Variational anisotropic model of Wannier excitons compared with fractional-dimensional space approach

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Binding energy of Wannier excitons in a quantum well of thickness L is studied using two models: a two-parameter trial wave function and a fractional-dimensional space with dimension $2 \leqslant \alpha \leqslant 3$. Since both models provide quantitative measures of the exciton spatial anisotropy as L changes, we give physical arguments for a plausible definition of $\alpha = \alpha(L)$.

Keywords: Electron states and collective excitations in multilayers; quantum wells; mesoscopic and nanoscale systems.

Se estudia la energía de amarre de excitones de Wannier en un pozo cuántico de ancho L utilizando dos modelos: una función de onda de prueba con dos parámetros y un espacio de dimensión fraccional con dimensión $2 \leqslant \alpha \leqslant 3$. Ya que ambos modelos proporcionan medidas cuantitativas de la anisotropía espacial del excitón al cambiar L, damos argumentos físicos para una plausible definición de $\alpha = \alpha(L)$.

Descriptores: Estados electrónicos y excitaciones colectivas en multicapas; pozos cuánticos; sistemas mesoscópicos y de escala nanoscópica.

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1. 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. On the other hand excitons are important excitations [1] that strongly affect the electronic and optical properties of low-dimensional solids [2].

The purpose of this paper is two-fold; in the first place we present a variational model calculation for large excitons (Wannier-Mott excitons) in a semiconducting quantum well structure as a function of the width of the quantum well to exhibit their behavior between two and three dimensions (2D and 3D). Secondly, we compare the variational exciton binding energy with the energy of an exciton in a space of alfa dimensions (αD) where α is a real number between 2 and 3. In general, a fractional-dimensional space is an interesting mathematical concept where the dimension is determined by the degree of anisotropy. In other words the anisotropic interaction in a 3D space becomes isotropic in a lower fractional-dimensional space.

A mathematical basis for spaces with "non integer dimension" was developed by Stillinger [3] with five axioms; four of them topological and the fifth of them specifies an integration measure. In this formalism the dimension α is not restricted to the positive integers but α is a real positive number and the α-dimensional space behaves like a conventional Euclidean vector space. The article of Stillinger is interesting from the mathematical point of view but it is probably more indicated for mathematicians than for physicists since it deals with concepts such as metric space, integration measure, density of mutually perpendicular lines, etc. Also we should mention a paper by Wilson [4], which offers a similar axiomatic description of spaces with non integer dimensions. There exists interesting work on isotropic interactions in solids making use of fractional dimensionality [5–7]. In particular, we will employ here some of the results of a paper by He [7] where a simple hydrogenic Schrödinger equation is solved in the fractional dimensional space yielding exciton wave functions, bound energies and associated optical spectra as a function of spatial dimensionality.

The structure of this paper is the following; in Sec. 2 we present a variational approach of an isotropic exciton in a quantum well. In Sec. 3 we present results of fractional-dimensional spaces for excitons and Sec. 4 is devoted to comparison of results of Secs. 2 and 3 and discussion.

2. Trial wavefunction for excitons between 2D and 3D.

The two-particle Hamiltonian in a quantum well can be written as

$$\widehat{H}\Psi(x_1,y_1,z_1,x_2,y_2,z_2)=E_t\Psi(x_1,y_1,z_1,x_2,y_2,z_2)\,, \quad (1)$$

where E_t is the total energy of the system and we use the labels 1 and 2 for particles p_1 and p_2 (electron and hole). $\widehat{H}$ is defined as

$$\widehat{H} = \widehat{H}_1 + \widehat{H}_2 + \widehat{V}_{int}, \quad (2)$$

and the Hamiltonian of each particle is

$$\widehat{H}_\nu = \frac{-\hbar^2}{2m_\nu}\nabla_\nu^2 + V_\nu\left(z_\nu\right), \quad (3)$$

with ν =1, 2, m_ν are the effective masses, $V_\nu(z_\nu)$ is the transverse confinement potential of each carrier and the Coulomb interaction potential is

$$\widehat{V}_{int}(\overrightarrow{r_1}-\overrightarrow{r_2})=\frac{q_1q_2}{\epsilon\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}}, \quad (4)$$

where ϵ is the appropriate dielectric screening of the semiconductor media.

