Wannier-Mott exciton formed by electron and hole separated in parallel quantum wires

J. A. Reyes*
Liquid Crystal Institute, Kent State University, Kent, Ohio 44242

M. del Castillo-Mussot
Instituto de Física, Universidad Nacional Autonoma de México, Apartado Postal 20-364, 01000 México, D.F., México

(Received 24 January 1997; revised manuscript received 25 August 1997)

We analyze a Wannier-Mott exciton in which the electron and hole are constrained to move in two separated and parallel quantum wires. We expand the electron-hole interaction potential in terms of multipoles by assuming that both the electron and hole experience transverse harmonic confinements in the x and y directions, both being in their respective transverse ground states. For the resulting z-dependent Schrödinger equation, we calculate in detail eigenenergies and eigenfunctions for the exciton ground and first excited states as functions of the transverse dimension of the wires and their separation distance. Also, we calculate the higher eigenenergies and eigenfunctions approximately by using a WKB formalism. [S0163-1829(97)04048-4]

I. INTRODUCTION

The electronic properties of highly inhomogeneous systems such as confined systems have received much attention due, among other reasons, to the possibility of growing high-quality nanostructures with prescribed configurations, allowing the control of physical properties such as carrier densities, band gaps and bandwidths, and even dimensionality. In the case of quasi-one-dimensional systems or quantum wires, the Fermi energy is comparable to the interlevel energy separation associated with the strong transverse configuration. In strictly one dimensional (1D) systems, the carrier density is such that only the levels associated with the ground-state energy of the transverse confinement are occupied. For experimental and theoretical reviews on these systems, see Refs. 1 and 2, respectively.

The purpose of this paper is to present model calculations of large excitons in a structure consisting of two parallel strictly 1D quantum wires, with the electron being confined in one wire and the hole being confined in another parallel wire (see Fig. 1). We shall calculate the eigenenergies and eigenfunctions as a function of the distance that separates both wires. Here we do not address the issue of how this kind of system could be induced, but in analogy to 2D cases we think of different ways of favoring such an arrangement: (i) etching a 2D double quantum well to make it 1D; (ii) placing a quantum wire in the neighborhood of the interface of two media to produce electrostatic image forces; and (iii) applying an electric field to increase tunneling and thus physical separation between electron and holes.

Some studies of 2D systems with spatial separation between the electron and holes were reported in the following papers. Beresford *et al.*[3] studied type-II heterojunctions based upon materials such as InAs and GaSb, where neighboring layers of electrons and holes were produced. Brum and Ferrara[4] calculated the ground exciton state of the GaSb-InAs-GaSb heterostructure, in which electrons and holes are present in spatially separated regions. The dielectric function and collective modes of 2D interacting bosons (excitons) were theoretically investigated by Kachintev and Ulloa.[5] On the other hand, there is a related relevant theoretical work in three dimensions on layer structures, and near an interface of two media for small and large electron-hole separation.[6]

In the pioneering theoretical work of Loundon[8] on a 1D hydrogen atom, anomalous behaviors of both eigenfunctions and eigenenergies were found due to a nonphysical electronic distribution, since the transverse dimensions of the wire were neglected. Later Banyai *et al.*[7] took into account the finite width of the wire, and made use of parametrized

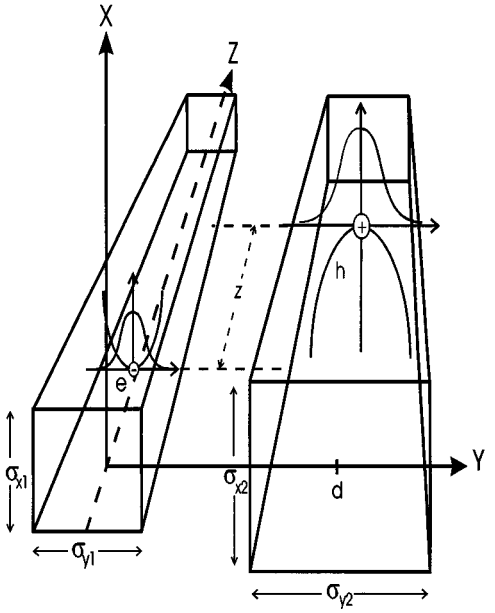

FIG. 1. Diagram of a section of the system formed by two infinite parallel quantum wires where their centers are separated by distance d. Both electron e and hole h experience transverse harmonic potential confinements in the x and y directions (of which we only show schematically the potential in y). The dimensions of the wires are given in terms of standard deviations $\sigma_{x\nu}$ and $\sigma_{y\nu}$ ($\nu=1$ and 2) of both electron and hole as defined in the text. These constants are inversely proportional to the stiffness of the harmonic potential.

trial electron-hole potential to adjust the effective potential numerically.

This paper is structured as follows; in Sec. II we derive the effective 1D interaction potential between two particles, when each one is in one of the parallel quantum wires and when both particles experience a harmonic potential for the transverse confinement. Then we proceed to make a multipolar expansion in which the zeroth-order solution is (in the case of the electron-hole pair) Loundon's anomalous solution. In Sec. III we solve the resulting Wannier-Mott exciton equation, in Sec. IV we explicitly present our results in terms of typical parameters of a semiconductor heterostructure, and in Sec. V we present a brief analysis of the higher eigenestates and eigenenergies of the system by using the WKB approximation. Finally, Sec. VI is devoted to summarizing our work and presenting our results.

