Bulk anisotropic excitons in type-II semiconductors built with 1D and 2D low-dimensional structures

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We used a simple variational approach to account for the difference in the electron and hole effective masses in Wannier-Mott excitons in type-II semiconducting heterostructures in which the electron is constrained in an one-dimensional quantum wire (1DQW) and the hole is in a two-dimensional quantum layer (2DQL) perpendicular to the wire or viceversa. The resulting Schrödinger equation is similar to that of a 3D bulk exciton because the number of free (nonconfined) variables is three; two coming from the 2DQL and one from the 1DQW. In this system the effective electron-hole interaction depends on the confinement potentials.

Keywords: Groundstate energy of screened excitons; low-dimensional structures; semiconductors.

Utilizamos un método variacional para tomar en cuenta la diferencia entre las masas efectivas del electrón y del hueco en excitones Wannier-Mott en heteroestructuras semiconductoras tipo II en las que el electrón está constreñido en un alambre cuántico unidimensional (AC1D) y el hueco en un pozo cuántico bidimensional (PC2D) perpendicular al alambre o viceversa. La ecuación de Schrödinger resultante es similar a la de un excitón en el bulto en 3D porque el número de variables libres (no confinadas) es tres; dos que provienen del PC2D y una del AC1D. En este sistema interacción efectiva electrón-hueco depende de los potenciales de confinamiento.

Descriptores: Energía del estado base de excitones apantallados; estructuras de baja dimensionalidad; semiconductores.

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1. Introduction

Man-made low-dimensional solids yield new challenges in microstructure materials science. In general, excitons in confined systems are interesting due to their effects on the electronic and optical properties of high-quality nanostructures with prescribed configuration and dimensionalities. Size quantization in man-made semiconductor structures of less than three-dimensions leads to exciting new electronic properties which are important for fundamental physics and for the development of novel device concepts. Fundamental research as well as device applications based on these low-dimensional semiconductor structures requires methods of fabricating the structures and of controlling their geometrical size on the nanometer scale in a reproducible manner [1]. Typical examples of low-dimensional systems are one-dimensional quantum wires (1DQW) and two-dimensional quantum layers (2DQL). On the other hand, it is possible to construct more complicated artificial structures by assembling low-dimensional subsystems to study few-particle systems with tailored interaction potentials. For instance, now it is possible to join and assemble nanotubes to form more complex skeletons [2, 3].

In recent papers [4] (hereafter referred to as I) and Ref. 5, Wannier-Mott excitons were analyzed in a novel system in which the electron is constrained to move along a one-dimensional quantum wire (1DQW) and the hole is confined to a two-dimensional quantum layer (2DQL) perpendicular to the wire. An analogous system is obtained by exchanging the particles. The motivations for studying this system are threefold. First, as mentioned above, it is now feasible to construct these types of artificial structures in laboratories. Secondly, as will be shown, our system makes it possible to tailor the electron-hole interaction by geometrical means. Finally, up to now most research has been devoted to type-I semiconducting structures (in which electrons and holes share the same spatial region), while type-II semiconducting structures have received less attention. In the latter structures, the electron is confined to one material and the hole in another material due to band lineups in the two materials, which make this arrangement energetically favorable. For example, Rorison [6] calculated exciton binding energy and oscillator strength for quantum wires in type-II semiconductor systems consisting of a cylindrical wire of one semiconductor embedded in a second semiconductor. Excitons in type-II structures in which the electron is in 1DQW and the hole is in

another parallel [7] or perpendicular 1DQW [8], have been studied. More recently, exciton properties in type-II quantum disks and dots (QD) have been studied by Janssens *et al.* as a function of a perpendicular magnetic field [9, 10] and also including strain fields in and around the QDs [11]. Strain is important since it can have a large impact on the QD band structure and corresponding optical properties [11]. Under intense light excitation, dynamical processes on indirect and direct excitons at high density in $Al_xGa_{1-x}As$-AlAs 1DQW structures have been investigated [12], and a large blue-shift of the indirect exciton photoluminescence appears under a heavy excitation density, but that of the higher lying direct one hardly does. This is due to the phase space filling effects on the conduction and valence bands as well as the electric field effect due to the separation mechanism of the carriers in the type-II structure.

