Theoretical model of excitons for type-II quantum-wire systems

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A calculation of the exciton binding energy (E_x) and oscillator strength (OS) for quantum wires in type-II semiconductor systems is presented. These structures consist of a cylindrical wire of one semiconductor embedded in a second semiconductor. In the type-II exciton systems in quantum wells the electron is confined in one semiconductor and the hole in the other is due to band lineups in the two materials, which make this arrangement energetically favorable. We use an approach which initially decouples the ρ and z components. We use a variational approach for motion in the ρ direction which allows for correlation of the free particle, and solve for the one-dimensional exciton in the z direction using an effective Coulomb interaction. The solutions are then coupled self-consistently to produce E_x, where $E_x(\rho,z)=E(\rho)+E(z)$, and a product wave function which is used to calculate the OS. We consider the idealized situation of infinite confining barriers and the more realistic case of finite barriers for the system GaAs/AlAs, where the electron is confined in the X state in the AlAs while the hole is confined in the Γ state in the GaAs wire (for a wire diameter of less than 43 Å). For finite barriers E_x peaks at 33 meV for a wire diameter of 16 Å, which represents a large enhancement over the infinite-barrier case due to the strong wave-function correlation possible in two dimensions.

Now that it is possible to fabricate or grow semiconductor quantum wires[1] it is of increasing relevance to consider excitons, both type I and type II in these systems. Excitons in type-I wires have been considered by Banyai *et al.*[2] within a variational calculation. They find that, again assuming infinite confining barriers, the exciton binding energy is vastly increased in these structures compared with the three-dimensional (3D) and two-dimensional (2D) cases. The case of excitons in quantum wires has also been considered by Brown and Spector[3] and Kodama and Osaka[4] among others with similar results. More recently, Kayanuma[5] has considered a general variational wave function to deal with excitons in quantum wells, wires, and dots. In addition, Byrant[6] has dealt with the similar system of a hydrogenic impurity in a quantum wire with finite barriers. To my knowledge, no one has considered the type-II exciton in quantum-wire (QW) systems. Here we present calculations on the type-II QW systems GaAs/AlAs, which is type II for a wire diameter of less than 43 Å having considered the case of type-II quantum dots (QD) in previous studies.[7]

We consider a 1D wire of cylindrical symmetry where z is parallel to the wire, $\boldsymbol{\rho}=(\rho\cos\Theta,\rho\sin\Theta)$ are the coordinates in the cylindrical plane and a is the diameter of the wire. The Hamiltonian for this type-II exciton wire with cylindrical symmetry is

$$H(\mathbf{r}_c,\mathbf{r}_f)=H(\boldsymbol{\rho}_c)+H(\boldsymbol{\rho}_f)+H(z_c)+H(z_f) - V(\boldsymbol{\rho}_c)+V(\boldsymbol{\rho}_f)-1/[\varepsilon(\mathbf{r}_c,-\mathbf{r}_f)] , \quad (1)$$

where $\mathbf{r}^2=(\boldsymbol{\rho}^2+z^2)$. The first term is the kinetic energy of the confined (c) particle in the $\boldsymbol{\rho}$ direction, the second is the kinetic energy of the free (f) particle in the $\boldsymbol{\rho}$ direction, the third and fourth terms are the kinetic energy of the corresponding particles in the free z direction, the fifth and sixth terms are the potentials for the confined and free particle, respectively, and the seventh is the Coulomb term which couples all the components. (Throughout this paper in all equations we use atomic units taking $\hbar=1$, $e=1$, and $m_0=1$.) The Hamiltonian separates into

$$H'(\rho_c)=-1/(2m^*_{\rho c})[1/\rho_c(\partial/\partial\rho_c)\rho_c\partial/\partial\rho_c]-V(\rho_c) , \quad (2a)$$

where $V(\rho_c)=$const for $\rho_c<a$ and $V(\rho_c)=0$ for $\rho_c>a$, where a is the diameter of the wire and

$$H'(\rho_f)=-1/(2m^*_{\rho f})[1/\rho_f(\partial/\partial\rho_f)\rho_f\partial/\partial\rho_f]+V(\rho_f) , \quad (2b)$$

