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Modeling of Coulomb interaction in parabolic quantum wires

C. González-Santander *, F. Domínguez-Adame

GISC, Departamento de Física de Materiales, Universidad Complutense, E-28040 Madrid, Spain

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ABSTRACT

We study the exciton states in a parabolic quantum wire. An exactly solvable model is introduced for calculating the exciton state and the binding energy as a function of the radius of the quantum wire within the envelope-function approximation. In the calculation, we replace the actual Coulomb interaction between the electron and the hole by a Gaussian nonlocal separable potential and obtain closed expressions for both the envelope-function and the binding energy. Results are compared with those obtained by perturbative methods.

1. Introduction

Advances in nanometer-size semiconductor techniques have made possible to fabricate low-dimensional devices, like quantum wells and quantum wires (QWs), with high crystalline quality. Due to the high crystal quality, interface roughness is often negligible and electrons and holes are free to move along the wire direction. Therefore, Coulomb interaction between them plays a crucial role for an electron and a hole to stay close to each other to form a Wannier exciton [1–4]. The interplay of Coulomb interaction and the lateral confinement has attracted much attention due to remarkable properties of the exciton transitions in QWs. In particular, it has been found an enhancement of the optical gain and low threshold current in QW lasers having exciton transitions as compared to those having free-carrier transitions [5,6].

There are several theoretical works on the calculation of the binding energy of electrons and holes due to Coulomb interaction in QWs [1–6]. The binding energy is usually computed within the framework of the envelope-function approximation [7–9]. This approach holds when the diameter of the QW is much larger than the spacing of the crystal lattice, which is not a serious restriction in QWs available nowadays. Neglecting the coupling to far bands and many body effects, the exciton envelope-function in wide gap semiconductors obeys a Schrödinger equation. Since no analytical solutions are available in many geometries of interest, the exciton envelope-function and the binding energy are often obtained by means of variational or numerical techniques.

The nonlocal separable potential (NLP) method [10–12] presents an alternative way to obtain accurate solutions of the Schrödinger equation when exact solutions are not available. To this end, the actual potential is replaced by a projection operator, leading to an exactly solvable equation and the energy of the states can be obtained in a closed form with little computational effort. More important, it is always possible to find a NLP (or a sum of them) which reproduces exactly the states in the original local potential [12]. Consequently, there is no theoretical limitation to the numerical accuracy with which physical results can be obtained. The NLP method has already been successfully used to determine the binding energy of confined excitons in two-dimensional quantum dots in a closed form [13] by replacing the actual Coulomb potential between the electron and the hole by a Yamaguchi's NLP [14], which is nothing but the Coulomb local potential times the ground state wave function for this local potential [15].

In this work we consider a single exciton in a parabolic QW and study the corresponding states within the envelope-function approach, replacing the Coulomb potential between the electron and the hole by a suitable NLP. The problem has some resemblances to the above-mentioned confined excitons in two-dimensional quantum dots [13]. However, the solution to the problem of an exciton in a QW is more complex because the mixing of perpendicular and parallel degrees of freedom and

* Corresponding author.
E-mail address: cglezsantander@fis.ucm.es (C. González-Santander).

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the resulting potential for the relative motion of the electron and the hole cannot be separated. The same shortcoming appears after replacing the Coulomb potential by the Yamaguchi's NLP [14]. These difficulties can be overcome by introducing a Gaussian NLP [16], as shown below.

2. Model Hamiltonian

Consider an electron bound to a hole within the effective-mass approximation. The exciton is embedded in a parabolic QW along the Z axis and relative dielectric constant ε made of a wide-gap semiconductor which, for simplicity, will be considered of infinite length. Within these approximations, the two-particle Hamiltonian can be written as

$$\mathscr{H} = \sum_{i=e,h}\left[\frac{p_i^2}{2m_i} + V_i(x_i, y_i)\right] - \frac{e^2}{\varepsilon|\boldsymbol{r}_e - \boldsymbol{r}_h|}, \tag{1}$$

where the sum index i refers to the electron (e) and the hole (h) with effective masses m_e and m_h, respectively. The lateral confinement potential is written as $V_i(x_i, y_i) = (1/2)m_i\omega^2(x_i^2 + y_i^2)$, where ω determines the lateral size of the QW.