We assume that the electron and the hole are confined by an infinite square well potential of thickness L

$$V_\nu(z_\nu)=\begin{cases} 0 & |z_\nu|<L/2 \\ \infty & |z_\nu|>L/2 \end{cases},$$

and propose in cylindrical coordinates a binding variational calculation of an exciton through the use of a two-parameter trial wave function [8]

$$\Psi = N\cos(\pi z_1/L)\cos(\pi z_2/L) \times \exp\left\{-\left[\beta^2\rho^2+\gamma^2(z_1-z_2)^2\right]^{1/2}\right\}. \quad (5)$$

where ρ and z_1-z_2 describe the relative motion of the electron-hole pair in the exciton, N is the normalization constant and γ and β are parameters chosen in such a way that they minimize the exciton binding energy. Notice that the argument of the exponential in Eq. (5) describes in general an anisotropic wavefunction. The system assumes that in the confinement z-direction both charged particles p_1 and p_2 (electron and hole) are in their respective groundstate and they are free to move perpendicularly to the z-direction interacting through a screened Coulomb potential

$$\hat{V}_{\text{int}} = -e^2/\epsilon\,|\vec{r}_1-\vec{r}_2|\,.$$

A similar calculation of the exciton binding energy was performed by Bastard, *et al*. [9] with two types of trial function. One of them describes a 2D exciton since the main dependence is on the 2D relative coordinate ρ and corresponds to our Eq. (5) with $\gamma=0$. By a 2D system we mean an exciton which is the solution of a bidimensional Schrödinger equation with a coulombic interaction term proportional to ρ^{-1} in polar coordinates. The second one describes 3D exciton since the dependence is on the 3D relative coordinate

$$\left[\rho^2+(z_1-z_2)^2\right]^{1/2}$$

corresponds to our Eq. (5) with $\gamma=\beta$. Although the real Coulomb potential proportional to $\left[\rho^2+z^2\right]^{1/2}$ can not be exactly separated in ρ and z coordinates, the 2D approach is a good approximation when the confinement in the z-direction is very strong and the wave functions in that direction are in their groundstate (very narrow 2D quantum layers) [10].

The exciton binding energy is obtained by minimizing with respect to γ and β the following expression:

$$F(\gamma,\beta)-E_g=-\frac{\hbar^2\beta^2}{4\mu}+\frac{2^{1/2}e^2\beta^3}{\kappa\gamma^2G_1(\gamma)}\int_0^\infty\frac{dq}{(q^2+2\beta^2)^{3/2}}\left[qG_0(s)+\frac{\gamma}{\beta}\left(q^2+2\beta^2\right)^{1/2}sG_1(s)\right], \quad (6)$$

where F is an energy measured from the top of the valence band. E_g is the band gap, $s=q+\frac{\gamma}{\beta}\left(q^2+2\beta^2\right)^{1/2}$,

$$G_0(s)=\frac{\pi}{s^2+\left(\frac{2\pi}{L}\right)^2}\left\{\frac{4\pi^2}{Ls^2}+\frac{3L}{2}-\frac{32\pi^4}{L^4s^3}\frac{\exp(-\frac{sL}{2})\sinh(\frac{sL}{2})}{s^2+\left(\frac{2\pi}{L}\right)^2}\right\},$$

$$G_1(s)=\frac{2\pi}{s\left(s^2+\left(\frac{2\pi}{L}\right)^2\right)^3}\left\{\frac{14\pi^2s^2}{L}+\frac{3s^4L}{2}+\frac{48\pi^4}{L^3}+\frac{64\pi^6}{L^5s^2}-\frac{56\pi^4}{L^4s}-\frac{96\pi^6}{L^6s^3}\right\} + \frac{2\pi}{s\left(s^2+\left(\frac{2\pi}{L}\right)^2\right)^3}\left\{\frac{56\pi^4}{L^4s}+\frac{96\pi^6}{L^6s^3}+\frac{8\pi^4}{L^3}+\frac{32\pi^6}{L^5s^2}\right\}\exp(-sL),$$