where $V(\rho_f)=$constant for $\rho_f<a$ and $V(\rho_f)=0$ for $\rho_f>a$ and

$$H(z_c,z_f,\boldsymbol{\rho}_f,\boldsymbol{\rho}_c)=-1/(2m^*_{zc})(\partial/\partial z_c^2) -1/(2m^*_{\|f})(\partial/\partial z_f^2) -V(\boldsymbol{\rho}_f,\boldsymbol{\rho}_c,z_c,z_f) , \quad (2c)$$

where $V(\boldsymbol{\rho}_f,\boldsymbol{\rho}_c,z_c,z_f)=-1/\{\varepsilon[(\rho_f\cos\Theta-\rho_c\cos\Theta)^2+(\rho_f\sin\Theta-\rho_f\sin\Theta)^2+(z_c-z_f)^2]^{1/2}\}$.

If the confinement in Eq. (2a) is large, the Coulomb interaction will be a small perturbation upon this solution so that to decouple it from the z component is a good approximation.[2] This will not be the case in Eqs. (2b) and (2c) where the solutions neglecting the Coulomb term will be free wave functions, which are very sensitive to perturbation. The motion in the z coordinate will be the most

sensitive to the Coulomb interaction since motion in this direction is totally free for both the electron and hole (neglecting the Coulomb interaction). We can, therefore, follow the approach of Ref. 2 and decouple the ρ dependence from the z dependence in Eq. (2c) (by integrating over the ρ_f and ρ_c coordinates) and using an averaged Coulomb interaction, which is defined as $V_{\text{eff}}(z)$ where $z=|z_c-z_f|$. We propose to take a separable wave function as the solution to Eq. (1) of the form

$$\Psi(\mathbf{r}_c,\mathbf{r}_f)=\Psi(\rho_c)\Psi(\rho_f)\Phi(z)\ , \tag{3}$$

where $\Psi(\rho_c)$ is the solution to (2a), $\Psi(\rho_f)$ is the solution to (2b), and $\Phi(z)$ is the solution to (2c) with $V(\rho_f,\rho_c,z_c,z_f)$ being approximated by $V_{\text{eff}}(z)$. Since the solutions to Eqs. (2b) and (2c) (neglecting the Coulomb interaction) are strongly perturbed by the Coulomb interaction, these two solutions are strongly coupled; once a solution of the form of Eq. (3) is achieved, it must be iterated to allow for the coupling of $\Psi(\rho_f)$ and $\Phi(z)$.

What we shall focus on is the GaAs/AlAs system where a wire of GaAs is surrounded by AlAs. In Fig. 1 (Ref. 7), we show the band lineup in the GaAs/AlAs system for a QD system. This is also the energy band lineup for the QW system. The potentials can be estimated from the data given in Ref. 8. The m^*_{zf} and $m^*_{\rho f}$ correspond to $m^*_{\parallel}$ $(1.56m_0)$ and $m^*_{\perp}$ $(0.19m_0)$ of the X valley in the AlAs when the direction parallel to the wire is $\langle 110\rangle$.[8] The heavy-hole mass is taken as $m^*_c=0.34m_0$.[8] Other approximations are as used in Ref. 7.

We shall first examine the approximation of using infinite confining potentials. For this case, the wave functions are completely confined in their appropriate semiconductors. The wave function and corresponding energy for the ground state of the confined particle are[9]

$$\Psi(\rho_c)_{n=1,l=0,m=0}=J_0(\alpha_0\rho_c/a)/[aJ_1(\alpha_0)\sqrt{\pi}] \tag{4a}$$

with corresponding binding energy

$$E=\alpha_0^2/(2a^2m^*_{\rho c})\ , \tag{4b}$$

where J_0 is the zeroth-order Bessel function, which has its first zero at $\rho=a$ and $\alpha_0=2.405$ is the value of the first zero. The exact form of the wave function of the unconfined particle [Eq. 2(b)] has not been evaluated in detail. It is free-particle-like everywhere except in the region $\rho<a$, where it is forced to zero. The energy of this state will be zero since it is unconfined.