II. EFFECTIVE INTERWIRE INTERACTION

We will consider the general case of two particles confined to move in a semiconductor heterostructure in such a way that each particle lies in one of the two parallel and infinite (or very large) quantum wires. We depict this situation in Fig. 1 for the case of an electron and a hole. If we neglect all possible variations and defects which could be present in the quantum wire walls, the Hamiltonian of the system can be written as

$$\hat{H}=\hat{H}_1+\hat{H}_2+\hat{V}_{\text{int}}, \tag{2.1}$$

where $\hat{H}_\nu$, with $\nu=1$ and 2 (we can use in general the labels 1 and 2 for particles p_1 and p_2, but later we will study the particular case of an electron and a hole), are defined as

$$\hat{H}_\nu=\hat{T}_{\nu x}+\hat{T}_{\nu y}+\hat{T}_{\nu z}+\hat{V}_\nu(x_\nu,y_\nu), \tag{2.2}$$

where $T_{\nu i}$, with $i=x$, y, and z, is the kinetic energy and V_ν is the transverse confinement potential of each carrier. On the other hand, the electric interaction potential is given by

$$\hat{V}_{\text{int}}(\vec{r}_1-\vec{r}_2)=\frac{q_1q_2/\epsilon}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}}, \tag{2.3}$$

where ϵ is the appropriate dielectric screening of the semiconductor media, and q_1 and q_2 are the magnitude of the charges of particles p_1 and p_2.

In order to find one-dimensional eigenfunctions of the Hamiltonian given by Eq. (2.1), let us assume that the transverse dimensions of the wires are small enough so that their associated ground-state energies are the only relevant levels for the energy range we consider. We also suppose that the wave function is variable separable; thus it can be written as

$$\psi=\psi_1^0(x_1,y_1)\,\psi_2^0(x_2,y_2)\,\psi(z_{\text{cm}})\,\phi(z), \tag{2.4}$$

where z_{cm} and z are the usual mass center and relative coordinate defined as $z_{\text{cm}}=(m_1z_1+m_2z_2)/(m_1+m_2)$ and $z=z_1-z_2$. Here $\psi_1^0(x_1,y_1)$ $\psi_2^0(x_2,y_2)$ and $\psi(z_{\text{cm}})$ are functions such that $(\hat{T}_{\nu x}+\hat{T}_{\nu y}+\hat{V}_\nu)\psi_\nu^0=E_{\nu 0}^t\psi_\nu^0$, (the index 0 denotes a ground-state) and $(d^2/dz_{\text{cm}}^2)\psi(z_{\text{cm}})=[(\hbar k)^2/2m]\psi(z_{\text{cm}})$, k being the wave vector of the pair p_1-p_2 (which is the exciton wave vector for the electron-hole pair) in the z direction, $\mu=m_1m_2/(m_1+m_2)$ its reduced mass, and $\phi(z)$ the wave function part associated with the relative coordinate. In the same way as Banyai *et al.*[7] did, we calculate the bracket $\langle\psi_1^0\psi_2^0\psi(z_{\text{cm}})|\hat{H}|\psi_1^0\psi_2^0\psi(z_{\text{cm}})\phi(z)\rangle$, where $\hat{H}$ is given by Eq. (2.1). This leads to the expression

$$-\frac{\hbar^2}{2\mu}\frac{d^2\phi}{dz^2}+V_{\text{eff}}(z)\,\phi(z)=E^{1\text{D}}\phi(z), \tag{2.5}$$

where the effective potential V_{eff} for the one-dimensional problem is defined as

$$V_{\text{eff}}(z)=\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2\int_{-\infty}^{\infty}dy_1\int_{-\infty}^{\infty}dy_2 \times|\psi_0(1)|^2|\psi_0(2)|^2\hat{V}_{\text{int}}(\vec{r}_1-\vec{r}_2) \tag{2.6}$$

and

$$E^{1\text{D}}=E-E_{10}^t-E_{20}^t-\frac{(\hbar k)^2}{2M}, \tag{2.7}$$

where E is the eigenenergy of the whole system, and $M=m_1+m_2$ is the total mass. Notice that V_{eff} is simply an average over the transverse coordinates of both electron and hole, and depends only on the relative coordinate z. Banyai *et al.*[7] established an expression similar to $V_{\text{eff}}(z)$, and adjusted it numerically to the trial potential $V_{\text{adj}}=1/(|z|+\gamma)$ by adequately choosing the parameter γ. Although this procedure provides a global behavior of $V_{\text{eff}}(z)$, it does not take into account correctly the spatial distributions of the density probabilities of both charge carriers in the vicinity of the origin; in fact their V_{adj} has a discontinuity of its first derivative that is not shown by $V_{\text{eff}}(z)$ given here.

In order to use the density probabilities explicitly, we proceed to perform a multipolar expansion of V_{eff}. At this point it is necessary to know the transverse confinement explicitly. We shall restrict our model to harmonic potentials mainly for two reasons: in the first place it could represent either soft or hard confinements, and, second, all the moments of the harmonic oscillator calculated in the ground-state can be expressed in terms of the powers of its standard deviation. However, our treatment is valid for any transverse confinement potential whose moment integrals are well defined and known, and for any pair of particles p_1 and p_2 (although in this work we will apply it to the exciton problem, so p_1 and p_2 will be the electron and the hole).

To find the multipolar expansion it is useful to write the ground-state joint density probability of the bidimensional harmonic oscillator in terms of its standard deviations $\sigma_{x\nu}=\langle(x^\nu)^2\rangle_0$ and $\sigma_{y\nu}=\langle(y^\nu)^2\rangle_0$, with $\nu=1$ and 2 (which are inversely proportional to the fourth power of the stiffness of the harmonic potential), as follows:

$$|\psi_0(1,2)|^2=|\psi_0(1)|^2|\psi_0(2)|^2$$
$$=\frac{e^{-[y_1^2/(\sigma_{y1})^2]-[x_1^2/(\sigma_{x1})^2]}}{\pi\sigma_{y1}\sigma_{x1}}$$
$$\times\frac{e^{-[(y_2-d)^2/(\sigma_{y2})^2]-[x_2^2/(\sigma_{x2})^2]}}{\pi\sigma_{y2}\sigma_{x2}}. \tag{2.8}$$

