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Non-local potential approach to the ground state of confined excitons in quantum dots

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Abstract
An interacting electron–hole pair in a two-dimensional quantum dot is studied within the framework of the effective-mass approximation. It is shown that non-local separable potentials may be used to obtain the ground state of confined excitons. To this end, we replace the actual Coulomb potential by a projective operator to determine in a closed form the exciton energy as a function of the quantum dot size. Several potential functions are considered and results are compared to well-established approaches. Improvements to the present method are also discussed.

1. Introduction

In recent years quantum dots (QDs) have been intensively investigated as a source of novel physical properties in zero-dimensional structures. This interest also originates from their quantum device applications since high component density and very high speed performance are possible. Electron confinement within the QD can be fairly well approximated by a parabolic potential with only one adjustable parameter (confining frequency) [1]. Due to this spatial confinement, the binding energy of the excitons is strongly enhanced, as compared to its value in bulk semiconductors or even in quantum wells. Within the effective-mass approximation, the interacting electron–hole pair is then described by a Hamiltonian including the Coulomb potential plus the confining parabolic potential. The Hamiltonian is separable upon introducing the centre-of-mass and relative coordinates. Finally, one is faced with a Schrödinger-like equation for the relative part, where the effective potential consists of a Coulomb potential coupled to a harmonic oscillator. Since no general analytical solutions are available, the relative Hamiltonian is to be solved numerically [2], by means of the shifted $1/N$ expansion [3] and WKB treatment [4] or even analytically for particular values of the ratio of the strengths of the Coulomb and harmonic oscillator terms [5].

In this paper we present a novel approach based on the non-local (separable) potential (NLP) method, in which the actual potential is replaced by a projective operator [6, 7]. This method yields an exactly solvable Schrödinger-like equation from which the binding energy can be readily obtained without tedious and elaborated calculations. What is more important, it is always possible to find an NLP (or a sum of them) able to reproduce any set of given electronic states [8] and, 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 in a closed form the binding energy of an electron in the H_2^+ ion within the Born–Oppenheimer approximation and the electron effective-mass in polyacetylene [9]. For a brief summary of applications of NLP in condensed matter physics see [10].

2. Model Hamiltonian

Consider an interacting electron–hole pair confined in a two-dimensional (2D) QD. In the framework of the effective-mass approximation, the Hamiltonian of the electron–hole pair can be written as $\mathcal{H} = H_R + H_r$, where [3]

$$H_R = \frac{P^2}{2M} + \frac{1}{2}M\omega^2 R^2 \qquad (1a)$$

$$H_r = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2 - \frac{e^2}{\epsilon r}. \qquad (1b)$$

Here the pairs $(\boldsymbol{P}, \boldsymbol{R})$ and $(\boldsymbol{p}, \boldsymbol{r})$ are the usual centre-of-mass and relative momenta and coordinates, respectively. The exciton mass is $M = m_e^* + m_h^*$ and the reduced mass is $m = m_e^* m_h^*/(m_e^* + m_h^*)$. The QD is assumed to be parabolic with confining frequency ω and the Coulomb potential is screened by the background dielectric constant ϵ. The exciton wavefunction is expressed as $\Psi(\boldsymbol{R})\psi(\boldsymbol{r})$. The centre-of-mass wavefunction $\Psi(\boldsymbol{R})$ is exactly solvable since $\mathcal{H}_R$ is the standard harmonic oscillator Hamiltonian. Thus, we will deal only with the relative wavefunction $\psi(\boldsymbol{r})$ in what follows.

Inspired in our previous treatment of Coulomb forces in the H_2^+ ion [9], we replace the Coulomb term in (1b) by an NLP. Consequently, the Schrödinger equation arising from (1b) is replaced by

$$\left(\frac{p^2}{2m}+\frac{1}{2}m\omega^2r^2+V_{\mathrm{NL}}\right)\psi(\boldsymbol{r})=E\psi(\boldsymbol{r}) \qquad (2a)$$

where

$$V_{\mathrm{NL}}\psi(\boldsymbol{r})\equiv-\frac{\alpha\hbar^2}{2m}v(r)\int\mathrm{d}^2\boldsymbol{r}'v(r')\psi(\boldsymbol{r}'). \qquad (2b)$$

Here α is the coupling constant and v is the potential function. It is usual to assume, as a first approximation, that the potential function v is spherically symmetric, although other symmetries can be also considered within the NLP approach.

At this point it is important to stress that the substitution $-(e^2/\epsilon r)\psi(\boldsymbol{r})\to V_{\mathrm{NL}}\psi(\boldsymbol{r})$ is exact provided the appropriate potential function v is used in (2b). The main shortcoming of the NLP method is that the *exact* potential function v is expressed in terms of the eigenenergies and eigenfunctions of the original Schrödinger equation [8]. Interestingly, equation (2a) is exactly solvable for any *arbitrary* potential function v. Therefore, the crucial point within the NLP is to choose a potential function that reproduces the observed energy values of the physical system being considered. Typically naive functions with very few adjustable parameters are good candidates [9, 11].