The confined particle will not be altered by the Coulomb interaction since $E(\text{confinement})\gg E(\text{Coulomb})$ for infinite barriers. The unconfined or free particle will be affected by the Coulomb interaction, and its wave function will peak near the wire and will be forced to vanish at $\rho=a$ for infinite barriers. For infinite barriers, we propose a variational wave function of the form[10]

$$\Psi(\rho_f)=(\rho_f-a)\exp[-(\rho_f-a)b/2]/\sqrt{2\pi(6/b^4+2a/b^3)} \quad \text{for } \rho_f>a\ , \tag{5}$$

$$\Psi(\rho_f)=0 \quad \text{for } \rho_f<a\ ,$$

where b is the variational parameter, which is $b=2/a_0$, where a_0 is the effective orbital size. We use numerical techniques to solve for $E_x(z,\rho)$ by minimizing $E_x(\rho)$ with respect to the variational parameter b in Eq. (5) taking $z=0$ in the Coulomb term. This produces an initial $E_x(\rho)$ and $\Psi(\rho_f)$ from which we can evaluate an effective Coulomb interaction for the 1D exciton[10] using Eq. (3). We evaluate $E_x(z)$ for the 1D hydrogenic system[11] and evaluate $\langle z\rangle$ according to

$$E=1/(2\mu a_0^2)\ , \tag{6}$$

where $a_0=\langle z\rangle$ and μ is the reduced mass of the system. We then iterate until convergence is achieved. In Fig. 1, $E(z)$, $E(\rho)$, and their sum $E_x(\rho,z)$ are shown for the case of infinite barriers and the parameters introduced earlier.

If we consider the more realistic case of finite barriers, which are 0.526 eV for the confined hole and 0.278 eV for the free electron in the GaAs/AlAs system, this leads to penetration of the confined wave function out of the wire and of the free particle into the wire. This should greatly increase the Coulomb energy. This leakage can be represented as an exponential type of decay into the other semiconductor similar to the approach followed in Ref. 7. The calculation is similar to that followed for the infinite barrier and produces $E(\rho)$, $E(z)$, E_x, $\Psi(\rho_c)$, and $\Psi(\rho_f)$. The results for the GaAs/AlAs system are shown in Fig. 2.

The radiative recombination rate of both band-to-band and excitonic transitions is directly related to its oscillator strength, which for the type-II QW takes the form[7,12]

$$R\sim\|p_\rho\|^2\|p_z\|^2\langle\Psi(\rho_f)|\Psi(\rho_c)\rangle^2\langle\Phi(z=0)\rangle^2\Omega\ , \tag{7}$$

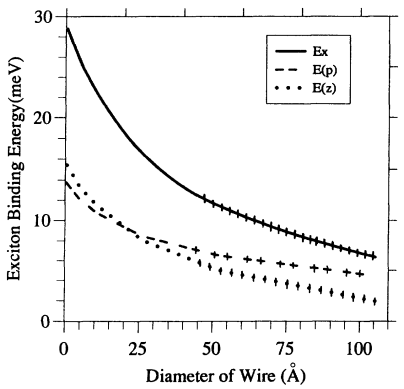

FIG. 1. The exciton binding energy $E_x=E(\rho)+E(z)$ in meV is shown as a full line as a function of the diameter of the quantum wire in Å for the system GaAs/AlAs assuming infinite barriers. The dashed line shows $E(\rho)$ using an exciton reduced effective mass of $0.12m_0$. This curve can be compared to a bulk exciton binding energy of 13.0 meV and a bulk hydrogenic impurity binding energy E_r of 20.2 meV. The dotted line shows $E(z)$ as a function of wire diameter using an exciton reduced mass of $0.28m_0$ and can be compared with a bulk exciton binding energy of 29.8 meV. (These values can also be compared with an averaged isotropic bulk exciton binding energy of 16.3 meV.) The system becomes type I for $a>43$ Å and so the finite and infinite curves are not valid for $a>43$ Å, which is indicated by the lines being crossed.