Here d is the distance between the center of the wires, as shown in Fig. 1, and the indexes 1 and 2 indicate particles p_1 and p_2. It is well known that $|\psi_0(\nu)|^2$ tends to the Dirac's δ function as $\sigma_{x\nu}$, $\sigma_{y\nu}\to 0$. Then we can approximate the electrostatic potential as a Taylor expansion around the maximum of $|\psi_0(1,2)|^2$ with respect to its four transverse variables. This yields

$$V_{\text{eff}}=\frac{q_1q_2}{\epsilon}\sum_{ijkl}\frac{I(\sigma_{x1},\sigma_{x1},\sigma_{y2},\sigma_{y2})}{(i+j+k+l)!}\frac{\partial^{i+j+k+l}}{\partial y_1^i\partial y_2^j\partial x_1^k\partial x_2^l}$$
$$\times[(x_1-x_2)^2+(y_1-y_2)^2$$
$$+(z_1-z_2)^2]^{-1/2}|_{x_2=x_1=y_2=0,y_1=d}, \tag{2.9}$$

where $I(\sigma_{x1},\sigma_{x2},\sigma_{y1},\sigma_{y2})$ are the moments of the joint density probability of the ground-state given by

$$I(\sigma_{x1},\sigma_{x2},\sigma_{y1},\sigma_{y2})=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dx_1dx_2dy_1dy_2$$
$$\times|\psi_0(1,2)|^2y_1^i(y_2-d)^jx_1^kx_2^l. \tag{2.10}$$

The calculation of $I(\sigma_{x1},\sigma_{x2},\sigma_{y1},\sigma_{y2})$ is straightforward, and we rewrite the multiple partial derivative involved in Eq. (2.9) in terms of orthogonal polynomials. By using the generating function of the Legendre polynomials, it is easily shown that[9]

$$\frac{\partial^{i+j}}{\partial x_1^i\partial x_2^j}[(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2]^{-1/2}|_{x_1=x_2=0}$$
$$=\frac{(-1)^j(i+j)!P_{i+j}(0)}{[(y_1-y_2)^2+(z_1-z_2)^2]^{(1+i+j)/2}}, \tag{2.11}$$

where P_n are the Legendre polynomials ($n=0,1,\ldots$). Since $P_n(0)=0$ for odd n, in what follows we set $2n=i+j$. If we now take the partial derivatives of Eq. (2.11) with respect to y_1 and y_2, and write the resulting expression in terms of the Gegenbauer polynomials by means of its generating function,[10] we find that

$$\left.\frac{\partial^{k+l}[(y_1-y_2)^2+(z_1-z_2)^2]^{-(1/2)-n}}{\partial y_1^k\partial y_2^l}\right|_{y_1=0,y_2=d}$$
$$=\frac{(-1)^l2^{k+l}(k+l-1/2)!}{\sqrt{\pi}(d^2+z^2)^{n+[(1+k+l)/2]}}T_n^{k+l}\left(\frac{d}{\sqrt{d^2+z^2}}\right), \tag{2.12}$$

where T_n^{k+l} denotes the Gegenbauer polynomials. By substituting Eq. (2.12) into Eq. (2.9) and expressing $I(\sigma_{x1},\sigma_{x2},\sigma_{y1},\sigma_{y2})$ in terms of the Γ function, we arrive at the following general expression for V_{eff}:

$$V_{\text{eff}}=q_1q_2\sum_{n,m}^{\infty}\frac{C(\sigma_{x1},\sigma_{x2})D(\sigma_{y1},\sigma_{y2})T_n^m(d/\sqrt{d^2+z^2})}{(2n+2m)!(d^2+z^2)^{n+m+1/2}}, \tag{2.13}$$

where we have set $m=k+l$ and introduced the abbreviations $C(\sigma_{x1},\sigma_{x2})$ and $D(\sigma_{y1},\sigma_{y2})$ defined as

$$C(\sigma_{x1},\sigma_{x2})=\sum_{j=0}^{n}\frac{(-1)^jn!P_{2n}(0)}{\pi^2}\Gamma(n-j-\tfrac{1}{2})\Gamma(j+\tfrac{1}{2})$$
$$\times(\sigma_{y1})^{2n-j}(\sigma_{y2})^j, \tag{2.14}$$

$$D(\sigma_{y1},\sigma_{y2})=\sum_{l=0}^{m}\frac{(-1)^l(2m-1/2)!}{\sqrt{\pi}}2^m\Gamma(m-l-\tfrac{1}{2})$$
$$\times\Gamma(l+\tfrac{1}{2})(\sigma_{x1})^{2m-l}(\sigma_{x2})^l, \tag{2.15}$$

where Γ is the gamma function. Note that expansion (2.13) is valid for any values of the length parameters d and the four σ's. However, when $d=0$ and all the σ's are nonvanishing, this expansion is just valid for $z>\max\{\sigma\}$, so that our procedure cannot describe the eigenfunctions in the special case when $d=0$.

For the sake of simplicity we assume in what follows that the confinements are chosen in such way that $\sigma_{x1}=\sigma_{x2}$ and $\sigma_{y1}=\sigma_{y2}$, and we keep only the dominant term of the potential and the first correcting term which takes into account the finite wire dimensions. This yields

$$V_{\text{eff}}=\frac{q_1q_2}{\epsilon\sqrt{z^2+d^2}}\left[1-\frac{3.16\sigma_x^4}{(z^2+d^2)^2}\right]. \tag{2.16}$$

Since we are interested in solving the exciton problem, we set $q_1q_2=-e^2$ from now on. It is important to remark that in the cases $\sigma_{x1}=\sigma_{x2}$ and $\sigma_{y1}=\sigma_{y2}$, the bipolar term of this expansion vanishes, since it is proportional to the difference of thickness of both wires $\sigma_{x_i1}=\sigma_{x_i2}$, so the first nonvanishing correcting term is proportional to σ_x^4 (quadrupolar term), as shown in Eq. (2.16). Also, to this order of approximation V_{eff} does not depend on σ_y.