2. The system

In our system, in which the electron is constrained in a 1DQW and the hole is in a 2DQL perpendicular to the wire (or viceversa), the number of free (nonconfined) variables is three; two coming from the 2DQL and one from the 1DQW. This arrangement of the particles is original and interesting because, as shown in I, this system can be mapped on to a one- particle system moving in a three-dimensional (3D) free space which interacts through an effective potential V_{eff} with another particle fixed at the origin. Thus, except for the fact that the interaction potentials are different, a 3D exciton is analogous to our novel system. Since the V_{eff} in I is defined as an interaction between the charged density probabilities of the electron and the hole, then it involves an average over some transverse coordinates, and thus V_{eff} between confined particles depends on the kind of transverse confinement. For instance, here we will employ a parabolic transverse confinement potential which allow us to obtain analytical expressions for V_{eff}. In I, the resulting 3D exciton Schrödinger equation in the laboratory frame of reference was solved in terms of the common 3D exciton states by taking into account the finite width of both 1DQW and 2DQL. For vanishing 1DQW and 2DQL widths, the solution is formally identical to a 3D exciton.

However, calculations in I were performed by assuming, for simplicity's sake, that the effective masses of the electron and the hole were identical. This approximation is almost never valid. Since generally these effective masses are different in semiconductors, the purpose of this paper is to present a more realistic calculation that takes into account the fact that these effective masses are different. As in I, let us consider the general case of two quasiparticles confined to move in a heterostructure in such a way that one quasiparticle lies in an infinite 1DQW with the axis along the z-direction and the other lies in an infinite 2DQL parallel to the xy plane (see Fig. 1). We assume strong confinement so that in the confining directions (x and y for one quasi-particle in the 1DQW and z for the other), both quasi-particles are in their respective ground states. The widths of the 1DQW are σ_{x1} and σ_{y1}, and σ_{z2} is the width of the 2DQL.

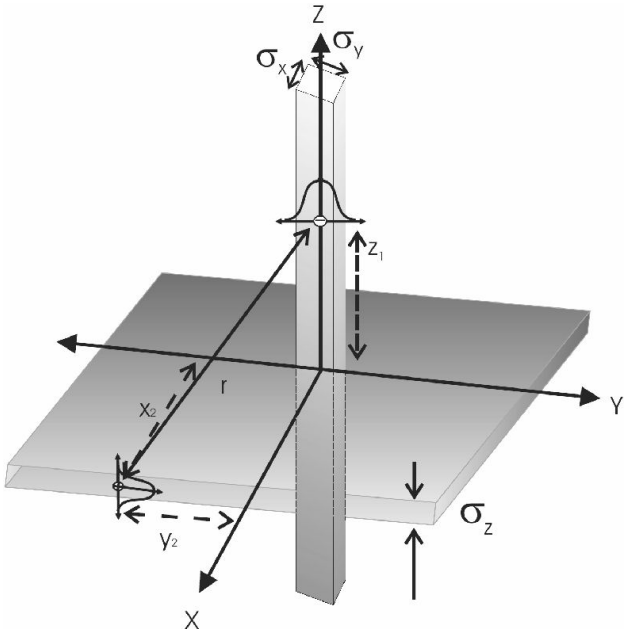

FIGURE 1. Schematic diagram of a system formed by an infinite 1DQW in which an electron is confined crossing a perpendicular 2DQL in which a hole is confined. Their widths are given in terms of the standard deviations as defined in the text.

3. Theory

As in I, we separate the two-particle wave function as

$$\Psi(x_1, y_1, z_1, x_2, y_2, z_2) = \Psi_1^0(x_1, y_1)\Psi_2^0(z_2)S(z_1, x_2, y_2), \quad (1)$$

where $\Psi_1^0(x_1, y_1)$ and $\Psi_2^0(z_2)$ are the groundstate wavefunctions of the quasiparticles with charges q_1 and q_2, with corresponding transverse confinement energies E_1^{0t} and E_2^{0t}. $S(x_2, y_2, z_1)$ is the part of the wavefunction that contains the interparticle Coulomb potential which satisfies the Schrödinger equation

$$\left[\frac{-\hbar^2}{2}\left(\frac{1}{m_1}\left(\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial y_2^2}\right)+\frac{1}{m_2}\frac{\partial^2}{\partial z_1^2}\right)+E_1^{0t} + E_2^{0t}+V_{eff}\right] S(x_2, y_2, z_1) = E_t S(x_2, y_2, z_1) \quad (2)$$

where m_1 and m_2 are the effective masses of the quasiparticles and

$$V_{eff}(x_2, y_2, z_1) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \left|\Psi_1^0(x_1, y_1)\right|^2 \times \left|\Psi_2^0(z_2)\right|^2 \widehat{V}_{int} dz_2 dy_1 dx_1 \quad (3)$$