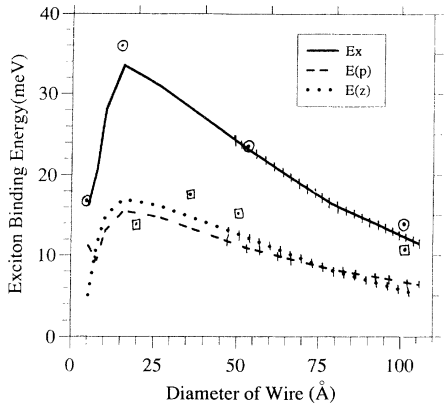

FIG. 2. The same as Fig. 1 with finite barriers (Ref. 11). These values of E_x should be compared to the binding energy of a hydrogenic impurity in bulk E_r, which is 36.3 meV, and the bulk exciton binding energy, which is 23.6 meV. Four values of E_x for the type-I system (Ref. 7) are shown for comparison as ⊡ , while four values of a hydrogenic impurity in a wire (Ref. 10) are shown as ⊙ for comparison.

where $\|p\|$ is the numerical version of the momentum matrix elements between Bloch functions and Ω is the wire atomic volume. For the type-II wire system, the overlap factor $\langle\Psi(\rho_f)|\Psi(\rho_c)\rangle$ will be small since it depends on the overlap of the exponential tails into and out of the well while the overlap factor $\langle\Phi(z=0)\rangle^2$ (Ref. 13) will be close to one since this is a type-I exciton overlap. Within this level of approximation, the exciton recombination in type-II systems with infinite barriers is zero. For finite barriers, the exponential tails contribute and as the dot gets smaller, pushing the ground state upwards, this exponential contribution increases sharply until the "confined" particle becomes unbound when the overlap should increase strongly. The overlap factor squared $\langle\Psi(\rho_f)|\Psi(\rho_c)\rangle^2$ is shown in Fig. 3. As mentioned previ-

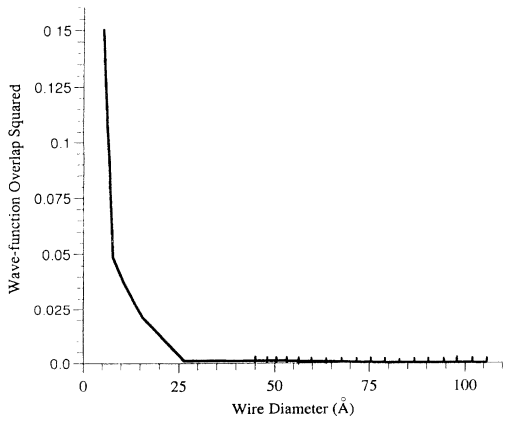

FIG. 3. The wave-function overlap squared $\langle\Psi(\rho_f)|\Psi(\rho_c)\rangle^2$ as a function of the diameter of the quantum wire in Å for the GaAs/AlAs system. This factor enters into the definition of the oscillator strength as given in Eq. (8) and will be the dominating factor in this equation. The system becomes type I when $a>43$ Å so the results shown for the type-II system for this region are shown crossed.

ously, the GaAs/AlAs system is indirect in k space as well as in real space. This complicates the analysis significantly, but the effect will be to reduce the oscillator strength (OS) further.[7]

Figures 1 and 2 show E_x [and $E(\rho)$ and $E(z)$] for infinite and finite barriers, respectively. In both cases E_x is small when a, the diameter of the wire, is large since the particles are kept apart so that the Coulomb interaction is small. As the diameter of the QW is reduced, the particles are allowed to approach each other in the ρ dimension and can therefore have a stronger interaction with the free electron correlating more with the confined hole, increasing E_x. For the infinite-barrier case, E_x increases smoothly to a value of 29.5 meV as $a\rightarrow 0$. For the finite-barrier case, as the size of the wire is decreased, E_x increases greatly above the E_x of the infinite barrier due to wave-function leakage into and out of the wire, which increases the Coulomb interaction. As a is decreased, E_x reaches a maximum of 33.5 meV at $a=16$ Å and then decreases. This decrease is due to the confined hole leaking out into the AlAs reducing its effective confinement and making the wave-function AlAs-like. For $a=7$ Å, the confined state moves out of the wire potential and becomes unbound. It is useful to decompose E_x into its $E(\rho)$ and $E(z)$ components and to discuss them separately. The ρ component contains the essential type-II behavior while the z component behaves much more like a 1D exciton with a modified Coulomb interaction.

