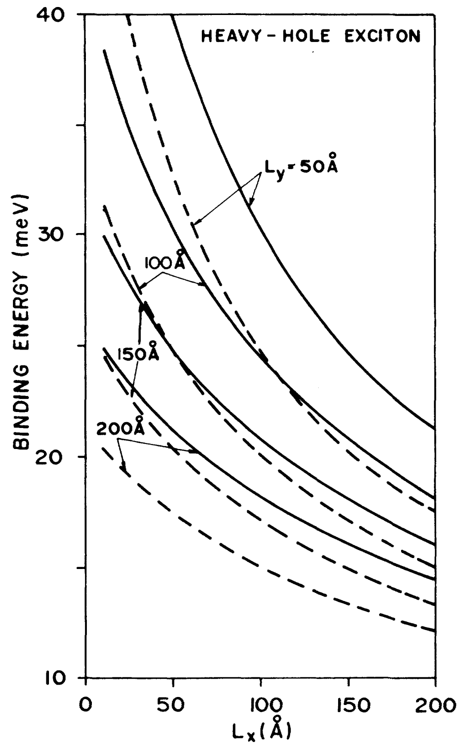

FIG. 1. Heavy-hole exciton binding energy of GaAs quantum wires as a function of the size of the wires. The solid and dashed curves represent the exciton binding energies with and without the presence of phonons, respectively.

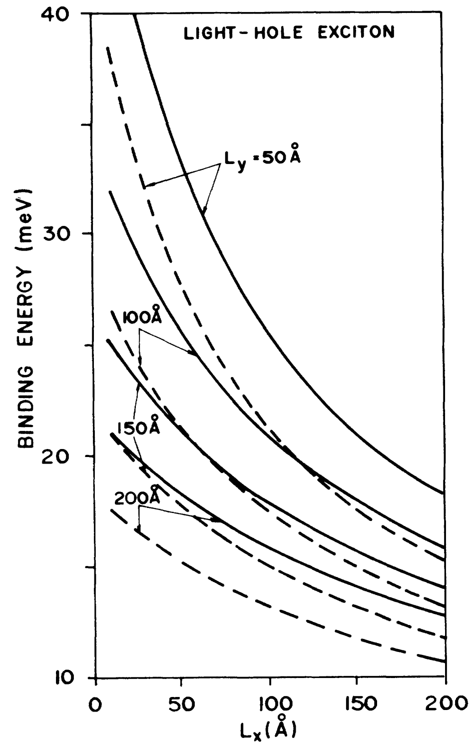

FIG. 2. Binding energies for the light-hole exciton in GaAs quantum-well wires as a function of the size of the wires. The solid and dashed curves represent the energies of the exciton with and without the presence of the phonons, respectively.

cally as the wire expands in one direction while remaining fixed in the other direction. After sufficient expansion of one side, the exciton binding energy approaches the value expected for the binding energy of an exciton in a two-dimensional quantum well.[13] It should be noted that the changes in the energy shown in Figs. 1 and 2 are similar for comparable changes in the dimensions of the wire. For example, the heavy-hole exciton binding energy for a 100×100 Å^2 wire changes by the same amount when one side doubles or is reduced by one-half in length. In a very close similarity with the impurity-state problem in quantum wires as worked out by Bryant,[8] the exciton binding energies are correlated to the cross-sectional area of the wire rather than to the sizes of the rectangular cross section. This insensitivity to the shape of the wire is much more evident for large wires which are less sensitive to the boundary effects.

From Figs. 1 and 2 we may note that the values of the exciton binding energies are larger than those in comparable two-dimensional quantum wells.[13] These results are consistent with the cathodoluminescence observed by Petroff *et al.*[2] in quantum-well wires, which was attributed to transitions involving exciton states. They observed the value of the exciton binding energy at 8–10 meV higher than that in two-dimensional quantum wells. We also can see that the heavy-hole exciton in a GaAs quantum-well wire is more strongly bound than the light-hole exciton, in contrast to the two-dimensional analog. The reason for this behavior is easy to understand. Both the heavy-hole mass and the electron–heavy-hole reduced mass are heavier than the light-hole mass and the electron–light-hole reduced mass, respectively, leading then to an enhancement of the binding energy.

In Figs. 1 and 2 are also included the contribution of the electron- and hole-optical–phonon interaction to the exciton binding energies in GaAs quantum-well wires as a function of the sizes of the wires. The relative shift of the exciton binding energies, i.e., $\Delta E_B = (E_B^* - E_B)/E_B$, where E_B^* and E_B are the binding energies with and without the exciton-phonon coupling, respectively, decreases when one of the dimensions of the wire increases. The polaronic contribution is larger for wires of small dimensions, and ranges from about 23% for a 10×50 Å^2 wire, for the heavy-hole exciton, to 19% for a 200×200 Å^2 wire, for the light-hole exciton.

The importance of the electron- and hole-optical phonon interaction is more pronounced as the exciton binding energy becomes larger. Then, for a given size of the wire, the largest polaronic contribution to the exciton binding energy comes from the heavy-hole exciton which is more strongly bound.

In conclusion, we have calculated the binding energies for the heavy-hole and the light-hole excitons in GaAs quantum-well wires with rectangular cross section as a function of the size of the wires. We find that the binding energies increase on decreasing one dimension of the wire. The binding energies approach the value expected for two-dimensional quantum wells of finite thickness by expanding one side while keeping the other fixed. We find that the exciton binding energies are more correlated to the cross-sectional area of the wire than to the sizes of the cross section. We have also investigated the effects of the electron- and hole-optical phonon interaction on the exciton binding energies. Our results explicitly show the quantitative importance of the polaronic contribution in increasing substantially the exciton binding energies.

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