is the effective interparticle Coulomb potential, the Coulomb interaction potential being

$$\widehat{V}_{int}\left(\overrightarrow{r_1}-\overrightarrow{r_2}\right)=\frac{q_1 q_2}{\epsilon\sqrt{\left(x_1-x_2\right)^2+\left(y_1-y_2\right)^2+\left(z_1-z_2\right)^2}}, \quad (4)$$

where ϵ is the appropriate dielectric screening of the semiconductor media. The excitonic energy E is defined as

$$E = E_t - E_1^{0t} - E_2^{0t}. \quad (5)$$

For the sake if convenience we choose harmonic transverse confining potentials for both particles, that is, $\hat{V}_1(x_1, y_1) = (k_1 x_1^2 + k_2 y_1^2)/2$ and $\hat{V}_2(z_2) = k_3 z_2^2/2$. The choice of harmonic confining potentials has the advantage over a hard-well potential that it could model either soft or hard possible confinements. In terms of standard deviations $\sigma_{x1} = \langle (x_1)^2 \rangle_0$, $\sigma_{y1} = \langle (y_1)^2 \rangle_0$ and $\sigma_{z2} = \langle (z_2)^2 \rangle_0$ (which are of the order of magnitude of the respective thickness of the 1DQW and 2DQL when subindex 0 indicates groundstate), these potentials yield the normalized groundstate transverse wavefunctions

$$\left|\Psi_1^0(x_1, y_1)\right|^2 = \frac{e^{-\left(\frac{x_1^2}{2\sigma_{x1}^2}+\frac{y_1^2}{2\sigma_{y1}^2}\right)}}{2\pi\sigma_{x1}\sigma_{y1}} \quad (6)$$

and

$$\left|\Psi_2^0(z_2)\right|^2 = \frac{e^{\frac{-z_2^2}{2\sigma_{z2}^2}}}{\sqrt{2\pi}\sigma_{Z2}} \quad (7)$$

Furthermore, it was found that for harmonic confinement potentials the effective potential (with $q_1 = e$ and $q_2 = -e$) is

$$V_{eff} = -\frac{e^2}{\epsilon r}\text{erf}\left(\frac{r}{\sqrt{2}\sigma}\right), \quad (8)$$

where, for the sake of simplicity, $\sigma = \sigma_{x1} = \sigma_{y1} = \sigma_{z2}$. Here erf$(x)$ is the error function defined as

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-s^2} ds.$$

As shown in I, when all widths σ_{x1}, σ_{y1} and σ_{z2} vanish, then V_{eff} becomes a simple screened Coulomb potential $-e^2/\epsilon r$, where $r = \sqrt{x_2^2 + y_2{}^2 + z_1^2}$. With this V_{eff}, Eq. (2) was solved in I for the case $m_1 = m_2$ (see Fig. 2). Notice that we can tailor V_{eff} in two ways. One way is due to the particular geometry, and the second one by choosing the type of confinement potential.

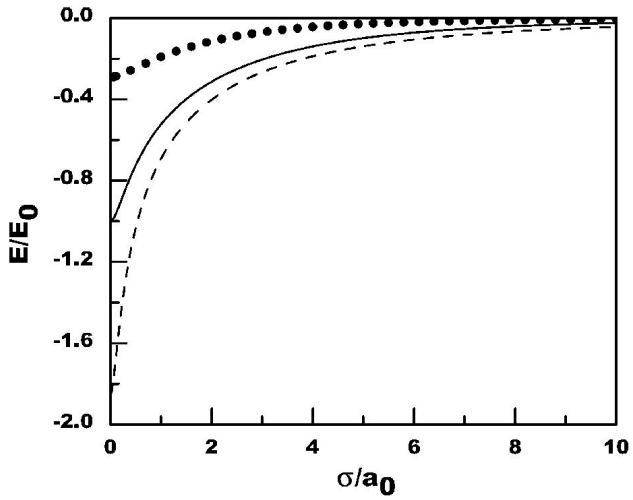

FIGURE 2. Comparison of the equal-mass case ($m_1 = m_2$, solid line) and the more realistic cases $m_1 \neq m_2$ (dashed and dotted lines) for the normalized groundstate energies E/E_o as a function of the width σ/a_o. The dashed curve corresponds to the electron in the 1DQW and the hole in the 2DQL, and the dotted line corresponds to an exchange of electron and hole. Here, $E_o = e^2/(2\epsilon a_o)$ is the $3D$ exciton binding energy, $a_o = \hbar^2\epsilon/(e^2\mu)$ is the exciton Bohr radius, and the reduced mass is $\mu = m_1 m_2/(m_1 + m_2)$.