III. 1D SCHRÖDINGER EQUATION FOR THE EXCITON

If we insert Eq. (2.16) into Eq. (2.5) for the case $q_1q_2=-e^2$, and write it in terms of the dimensionless variable $\zeta\equiv z\sqrt{-2\mu E_n^{1\text{D}}}/\hbar$, the effective exciton 1D Schrödinger equation for the electron-hole relative coordinate turns out to be

$$\frac{d^2\phi}{d\zeta^2}+\left(\frac{\gamma}{\sqrt{\zeta^2+\zeta_0^2}}\left[1+\frac{\beta}{(\zeta^2+\zeta_0^2)^2}\right]-1\right)\phi=0, \tag{3.1}$$

where $\zeta_0\equiv d\sqrt{-2\mu E_n^{1\text{D}}}/\hbar$, $\beta\equiv -3.06[-2\mu E_n^{1\text{D}}\sigma_{x2}/\hbar^2]^2$, and $\gamma\equiv(e^2/\epsilon\hbar)\sqrt{-2\mu/E_n^{1\text{D}}}$ are dimensionless parameters. Note that, as expected, Eq. (3.1) reduces to the one-dimensional Loundon's[8] hydrogen atom when β and ζ_0 are to be taken to be zero. This limit case is an anomalous one

since, as Loundon[8] showed, it has an infinite ground-state binding energy and exhibits degeneration between odd and even states. If we introduce the variables $u \equiv \sqrt{\zeta^2+\zeta_0^2}$ and $f(u) \equiv \phi(u)e^u$, then Eq. (3.1) takes the following form

$$u^2\frac{d^2f}{du^2}-2u^2\frac{df}{du}+\gamma uf+\frac{\gamma\beta f}{u^3}+\zeta_0^2\left[-\frac{d^2f}{du^2}+\left(2+\frac{1}{u}\right)\frac{df}{du}-\left(1+\frac{1}{u}\right)f\right]=0. \tag{3.2}$$

It is necessary to point out that although Eqs. (3.2) and (3.3) have the necessary structures to be treated by the conventional time-independent perturbation method, this method cannot be performed due to the fact that the corresponding unperturbed ground-state eigenenergy and eigenfunction ($\zeta_0=\beta=0$) are anomalous, as mentioned above. The former is infinite, and the latter is the Dirac's δ function.[8]

Notice that Eq. (3.2) can only describe the even eigenstates of the system, since the variable u is an even function of ζ, so we have to use another equation for describing the odd eigenstates. To this end let us introduce the function $g \equiv f(\sqrt{\zeta^2+\zeta_0^2})/\zeta$, which is itself an odd function of ζ. Thus, by using the definition of u, Eq. (3.1) turns out to be

$$u^2\frac{d^2g}{du^2}-2u(1+u)\frac{dg}{du}+(\gamma-2)ug+\frac{\gamma\beta}{u^3}g+\zeta_0^2\left[-\frac{d^2g}{du^2}+\left(2+\frac{1}{u}\right)\frac{dg}{du}-\left(1+\frac{1}{u}\right)g\right]=0. \tag{3.3}$$

Now, both Eqs. (3.2) and (3.3) can be solved by using a Frobenius series since, as can be shown directly, their coefficients do not present any fundamental singularity. Then by expanding both as f and g as $\Sigma_0^\infty C_n u^{-n-\eta}$ (where η is an index whose value is found to be equal to zero to satisfy the conditions $f,g \to 0$ as $|\zeta| \to \infty$), we can easily show that their recurrence relations are of the form

$$C_{n-1}A^\iota+C_nB^\iota+C_{n+1}D^\iota+C_{n+2}E^\iota+C_{n+3}F^\iota=0, \tag{3.4}$$

where $\iota=e$ and o (even and odd, respectively) and $A^e=(2+n)(n+1)-\zeta_0^2$, $A^o=(n+1)(n+4)-\zeta_0^2$, $B^{e,o}=\gamma-2n$, $D^{e,o}=-\zeta_0^2(2n+5)$, $E^{e,0}=-\zeta_0^2(n+5)(n-3)$, and $F^{e,o}=\beta$. Note that the last three of these coefficients are proportional to the parameters ζ_0^2 and β, which are also proportional to d and σ_x, the distance between wires and their transverse dimensions along the x direction. Furthermore, the solution of Eq. (3.4) reduces to $uL_n^1(u)$ where $L_n^1(u)$, $(n=1,2,\ldots)$ are the associated Laguerre polynomial when both ζ_0^2 and β are to be taken to be zero. This limit case corresponds to a 1D exciton or hydrogen atom.[8]

Here, to be consistent with the few-term expansion of V_{eff} given by Eq. (2.16), we restrict ourselves to take into account only small values of the length parameters ζ_0 and β, which amounts to having small values of d and σ_x. Let us numerically estimate ζ_0 and β, by taking $d=100$ Å and $\sigma=30$ Å, and suppose that $E_0^{1D} \approx meV$ (which is the typical magnitude order of the exciton energy) to obtain that $\zeta_0=0.1$ and $\beta=0.05$, which are indeed small values.