It is interesting to compare $E(\rho)$ to E_r, the binding energy of a hydrogenic impurity in the bulk system,[10] which has an enhanced binding energy due to the enhanced correlation of the free particle with the localized impurity. For infinite-barrier systems, $E(\rho)$ will always be less than E_r since the wave function of the correlating particle is excluded from the wire. For the QW, $E(\rho)=14$ meV at $a=0$. Comparison can be made with a type-II quantum well where the correlation is in only one dimension and $E(\rho)$ would be much less (~ 8 meV) and with a QD where correlation is possible in three dimensions producing $E(\rho)=36.3$ meV. A comparison of these values shows the large effect of the electron mass anisotropy and a comparison of these values to $E(\rho)$ show that the added correlation due to the localization of the hole in the wire is very significant.

For finite-barrier systems, there will be wave-function leakage, which will enhance the Coulomb interaction allowing $E(\rho)$ to increase above that of the infinite-barrier case for the same diameter of wire. However, the type of wave-function leakage will also effect E_x. If the wave-function leakage arises from tunneling of the free particle into the wire, this results in wave-function overlap of this wave function with the strongly peaked wave function of the confined particle producing a large enhancement of both E_x and OS. A similar effect is observed in the case of a hydrogenic impurity confined in a quantum well[14] or wire[15] where the wave function of the correlating particle is forced to be much more peaked about the impurity by the confinement which increases E_r. As the wire size increases in the finite-barrier case, wave-function leakage

from the confined state and from the free state decreases and the finite- and infinite-barrier cases approach each other. (The significant difference between the finite and infinite cases at large a arises from the strong coupling between the ρ and z components.)

We now consider the z component. $E(z)$ is given as a dotted line for the case of infinite barriers in Fig. 1 and for the case of finite barriers in Fig. 2. $E(z)$ for the finite infinite-barrier case has its maximum value of 16.0 meV at $a=0$. For the case of finite barriers, $E(z)$ increases in magnitude due to wave-function leakage, which reduces the ρ component in the Coulomb term and therefore increases $E(z)$. It follows the same behavior as $E(\rho)$ reflecting their coupling and has its maximum peak value of 17 meV at $a=16$ Å. This component can be compared with the calculations on a 1D exciton for both an infinite[2] and finite[3] barriers. If we consider the case of infinite barriers, we see that for a 1D type-I exciton the binding energy goes to infinity for $a\rightarrow 0$, while for the type-II system it remains finite. Whereas the type-I exciton goes to the 3D limit as $a\rightarrow\infty$, for the type-II system the limit as $a\rightarrow\infty$ is $E(z)\rightarrow 0$. This difference occurs because of the $\rho=a$ dependence in the Coulomb integral. For the finite-barrier type-I exciton,[6] E_x does not go to infinity but has a maximum of 17.5 meV at $a\sim 33$ Å for a barrier of $Al_xGa_{1-x}As$ with $x=0.4$ and a conduction-band offset of 85%. This is shown for comparison in Fig. 2.

We will now discuss E_x which is the sum of $E(\rho)$ and $E(z)$ and reflects the trends discussed above. A comparison of the hydrogenic impurity (type I) confined in a finite-barrier wire[6] and a type-I 1D exciton with finite barriers[3] are made with the type-II exciton system in Fig. 2. In both of these systems, the barrier material is $Al_xGa_{1-x}As$ with $x=0.4$ and type-I parameters are used. For the 1D exciton system, an 85% conduction-band offset is taken[3] but this should not affect the results significantly. We can see that the 1D type-I exciton peaks at a much lower E_x of 17.5 meV compared to the other two systems. This is because of the much lower effective mass of the electron in this system. The hydrogenic impurity is very similar in shape and overall magnitude to the type-II exciton system. This similarity arises because of the strong wave-function overlap into and out of the wire, particularly the latter.

In conclusion, we have calculated the exciton binding energy and envelope wave-function overlap required for the calculation of the oscillator strength in a type-II QW for the GaAs/AlAs system. It is found to be substantially larger than the exciton binding energy of a type-II quantum-well system or of a type-I 3D or 1D exciton in these systems for the appropriate wire sizes in which these systems naturally occur in the type-II configuration. The wave-function leakage in these systems enhances the exciton binding energy and also gives a finite value for the oscillator strength of these systems, which can be tuned by the wave-function leakage.

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