and it is found that $N^{-2}=\gamma^2/\beta^2G_1(\gamma)$. According to quantum variation method, with these expressions we proceed to find the values of γ_0 and β_0 that minimize the energy for different values of L to obtain the exciton binding energy $E_B\equiv|F(\gamma_0,\beta_0)-E_g|$ (which is defined as a positive quantity). In the Fig. 1 one of the curves (solid line) shows the exciton binding energy as a function of L. This figure shows that binding energies decreases as L increases, which is consistent with the values of the effective exciton Bohr radius $a_{1,2}=a_e/4$ for 2D and $a_{1,3}=a_e$ for 3D meaning a more spread groundstate wave function with increasing L.

3. Excitons in fractional-dimensional spaces.

In a space of α dimension (αD) the Laplace operator proposed by Stillinger [3] is

$$\nabla^2=-\frac{1}{r^{\alpha-1}}\frac{\partial}{\partial r}\left(r^{\alpha-1}\frac{\partial}{\partial r}\right)-\frac{l^2}{\hbar^2r^2},$$

where

$$\widehat{l}^2=-\frac{\hbar^2}{\sin^{\alpha-2}\theta}\frac{\partial}{\partial\theta}\left(\sin^{\alpha-2}\theta\frac{\partial}{\partial\theta}\right) \quad (7)$$

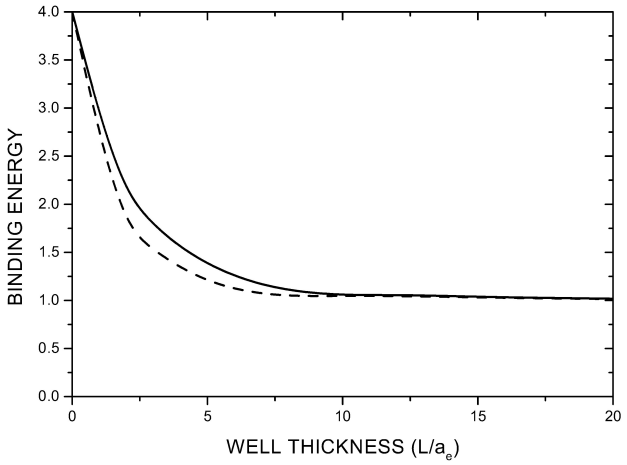

FIGURE 1. Normalized exciton binding energies vs normalized quantum well thickness L/a_e. Solid line indicates the variational energy E_B/E_e and dash line indicates the fractional-dimensional result $|E_{1,\alpha} - E_g|$.

corresponds to an angular momentum, $0 \leqslant r \leqslant \infty$ and $0 \leqslant \theta \leqslant \pi$ are the radial distance and the related angle measured relative to an axis passing through the origin. This laplacian is to be applied to any function $f(r,\theta)$ in an αD space where the integration measure can be calculated using the following formula:

$$\int_{\alpha D} d\mathbf{r} = \frac{2\pi^{(\alpha-1)/2}}{\Gamma\left(\frac{\alpha-1}{2}\right)} \int_0^{\infty} dr r^{\alpha-1} \int_0^{\pi} d\theta \sin^{\alpha-2}\theta,$$

where $\Gamma(x)$ is the gamma function [11] and $d\mathbf{r}$ represents the volume element in the αD space.

Therefore the Wannier-Mott exciton time-independent Schrödinger equation in an αD space can be expressed as follows:

$$\left[-\frac{\hbar^2}{2\mu r^{\alpha-1}}\frac{\partial}{\partial r}\left(r^{\alpha-1}\frac{\partial}{\partial r}\right) + \frac{\hat{l}^2}{2\mu r^2} - \frac{e^2}{\epsilon r}\right]\psi(r,\theta) = (E - E_g)\,\psi(r,\theta), \quad (8)$$

where $\hat{l}^2$ is given by Eq. (7), α is the dimension of a solid (here $1 < \alpha < 3$), radial distance r and related angle θ are two coordinates describing the relative distance vector $\mathbf{r}$ in the αD space, ϵ is the dielectric constant of the background, E is the exciton energy measure from the top of the valence band, and μ is the reduced mass.