Since ζ_0^2 and β are small quantities we can approximate the coefficients E and F iteratively, by using the recurrence relation of $uL_n^1(u)$, valid when both ζ_0^2 and β are zero, so that Eq. (3.4) can be written as a three-term recurrence relation. We will not use the same approximation to calculate the coefficient D since Eq. (3.4) would reduce to a two-term recurrence relation and then the associated eigenenergies would be the same as the one obtained by Loundon.[8] In this way, the three-term recurrence relation has the same A and B coefficients, but now the third coefficient C' is given by

$$C'=\zeta_0^2\left(-5-2n-\frac{(\gamma-2n-4)(n+3)(n+5)}{(n+3)(n+4)-\zeta_0^2}\right)+\beta\frac{(\gamma-2n-6)(\gamma-2n-4)}{[(n+4)(n+5)-\zeta_0^2][(n+3)(n+4)-\zeta_0^2]}. \tag{3.5}$$

To establish the equations for determining the eigenenergies, we use each of our three-term recurrence relation to find their associated continued fraction,[11] leading to the expressions

$$\frac{B_0}{A_0}-\cfrac{B_1}{A_1+\cfrac{C_1'B_2}{A_2+\cfrac{C_2'B_3}{A_3+\cfrac{C_3'B_4}{A_4+\cdots}}}}=0. \tag{3.6}$$

The solutions of these transcendental equations provides all the eigenenergies of the system.

IV. NUMERICAL RESULTS

For the sake of brevity, let us calculate only the ground-state E_0^{1D} and first excited E_1^{1D} binding energies by expanding Eqs. (3.6) in powers of ζ_0^2 and β around zero to yield

$$E_0^{1D}=-\frac{6^{2/3}}{[(8\sqrt{2\mu}\epsilon d^2/e^2\hbar)+1.34(2\mu/\hbar)^{3/2}\sigma_x^2]^{2/3}}, \tag{4.1}$$

$$E_1^{1D}=-\frac{\mu/2\,(e^2/\epsilon\hbar)^2}{\left\{1+\frac{8}{3}\left[(\mu d e^2/\epsilon h^2)^2+\frac{1}{15}(\mu\sigma_x e^2/\epsilon\hbar^2)^4\right]\right\}^2}. \tag{4.2}$$

Note that up to this order of approximation, the expression for E_0^{1D} and E_1^{1D} depend on σ_x and not on σ_y. This fact is reasonable since a larger front area (larger σ_x) increases the Coulomb interaction between both wires, whereas a variation of σ_y does not significantly change the average distance between the centers of charge of the two particles.

Finally, let us calculate the ground and first excited eigenfunctions ϕ_0 and ϕ_1. By inserting the eigenenergies E_0^{1D} and E_1^{1D} into the recurrence relation, we find the coefficients of

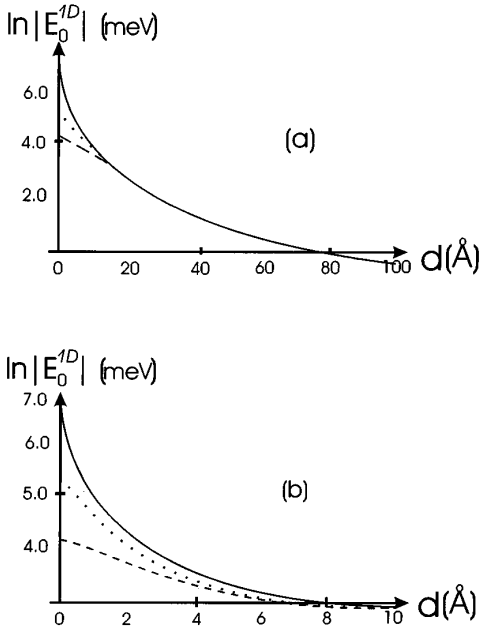

FIG. 2. Ground-state eigenenergies as function of d for various values of σ_x. We assume the same confinement for the electron and hole ($\sigma_{x1}=\sigma_{x2}$ and $\sigma_{y1}=\sigma_{y2}$). In panel (a) we plot $\ln|E_0^{1D}|$ for $\sigma_x=10$ Å (solid line), $\sigma_x=30$ Å (dotted line), and $\sigma_x=45$ Å (discontinuous line). Panel (b) is the same as panel (a), but for a minor range of d in the vicinity of the origin.

the Frobenius series of f and g, and then the eigenfunctions ϕ_0 and ϕ_1. These eigenfunctions, to first nonvanishing order in ζ_0^2 and β, turn out to be

$$\phi_0=Se^{-u}\left(-\frac{5}{4}\gamma\zeta_0^2+\frac{\beta}{10}-\frac{\gamma}{u}\right), \tag{4.3}$$

$$\phi_1=S'\zeta e^{-u}\left(-\frac{5}{4}\gamma\zeta_0^2+\frac{\beta}{10}-\frac{\gamma}{u}\right), \tag{4.4}$$

where S and S' are normalization constants such that $\int_{-\infty}^{\infty}\phi_0^2 d\zeta=1$ and $\int_{-\infty}^{\infty}\phi_1^2 d\zeta=1$, respectively.

We have assumed that the screening dielectric constant is the same inside and outside the quantum wires. This approximation is valid when the ratio ϵ_1/ϵ_2 is close to 1. Banyai *et al.*[7] studied the 1D excitonic ground-state energy and eigenfunction for one isolated quantum wire using the value $\epsilon_1/\epsilon_2=1.3$.

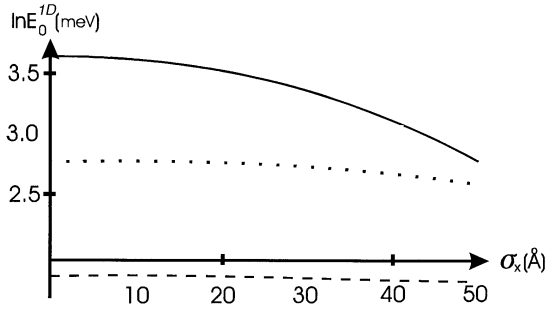

FIG. 3. Ground-state eigenenergies as function of σ_x for various values of d. We plot $\ln|E_0^{1D}|$ for $d=10$ Å (solid line), $d=30$ Å (dotted line), and $d=45$ Å (discontinuous line).