In our system the source of anisotropy is from the fact that the coefficients of the partial derivatives in Eq. (2) are not equal because, in general, the values of the effective masses of the electron and the hole are different (that is, $m_1 \neq m_2$). To solve Eq. (2), we employ the following variational function for the ground state

$$S(z_1, x_2, y_2) = \left(\pi a^2 b\right)^{-1/2} \exp\left[-\left(\frac{\rho_2^2}{a^2}+\frac{z_1^2}{b^2}\right)^{-1/2}\right], \quad (9)$$

which represents, with suitable choice of the constants a and b, a very good approximation to the exact solution [13]. In Ref. 13 this wavefunction modeled donor states in silicon. Here $\rho_2^2 = x_2^2 + y_2^2$, and the parameters a and b are chosen in such a way that they minimize the exciton binding energy (which is defined as the negative of the groundstate energy). This function was originally used by Kohn to solve a similar equation which describes donor states in semiconductors with different effective masses around the minima of the conduction band along the (1,0,0) axis and equivalent axes [13].

4. Results and discussion

To solve Eq. (2), we employed the simple variational wavefunction Eq. (9). However, for some cases this method may not be the most appropriate on for dealing with strong anisotropies. For instance, if one of the effective masses is very small compared with the others, we may use what is called adiabatical approximation. That is, one first solves the equation of the smallest effective mass particle (light particle) where the positions of the other particles are treated as parameters - as when we find the electric motion for fixed nuclear

positions in molecular problems. Then the slower dynamics of the rest of the particles is solved- as if one weresolving the nuclear motion in molecular problems. The same procedure is applied when two of the three effective masses are very small. In the particular case that the values of the three masses are all of different scales, then the same procedure is applied three times in succession.

In our case of semiconducting materials, the effective masses are not so different. Here we used the following values: the effective masses of the electron and hole are respectively $-0.067m$ and $0.7m$ [14] (m being the free electron mass), which correspond to quantum wells of $Al_xGa_{1-x}As$-AlAs. In Fig. 2, we show the corresponding results of the groundstate energy as a function of the width σ for isotropic and anisotropic cases. The results show that the exciton energy is not invariant with the exchange of particles since, in Eq. (2), m_1 contributes to the kinetic energy in the denominator of the two first terms, whereas m_2 contributes only in one kinetic energy component. Therefore, when $m_1$is smaller than m_2, the kinetic energy (and consequently the groundstate energy) of the system increases. Also, the exciton binding energy decreases as confinement becomes weaker. Therefore, confinement effects are always stronger for the ground state. This work presents a system that resembles a 3D anisotropic exciton Schrödinger equation. In the limit of vanishing thickness of both 1DQW and 2DQL ($\sigma_x = \sigma_y = \sigma_z = 0$), is similar to that of an anisotropic 3D exciton with screened Coulomb interaction, set for the relative coordinates in the center of mass reference. For arbitrary thickness, the electron–hole potential is no longer coulombic.

In summary, we have extended the work presented in I to take into account the more realistic cases in which the electron and hole effective masses are different. The ground state variational wavefunction used here is analogous to that employed in a 3D bulk system to study donor impurity states [13], but here we have solved the exciton Schrödinger equation of our heterostructure, which exhibits an important difference. In our case, the interaction potential is an effective Coulomb potential which depends on the type of confinement and on the 1DQW and 2DQL widths. We considered that, in the confinement directions, both electron and hole were in their respective groundstate of a harmonic potential which yielded an analytical expression for the effective interparticle Coulomb potential for the case $\sigma_x = \sigma_y = \sigma_z$. In general, we can modify the Coulomb potential with different choices of confinement potentials. It is interesting to note that the analogies between the system studied here and bulk excitons can be explained in terms of the equivalent degrees of freedom. A two-particle system like ours, with only one degree of freedom for one particle and two degrees of freedom for the other, behaves like a system where one particle is fixed at the origin and the other particle has the remaining three degrees of freedom.

The variational method employed here is simple, and accounts for the main features of the problem. Our quantitative results show that the difference between the cases $m_1 = m_2$ and $m_1 \neq m_2$ is large. We hope that this work may stimulate further experimental and theoretical efforts in the study of type-II novel semiconducting heterostructures.

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