Equation (8) can be separated as $\psi(r,\theta) = R(r)\,\Theta(\theta)$, to yield

$$R''(r) + \frac{\alpha-1}{r}R'(r) + \left[\frac{2\mu}{\hbar^2}\left((E - E_g) + \frac{e^2}{\epsilon r}\right) - \frac{l(l+\alpha-2)}{r^2}\right]R(r) = 0,$$

$$\Theta''(\theta) + [(\alpha-2)\,ctg\theta]\,\Theta'(\theta) + l(l+\alpha-2)\,\Theta(\theta) = 0,$$

where l is the angular-momentum quantum number which satisfies the same rule as in a 3D system, namely $l = 0, 1, 2, ..., n-1$.

The expressions (7) for all the resulting bound-state radial and angular wave functions in an αD space and the corresponding discrete bound-state energies are

$$E_{n,\alpha} = E_g - \frac{E_e}{\left(n + \frac{\alpha-3}{2}\right)^2}, \quad (9)$$

where n indicates the principal quantum number (starting with $n = 1$) and α the dimension. $E_e = \left(\mu/\epsilon^2 m_e\right) E_H$ is the effective Rydberg constant, $a_e = (m_e\epsilon/\mu)\,a_H$ is the effective exciton Bohr radius, where E_H and a_H are, respectively, the atomic Rydberg energy and atomic Bohr radius, and m_e is the free electron mass. It should be noted that the bound-state energy only depends on the principal quantum number and that the orbital energy degeneracy is the same for $1 \leqslant \alpha \leqslant 3$ [7]. Here we write only the groundstate wave functions [7]:

$$R_{1,0,\alpha}(r) = \left(\frac{2^{2\alpha}}{(\alpha-1)^{\alpha}\,\Gamma(\alpha)\,a_e^{\alpha}}\right)^{1/2} \exp\left[-\frac{2}{\alpha-1}\left(\frac{r}{a_e}\right)\right], \quad (10)$$

$$\Theta_{0,\alpha}(\theta) = \Gamma\left(\frac{\alpha}{2}\right)\left(\frac{2^{\alpha-2}(\alpha-1)}{\pi\Gamma(\alpha)}\right)^{1/2} \quad (11)$$

where the first subindex in R indicates the principal quantum number and the second subindex in R and the first subindex in Θ indicates l.

From Eq. (9) $E_{1,3} - E_g = -E_e$, $E_{1,2} - E_g = -4E_e$ and $E_{1,1} - E_g = -\infty$. This results are consistent with the well-known excitonic spectra in 3D [1], with the excitonic spectra in 2D [10] and with the theoretical result of the fictitious system in 1D first studied by Loudon [12]. As discussed above, a mathematical approach to excitons in 2D is a good approximation for very narrow quantum layers but the mathematical solution of excitons in 1D (vanishing both transverse dimensions) leads to nonphysical states [12].

4. Discussion

In order to compare the binding energy $|E_{1,\alpha} - E_g|$ as a function of dimension $2 \leqslant \alpha \leqslant 3$ with the results of the variational calculation of Sec. 2, we need a model of $\alpha = \alpha(L)$. For this purpose, from the variational wavefunctions we show in Fig. 2 our calculation of

$$\left(\left\langle |z_e - z_h|^2 \right\rangle_{1s}\right)^{1/2},$$

and

$$\left(\left\langle x^2 \right\rangle_{1s}\right)^{1/2},$$

(being equal to $\left(\left\langle y^2 \right\rangle_{1s}\right)^{1/2}$ from symmetry considerations), which yield measures of the exciton size in the $z-$ and