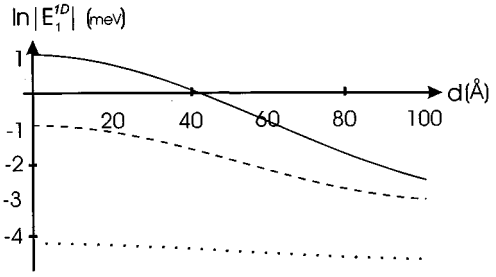

FIG. 4. Same as Fig. 2, but for the first excited state with only one panel.

In Figs. 2 and 3 we plot the absolute values of the ground-state for various parameters. For instance, for $\sigma_x=30$ Å, $\mu=0.05m_e$ (m_e is the electron mass), $\epsilon=12$, and $d=100$ Å (corresponding to the last point in Fig. 2), we find that $|E_0^{1D}|=0.73$ meV. This value is larger than the ones obtained for a three-dimensional exciton with the same reduced mass and dielectric screening constant, and smaller than the ones associated with the one-wire exciton for which $d=0$. These plots show how $|E_0^{1D}|$ would take their largest values for $d=0$ regardless of the values of σ_x. Notice also that $|E_0^{1D}|$ is more sensible than $|E_1^{1D}|$ for small values of d, since it changes by two orders of magnitude from its value at $d=100$ Å.

On the other hand, in Figs. 4 and 5 $|E_1^{1D}|$ is plotted as a function of σ_x and d. $|E_0^{1D}|$ and $|E_1^{1D}|$ tend to constant values as $\sigma_x\to 0$ by keeping d fixed. The dependence of the eigenenergies on d is stronger than the dependence on σ_x. For these eigenenergies increasing σ_x also increases the electrostatic interaction, since there is a larger front surface between the wires.

We plot the normalized probability density of the ground-states (Figs. 6 and 7) and first excited states (Figs. 8 and 9). $|\phi_0|^2$ only has a maximum in the origin, and decays exponentially far away from it, and is narrower for smaller values of d since the interaction is stronger and the charges tend to be as close as possible. On the other hand, $|\phi_1|^2$ has a node in the origin and two equal-distanced maxima around it. For instance, for $d=100$ Å those maxima are located at $\zeta_0=\pm 1.3$. These two maxima cause dipolar moments at an angle $\angle=\arctan\frac{1}{2}$, as measured relative to the wire direction, which could be observed when the exciton is on its first excited state. This angle is reduced for smaller values of d.

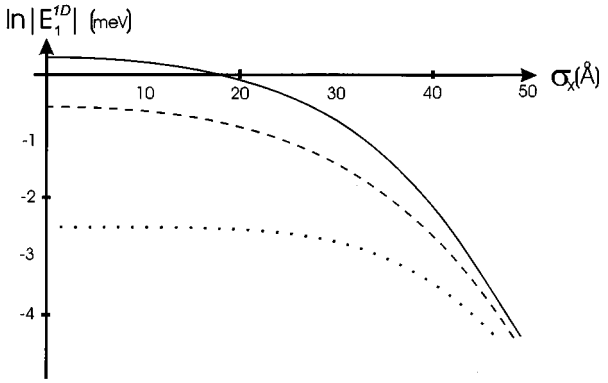

FIG. 5. Same as Fig. 3, but for the first excited state.

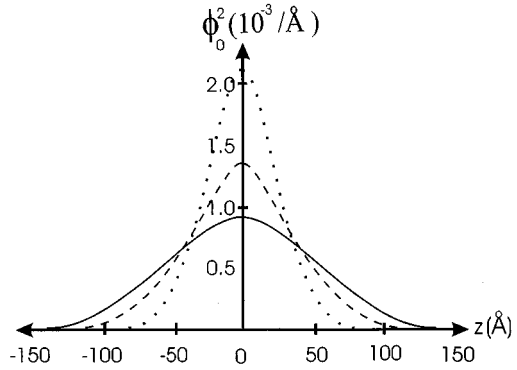

FIG. 6. Ground-state normalized density for different values of d and $\sigma_x = 30$ Å. We plot ϕ_0^2 for $d = 100$ Å (solid line), $d = 50$ Å (dotted line), and $d = 30$ Å (discontinuous line).

V. WKB APPROXIMATION

So far the eigenenergies and eigenfunctions were calculated for only ground and first excited exciton states, the purpose of this section is to study the higher-energy states of the exciton within the WKB approximation. In this way we intend to present a global view of the system within the limitations imposed by the WKB approximation. Clearly this overall view is useful from the experimental side in ideal systems (pure materials, low temperatures, etc.) for which many eigenstates could be able to manifest themselves.

We shall describe both eigenfunction ϕ_n and eigenvalues E_n^{1D} of Eq. (3.1) by using the well known WKB approximation.[12] For instance, the even ϕ_n, $(n = 0,2,4, \ldots)$ are given by

$$\phi_n = \begin{cases} C_n \dfrac{e^{-\left|\int_{\zeta}^{-\zeta_r} d\zeta' iS(\zeta')\right|}}{\sqrt{iS(\zeta)}}, & |\zeta| > \zeta_r \\ C_n \dfrac{\cos\left(\int_{-\zeta_r}^{\zeta} d\zeta' S(\zeta') - \pi/4\right)}{\sqrt{S(\zeta)}}, & |\zeta| < \zeta_r, \end{cases} \tag{5.1}$$

with a similar expression involving sine instead of cosine for the odd states ϕ_n $(n = 1,3 \ldots)$.[12] $\zeta_r = \sqrt{\gamma^2 - \zeta_0^2}$ yields the return point position, C_n is a normalization constant, and S is defined by

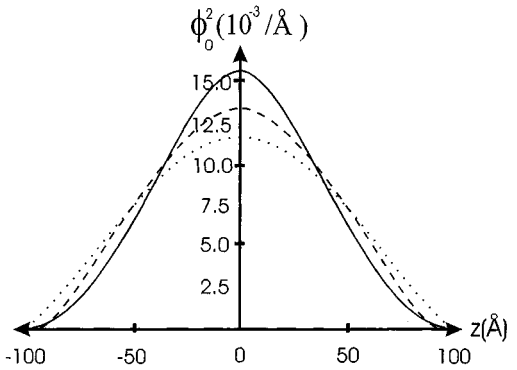

FIG. 7. Ground-state normalized density for different values of σ_x and $d = 100$ Å. We plot ϕ_0^2 for $\sigma_x = 10$ Å (solid line), $\sigma_x = 30$ Å (dotted line), and $\sigma_x = 45$ Å (discontinuous line).