For the parabolic potential it is convenient to separate the problem into center of mass and relative coordinates, described by $\boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_h$ and $\boldsymbol{R} = (m_e\boldsymbol{r}_e + m_h\boldsymbol{r}_h)/M$, where the total and reduced masses are $M = m_e + m_h$ and $m = m_e m_h/M$, respectively. The total Hamiltonian (1) can be expressed as $\mathscr{H} = \mathscr{H}_{CM} + \mathscr{H}_r$ with

$$\mathscr{H}_{CM} = \frac{P^2}{2M} + \frac{1}{2}M\omega^2(X^2 + Y^2), \tag{2a}$$

$$\mathscr{H}_r = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\rho^2 - \frac{e^2}{\varepsilon r} \equiv \mathscr{H}_0 - \frac{e^2}{\varepsilon r}, \tag{2b}$$

where $\boldsymbol{\rho} = (x, y)$, and $\boldsymbol{P}$ and $\boldsymbol{p}$ are the conjugate momenta of the coordinates $\boldsymbol{R}$ and $\boldsymbol{r}$. The center of mass problem (2a) is exactly solvable since $\mathscr{H}_{CM}$ correspond to a two-dimensional harmonic oscillator plus the kinetic energy of the free motion along the QW. A similar statement holds for $\mathscr{H}_0$ in Eq. (2b). However, the Coulomb term in Eq. (2b) mixes the parallel and perpendicular degrees of freedom, and the resulting Schrödinger equation cannot be exactly solved. The rest of this paper is devoted to find an accurate solution of the Schrödinger equation obtained from Eq. (2b).

We have previously shown that Coulomb forces in quantum dots [13] and molecular systems [15] can be accurately substituted by a suitable NLP. Consequently, the Schröndinger equation to obtain the envelope-function $|\chi\rangle$ from Eq. (2b) is replaced by

$$(\mathscr{H}_0 + V_{\mathrm{NL}})|\chi\rangle = E|\chi\rangle, \tag{3a}$$

where the NLP is defined by

$$V_{\mathrm{NL}} \equiv -\frac{\lambda\hbar^2}{2m}|\nu\rangle\langle\nu|. \tag{3b}$$

Here λ is the coupling constant and ν will be referred to as *shape function* hereafter. To proceed, we consider the resolvent of the Hamiltonian $\mathscr{H}_0$ as follows:

$$|\chi\rangle = -(\mathscr{H}_0 - E)^{-1}V_{\mathrm{NL}}|\chi\rangle = \frac{\lambda\hbar^2}{2m}\sum_\mu \frac{|\mu\rangle\langle\mu|}{E_\mu - E}|\nu\rangle\langle\nu|\chi\rangle, \tag{4}$$

where $|\mu\rangle$ labels the eigenstates of $\mathscr{H}_0$, E_μ being the corresponding eigenvalues. Projecting onto the ket $|\nu\rangle$ and assuming that $\langle\nu|\chi\rangle \neq 0$ we arrive at the following transcendental equation for the exciton energy:

$$\frac{\lambda\hbar^2}{2m}\sum_\mu \frac{|\langle\mu|\nu\rangle|^2}{E_\mu - E} = 1. \tag{5}$$

This equation is valid for any *arbitrary* shape function ν and coupling constant λ. Usually naive shape functions provide accurate results [15–17].

3. Free excitons

The coupling constant λ is not an adjustable parameter of the model. This can be understood from the fact that we might obtain the energy level $E_0 = -\mathrm{Ry}^*$ of the free exciton from Eq. (5) when the confining potential is switched off ($\omega \to 0$). Here Ry^* is the exciton effective Rydberg in three dimensions. The calculation of the coupling constant λ is easily achieved in momentum space when $\omega = 0$. The Hamiltonian of the relative particle reads in this case $\mathscr{H}_r = \boldsymbol{k}^2\hbar^2/2m + V_{\mathrm{NL}}$ and therefore $\mathscr{H}_0 = \boldsymbol{k}^2\hbar^2/2m$. The eigenstates of $\mathscr{H}_0$ are plane waves $\langle\boldsymbol{r}|\boldsymbol{k}\rangle = (2\pi)^{-3/2}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})$ with energy $E_{\boldsymbol{k}} = \hbar^2k^2/2m$. Thus, the energy spectrum is continuous and the summation appearing in Eq. (5) is replaced by integration in the momentum space. Defining $k_0^2 = 2m|E_0|/\hbar^2$, we get

$$\frac{1}{\lambda} = \int d^3\boldsymbol{k}\frac{|\langle\boldsymbol{k}|\nu\rangle|^2}{k^2 + k_0^2}. \tag{6}$$