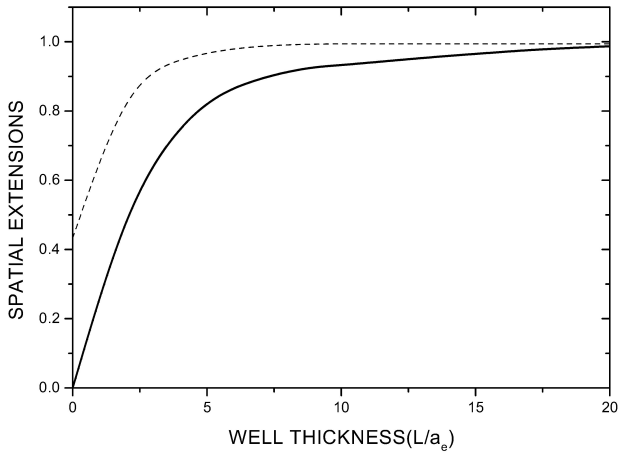

FIGURE 2. Variational calculation of $\left\langle |z_e - z_h|^2 \right\rangle_{1s}^{1/2}/a_e$ (solid line) and $\left\langle x^2 \right\rangle_{1s}^{1/2}/a_e$ (dashed line) vs L/a_e, which yield information of excitons spatial extensions.

$x-$directions. This figure shows how both quantities approach asymptotically the 3D bulk value for large L, as expected. On the other hand, since the exciton size is larger in 2D than in 3D,

$$\left(\left\langle x^2 \right\rangle_{1s}\right)^{1/2}$$

grows as L decreases until it reaches the 2D bulk value. Meanwhile

$$\left(\left\langle |z_e - z_h|^2 \right\rangle_{1s}\right)^{1/2}$$

decreases as L decreases until it vanishes for $L = 0$, since the choice of hard-walls as confinement potential does not allow any "spill over" of the wavefunctions outside the well.

Here we propose a simple way to find $\alpha(L)$ based on the range of values of

$$\left(\left\langle |z_e - z_h|^2 \right\rangle_{1s}\right)^{1/2},$$

and its monotonically behavior:

$$\alpha = 2 + \left(\left\langle |z_e - z_h|^2 \right\rangle_{1s}\right)^{1/2} \qquad (12)$$

which agrees with the values $\alpha = 2$ for $L = 0$ and $\alpha = 3$ for very large L. Substitution of this recipe of α in Eq. (9) yields the dashed curve in Fig. 1.

The agreement between the variational and the fractional dimension models is reasonable. Obviously the choice of $\alpha(L)$ is not unique since there exist several possible expressions for α satisfying the aforementioned requirements. In terms of

$$\left(\left\langle |z_e - z_h|^2 \right\rangle_{1s}\right)^{1/2}$$

and $\left(\left\langle x^2 \right\rangle_{1s}\right)^{1/2}$ it is possible to introduce other formulae with one or more adjustable parameters in order to obtain an even better agreement in Fig. 1. However, within the spirit of simplicity, we think that Eq.(12) contains the more important physical information.

With quantum mechanical theory it is relatively easy to accurately describe the transition of a 3D exciton to a low dimensional regime, and for this purpose we employed here a variational method. However, to assign a "fractional dimension" to a 3D anisotropic physical entity (such as an exciton) is not a straightforward task, despite the fractional dimensionality is a well define concept from the axiomatic mathematical point of view. Therefore it is necessary to resort heuristic arguments, as we did here. In other words, we expect to have given an outline of how to interpret physically the exciton spatial form in a fractional dimensional mathematical formalism.

In summary, we have compared two different approaches for anisotropic excitons in a quantum well. One of them is derived directly from conventional quantum mechanical methods, whereas the other is the result of a more or less sophisticated mathematical formalism. Although the latter approach is a relatively novel one and gives by construction the right results when the dimension is an integer, it is not clear how it can be employed. Here we gave a plausible definition of α for non integer values, which is not unique, but contains the main physical features of the system.

We hope that this article may stimulate further studies of both anisotropic systems and fractional-dimensional approaches in low-dimensional systems.

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