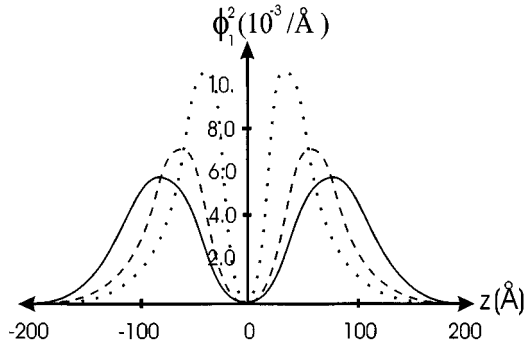

FIG. 8. Same as Fig. 6, but for the first excited state ϕ_1.

$$S(\zeta) = \sqrt{\frac{\gamma}{\sqrt{\zeta^2 + \zeta_0^2}}\left[1 + \frac{\beta}{(\zeta^2 + \zeta_0^2)^2}\right] - 1}. \tag{5.2}$$

E_n^{1D} are given by the quantization condition

$$2\zeta_0\left(\int_0^{\arccos(-\zeta_0/\gamma)} d\theta \frac{\sqrt{1 + (\gamma/\zeta_0)\cos\theta}}{\cos^2\theta} - 1.58\left(\frac{\sigma_x}{d}\right)^4 \int_0^{\arccos(-\zeta_0/\gamma)} \frac{d\theta \cos^3\theta}{\sqrt{1 + (\gamma/\zeta_0)\cos\theta}}\right) = \left(n + \frac{1}{2}\right)\pi, \tag{5.3}$$

where $\zeta = \zeta_0 \tan\theta$, and we have assumed that σ_x/d is a small number. Equation (5.3) can be written in terms of the first, second, and third class complete elliptic functions,[10] $K(\eta)$, $E(\eta)$, and $\Pi(\chi, \eta)$, respectively, in the following way:

$$2\sqrt{2\gamma\zeta_0}\left\{-\Pi\left(\frac{1}{2}, \frac{\gamma + \zeta_0}{2\gamma}\right) + \left[\frac{1}{2} + \frac{\zeta_0}{\gamma}\right]K\left(\frac{\gamma + \zeta_0}{2\gamma}\right) - E\left(\frac{\gamma + \zeta_0}{2\gamma}\right) - \frac{\zeta_0}{2\gamma}\right\} + i\pi\gamma - 4.2\zeta_0\left(\frac{\sigma_x}{d}\right)^4 = (n + \tfrac{1}{2})\pi. \tag{5.4}$$

Since the WKB approximation is valid for the higher energy levels, we restrict our analysis to large values of n. Now, since a physical acceptable eigenenergy $|E_n^{1D}|$ for an electrostatic system should decrease as n increases, then

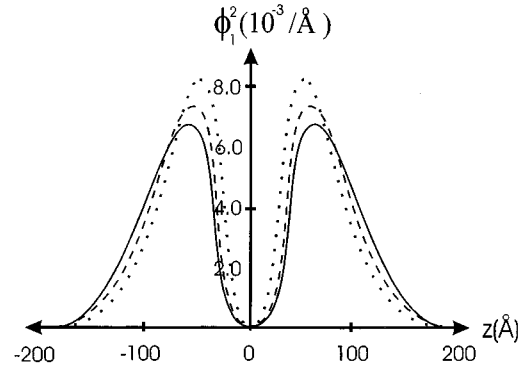

FIG. 9. Same as Fig. 7, but for the first excited state ϕ_1.

$\zeta_0/\gamma \propto |E_n^{1D}|$, and $\zeta_0(\sigma_x/d)^4 \propto \sqrt{|E_n^{1D}|}$ must be small numbers for large values of n. Therefore,

$$-\pi\sqrt{2\gamma\zeta_0}\alpha + i\pi\gamma - 4.2\zeta_0\left(\frac{\sigma_x}{d}\right)^4 = \left(n+\tfrac{1}{2}\right)\pi \quad (5.5)$$

where α is given by

$$\alpha = \frac{2}{\pi}[\Pi(\tfrac{1}{2},\tfrac{1}{2}) - \tfrac{1}{2}K(\tfrac{1}{2}) + E(\tfrac{1}{2})] = 4.3. \quad (5.6)$$

This means that E_n^{1D} can be written approximately as

$$E_n^{1D} \approx -\frac{(2e^2/\epsilon a_0')}{[\alpha\sqrt{d/a_0'}+n+\frac{1}{2}]^2}, \quad (5.7)$$

where $a_0' = \epsilon\hbar^2/\mu e^2$ is the 3D Bohr's radius of the exciton which, for typical semiconductors, is of the order of 300 times the atomic radius a_0. Even for $n=3$ the ratio ζ_0/γ is a small number, so Eq. (5.7) can be used for small n. To show that Eq. (5.7) reduces to Loundon's expression[8] for the eigenenergies when $d=0$, we recall that V_{eff} diverges at $\zeta=0$ in this limit. Thus, following the same reasoning as Loundon, any eigenfunction of Eq. (3.1) must vanish at $\zeta=0$ so that just the odd functions ϕ_n with $n=2j-1$ $(j=1,2,\ldots)$ have to be considered and then Eq. (5.7) turns out to be $E_j^{1D} \approx -e^2/2\epsilon a_0' j^2$ for odd states, which is the expression derived by Loundon for $d=0$.