It becomes apparent that the coupling constant can be calculated from the Fourier transform of the shape function $\langle\boldsymbol{k}|\nu\rangle$. Hereafter, we will consider the following Gaussian shape function $\nu(r) = (1/\sqrt{\pi}a)^3\exp(-r^2/a^2)$ [16]. Taking into account that $\langle\boldsymbol{k}|\nu\rangle = \exp(-k^2a^2/4)$ and performing the integration in Eq. (6) we arrive at

$$\lambda = 2\pi^2 a\left[\sqrt{\frac{\pi}{2}} - \frac{\pi}{2}\sqrt{\alpha}\,e^{\alpha/2}\mathrm{erfc}(\sqrt{\alpha/2})\right]^{-1}, \tag{7}$$

where $\mathrm{erfc}(z)$ is the complementary error function [18]. For brevity we have defined $\alpha = (a/a^*)^2$, where a^* is the effective Bohr radius of the exciton in three dimensions.

4. Excitons in a quantum wire

After having discussed the main features of the NLP, we now turn to its application to excitons in QWs ($\omega \neq 0$). In this case the normalized eigenfunctions of $\mathscr{H}_0$ in Eq. (2b) can be factorized in cylindrical coordinates as follows:

$$\varphi_{n\ell k_z}(\boldsymbol{r}) = R_{n\ell}(\rho)\frac{e^{i\ell\theta}}{\sqrt{2\pi}}\frac{e^{ik_z z}}{\sqrt{2\pi}}, \tag{8a}$$

with quantum numbers $\ell = 0, \pm1, \pm2, \ldots, n = 0, 1, 2, \ldots$ and k_z. The axial function corresponding to a two-dimensional harmonic oscillator is given by (see e.g. Ref. [19])

$$R_{n\ell}(\rho) = \sqrt{\frac{2n!}{(n + |\ell|)!}}\frac{\rho^{|\ell|}}{\mathscr{L}^{|\ell|+1}}\,e^{-\rho^2/2\mathscr{L}^2}L_n^{|\ell|}(\rho^2/\mathscr{L}^2), \tag{8b}$$

where $\mathscr{L} = \sqrt{\hbar/m\omega}$ is the QW radius for the exciton and $L_n^{|\ell|}$ denotes the generalized Laguerre polynomial [18]. The corresponding eigenenergies of the two-dimensional oscillator are $E_{n\ell} = \hbar\omega(2n + |\ell| + 1)$. Consequently, the total energy of eigenstate (8) is $E_{n\ell k_z} = E_{n\ell} + k_z^2\hbar^2/2m$.

To proceed we calculate $\langle\varphi_{n\ell k_z}|\nu\rangle$ and use Eq. (5), where the sum runs over the three quantum numbers n, ℓ and k_z. Due to axial symmetry of the shape function, $\langle\varphi_{n\ell k_z}|\nu\rangle$ is nonvanishing

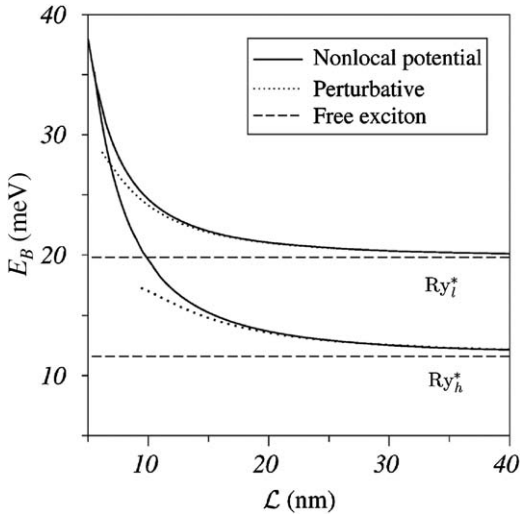

Fig. 1. Binding energy as a function of the QW width for light- and heavy-hole excitons (upper and lower solid lines, respectively). The binding energy of free excitons ($E_B = \mathrm{Ry}^*$) is indicated by dashed lines. Perturbative results are plotted as dotted lines for comparison.

only if $\ell = 0$. From Eq. (8) we get

$$\langle \varphi_{n\ell k_z} | \nu \rangle = \frac{2\mathscr{L}\gamma^2}{\sqrt{2}\pi a^2(1+\gamma^2)} \left(\frac{1-\gamma^2}{1+\gamma^2}\right)^n \exp\left(-\frac{k_z^2 a^2}{4}\right) \delta_{\ell 0}, \tag{9}$$

where $\gamma \equiv a/\sqrt{2}\mathscr{L}$.

After some lengthy but straightforward algebra, inserting Eq. (9) in Eq. (5) gives the following transcendental equation for the exciton energy:

$$1 = \frac{\lambda\gamma}{2\pi a(1+\gamma^2)^2} \sum_{n=0}^{\infty} \frac{1}{\xi_n} \left(\frac{1-\gamma^2}{1+\gamma^2}\right)^{2n} \mathrm{erfc}(\sqrt{2}\gamma\xi_n) \exp(2\gamma^2\xi_n^2), \tag{10}$$

where the coupling constant λ is given by (7). For brevity we have defined $\xi_n \equiv \sqrt{2n+1-E/\hbar\omega}$.

As an illustrative example of the NLP approach, we consider light- and heavy-hole excitons in a QW of width $\mathscr{L}$ based on $In_{0.06}Ga_{0.94}N$. The effective masses of electrons, light-holes and heavy-holes are $0.19m_0$, $0.17m_0$ and $0.78m_0$, respectively, in units of the free electron mass m_0. The relative dielectric constant is $\varepsilon = 10.24$. Consequently, the effective Bohr radii for light- and heavy-hole excitons are $a_l^* = 6.04\,\mathrm{nm}$ and $a_h^* = 3.54\,\mathrm{nm}$. The effective Rydberg is $\mathrm{Ry}_l^* = 11.6\,\mathrm{meV}$ and $\mathrm{Ry}_h^* = 19.8$ for light- and heavy-hole excitons, respectively. We then obtain the energy level E of the exciton inside the QW by solving Eq. (10) as a function of the QW width $\mathscr{L}$. In the absence of Coulomb interaction, the energy of the ground state of the electron and the hole is that of two independent harmonic oscillators in two dimensions, namely $2\hbar\omega$. When the Coulomb interaction is taken into account, the energy of the ground state is $\hbar\omega + E$, the first term arising from the center of mass motion [see Eq. (2a)]. The binding energy E_B is defined as the energy difference between the ground state energy of these two situations and therefore $E_B = \hbar\omega - E$. Fig. 1 shows the binding energy as a function of the QW width. We have taken $\alpha = (a/a^*)^2 = 0.01$ in Eq. (7) to perform the calculation, although we have checked that the results remain almost unchanged when $\alpha = 0.005$. The binding energy approaches the effective Rydberg ($E_B \to \mathrm{Ry}^*$) in wide QWs ($\mathscr{L} \gg a^*$), as expected. By decreasing the QW radius the binding energy increases due to confinement effects. This behavior can be understood as follows. Both $\hbar\omega$ and E, obtained after solving Eq. (10), increases upon reducing the QW radius because the wave function is pushed toward the center of the QW. However, the shift of the energy E of the relative particle is smaller since the corresponding wave function is already more localized around the center of the QW due to the presence of the Coulomb term in Eq. (2b). As a consequence, the difference $\hbar\omega - E = E_B$ increases, as observed in Fig. 1.

For comparison, we have also performed a first-order perturbative calculation, assuming that the confining potential is weaker than the Coulomb interaction. This approach holds when $a^* \ll \mathscr{L}$, namely in the weak confinement regime. The unperturbed envelope-function is written as $\chi^0(r) = (1/\sqrt{\pi a^{*3}}) \exp(-r/a^*)$ and the energy shift due to the parabolic confining potential is $\Delta E \equiv \langle \chi^0 | (1/2) m\omega^2 \rho^2 | \chi^0 \rangle = m\omega^2 a^{*2}$. Perturbative results are compared to those obtained by the NLP approach in Fig. 1. Remarkably, the perturbative calculation provides a reasonable value of the binding energy in the range $\mathscr{L} \gtrsim 3a^*$.

5. Conclusions

In this paper we have considered exciton states in parabolic QWs made of wide gap semiconductor within the framework of the effective-mass approximation. We introduced a solvable model that allows us to obtain the binding energy in a closed form with little computational effort. Our procedure is based on the NLP approach, in which the Coulomb potential between the electron and the hole is replaced by a nonlocal separable potential. It is important to realize that this technique can be made exact, and so there are no theoretical limitations on this approach. In addition, the solution can be found for any arbitrary NLP, as we actually demonstrated [see Eqs. (5) and (6)]. As our selection for a suitable NLP that allows for a closed solution, we have used a Gaussian shape function [10]. Once the solution is obtained, we have compared our predictions to the results obtained by a perturbative approach, and found that the latter gives a reasonable value of the binding energy in the range $\mathscr{L} \gtrsim 3a^*$.

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