On the other hand, if we consider $d \gg a_0$ the eigenenergy spectrum can be approximated as a set of equally separated levels (or harmoniclike spectrum) plus a constant term. This constant term represents the electric stored energy of the charge distributions.

Equation (5.7) shows, in contrast to the lower eigenenergy levels, that the width of the quantum wells (QWs), σ_x, do not affect the higher eigenenergy levels to this first approximation order. However, it is possible to perform another iteration which involves σ_x by substituting of Eq. (5.7) into the last term of the left-hand side of Eq. (5.4) to obtain

$$E_n^{1D} \approx -\frac{(2e^2/\epsilon a_0')}{[\alpha\sqrt{d/a_0'}+n+\frac{1}{2}]^2} + \frac{16.8(\sigma_x/d)^4(e^2/\epsilon a_0')^{3/2}}{[\alpha\sqrt{d/a_0'}+n+\frac{1}{2}]^3}, \quad (5.8)$$

which gives a better description for real systems than Eq. (5.7).

For completeness, let us briefly discuss the main features of the corresponding eigenfunctions by analyzing the behavior of the probability densities $|\phi|_n^2$. As can be seen from Eq. (5.1), for the interval which ranges from one return point $-\zeta_r$ to the other return point ζ_r, this consists of an oscillatory square cosine or sine functions, whose number of oscillation in this interval is determined by the principal quantum number n. These trigonometric function are modulated by the envelope $1/\sqrt{S}$ which, as usually found in the WKB approximation, diverges as $1/\sqrt{\zeta}$ at the return points. Finally the behavior beyond a return point is, as shown in Eq. (5.1), decaying one as $\exp[-2\zeta]$, which implies that the major probability density is concentrated between the origin and the return point.

VI. SUMMARY AND CONCLUSIONS

In summary, for a particle p_1 in a quantum wire and another particle p_2 in another parallel quantum wire, we have found multipole analytic expression for the effective 1D p_1-p_2 interaction. We hope that this expansion can be useful to study other similar problems in semiconductor heterostructures. Here in particular we used this expression for the electron-hole interaction. The conditions we assumed were, first, a transverse rectangular cross section with harmonic potential confinements for both transverse directions, and second, that both particles are in the transverse joint ground state. Therefore, our multipole expansion was performed in powers of the separation of the wires d and in power of the four standard deviations or moment intervals $\sigma_{x1}, \sigma_{x2}, \sigma_{y1}$, and σ_{y2} which are of the order of the dimensions of the wires when the particles are in the transverse ground-states. It is important to mention that our model can be applied to any type of transverse confinement potentials whose moment integral are known.

In order to obtain a relatively simple 1D Schrödinger equation for the Wannier-Mott exciton valid for small d and σ_x (assuming $\sigma=\sigma_{x1}=\sigma_{x2}$), we approximated the particle-particle (or electron-hole) potential by keeping just the dominant and the first correcting terms of the multipolar potential expansion. Since we could not use the usual perturbation theory to solve the corresponding Schrödinger equation, we had to resort to a Frobenius series method to find analytical expressions for the lowest eigenenergies and eigenfunctions, which, to the order of approximation we employed, obey the following behavior: (i) surprisingly, they do not depend on σ_y; (ii) they depend to first order on d and σ_x; and (iii) the dependence on d is stronger than on σ. These three features can be explained in terms of how the electrostatic energy of the charge distributions varies as function of the parameters of the system, as illustrated in our plots of the eigenenergies and eigenfunctions using typical values of semiconductor quantum wires. We also calculated higher eigenenergies and eigenfunctions by using the WKB approach yields and an overall view of the solution of the 2QW system. We hope that this work on the calculation of exciton states can stimulate further experimental and theoretical work on the study of heterostructure systems that exhibit spatial separation between the electron and the hole.

ACKNOWLEDGMENTS

We acknowledge useful discussions with R. A. Vázquez-Nava, and partial support by DGAPA-UNAM and CONACYT-México through Grant Nos. IN-107796 and 3042PE, respectively.

*On leave from Instituto de Física, UNAM, México, D.F., México. Author to whom correspondence should be addressed.

[1] W. Hansen, *in Quantum Coherence in Mesoscopic Systems*, Vol. 254 of *NATO Advanced Study Institute, Series B: Physics*, edited by B. Kramer (Plenum, New York, 1991), p. 23.

[2] G. Bastard, J. A. Brum, and R. Ferreira, in *Solid State Physics*,

Advances in Research and Applications, edited by H. Ehrenreich and D. Turnbull (Academic, New York, 1991), Vol. 44, p. 229.
[3] R. Beresford, L. F. Luo, K. F. Lonngenbach, and W. I. Wang, Appl. Phys. Lett. **56**, 953 (1990).
[4] G. Bastard, E. E. Mendez, L. L. Chang, and L. Esaki, Phys. Rev. B **26**, 1974 (1982).
[5] D. M. Kachintev and S. Ulloa, Phys. Rev. B **50**, 8715 (1994).
[6] Y. E. Lozovik and V. N. Nishanov, Fix. Tverd Tela (Leningrad) **18** 3267 (1976) [Sov. Phys. Solid State **18**, 1905 (1976)].
[7] L. Banyai, I. Galbraith, C. Ell, and H. Haug, Phys. Rev. B **36**, 6099 (1987).
[8] R. Loundon, Am. J. Phys. **27**, 649 (1959).
[9] G. Arfken, *Mathematical Methods for Physicists* (Addison-Wesley, Reading, MA, 1976), Sec. 12.1.
[10] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1965), Sec. 15.3.
[11] M. C. Bender and M. C. Arszog, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978), Sec. 8.5.
[12] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1977), Chap. 7.