3. Green function

We now calculate an explicit expression for the exciton energy for any arbitrary potential function v. This task is carried out within the Green function framework. The Green function for a 2D harmonic oscillator is determined by the equation

$$\left(\frac{p^2}{2m}+\frac{1}{2}m\omega^2r^2-E\right)G_\omega(\boldsymbol{r},\boldsymbol{r}';E)=\delta(\boldsymbol{r}-\boldsymbol{r}') \qquad (3a)$$

where in polar coordinates (r,ϕ)

$$\delta(\boldsymbol{r}-\boldsymbol{r}')=\frac{\delta(r-r')}{2\pi^2\sqrt{rr'}}\sum_{\ell=-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\ell(\phi-\phi')}. \qquad (3b)$$

The solution of (2a) can be cast in terms of the Green function

$$\begin{aligned}\psi(\boldsymbol{r})&=\int\mathrm{d}^2\boldsymbol{r}'G_\omega(\boldsymbol{r},\boldsymbol{r}';E)V_{\mathrm{NL}}\psi(\boldsymbol{r}')\\&=-\frac{\alpha\hbar^2}{2m}\mathcal{I}\int\mathrm{d}^2\boldsymbol{r}'G_\omega(\boldsymbol{r},\boldsymbol{r}';E)v(r')\end{aligned} \qquad (4a)$$

where we have defined the following constant:

$$\mathcal{I}\equiv\int\mathrm{d}^2\boldsymbol{r}\,v(r)\psi(\boldsymbol{r}). \qquad (4b)$$

After inserting (4a) in (4b), we arrive at the following implicit equation for the exciton energy E:

$$\frac{2m}{\alpha\hbar^2}=-\int\mathrm{d}^2\boldsymbol{r}\int\mathrm{d}^2\boldsymbol{r}'G_\omega(\boldsymbol{r},\boldsymbol{r}';E)v(r)v(r'). \qquad (5)$$

Now we perform the integration over the polar angle ϕ using the expansion

$$G_\omega(\boldsymbol{r},\boldsymbol{r}';E)=\frac{2m}{\hbar^2}\sum_{\ell=-\infty}^{\infty}\frac{g_\omega^\ell(r,r';E)}{2\pi^2\sqrt{rr'}}e^{i\ell(\phi-\phi')} \qquad (6)$$

so we can rewrite (5) as follows:

$$\frac{1}{2\alpha}=-\int_0^\infty\mathrm{d}r\int_0^\infty\mathrm{d}r'\sqrt{rr'}g_\omega^0(r,r';E)v(r)v(r') \qquad (7)$$

where, by virtue of (3), the function $g_\omega^0(r,r',E)$ is obtained by solving the following Sturm–Liouville problem:

$$\left(-\frac{\partial^2}{\partial r^2}-\frac{1}{4r^2}+\frac{r^2}{L^4}+\frac{4\varepsilon-2}{L^2}\right)g_\omega^0(r,r';E)=\delta(r-r') \qquad (8)$$

where we have introduced the QD size $L=\sqrt{\hbar/m\omega}$ and $\varepsilon=1/2-E/2\hbar\omega$. Therefore, using the Kummer functions [12], we get

$$\begin{aligned}g_\omega^0(r,r';E)&=-\frac{\Gamma(\varepsilon)}{2}\sqrt{rr'}\exp\left(-\frac{r^2+r'^2}{2L^2}\right)\\&\quad\times M(\varepsilon,1,r_<^2/L^2)U(\varepsilon,1,r_>^2/L^2)\end{aligned} \qquad (9)$$

where $r_<$ ($r_>$) stands for the smaller (larger) value of (r,r').

4. Coupling constant α

It is apparent that the coupling constant α is not an adjustable parameter of the model. The reason lies in the fact that we might obtain the binding energy $E_{2D}=-4\mathrm{Ry}^*$ of free excitons when the confining potential is switched off, Ry^* being the effective Rydberg in the bulk semiconductor. This step is easily achieved in momentum space, where the Schrödinger equation for the relative particle (2) for $\omega=0$ reads

$$\left(\frac{p^2}{2m}+|E_{2D}|\right)\psi(\boldsymbol{p})=\frac{\alpha\hbar^2}{2m}\mathcal{I}v(p). \qquad (10a)$$

with

$$\psi(\boldsymbol{p})=\frac{1}{2\pi\hbar}\int\mathrm{d}^2\boldsymbol{r}\,\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}/\hbar}\psi(\boldsymbol{r}) \qquad (10b)$$

$$v(p)=\frac{1}{\hbar}\int_0^\infty\mathrm{d}r\,rv(r)J_0(pr/\hbar). \qquad (10c)$$

Using the Parseval identity to write

$$\mathcal{I}=\int\mathrm{d}^2\boldsymbol{p}\,v^*(p)\psi(\boldsymbol{p}) \qquad (11)$$

and (10a) we obtain a closed expression for the coupling constant

$$\frac{1}{2\alpha}=\pi\hbar^2\int_0^\infty\mathrm{d}p\frac{p|v(p)|^2}{p^2+p_{2D}^2} \qquad (12)$$

where $p_{2D}^2=2m|E_{2D}|$. Let us stress that the Fourier transform of real and spherically symmetric functions is also real, but we retain the absolute value should nonspherical functions be considered.

We have found it most appropriate to introduce the Yamaguchi's NLP [13], as it correctly describes Coulomb coupling in the H_2^+ ion [9]. This potential function is simply the Coulomb local potential times the ground state wavefunction for this potential, namely $v(r) = (1/r)\exp(-r/a^*)$, a^* being the effective Bohr radius. Its Fourier transform (10*c*) reads $v(p) = \left(p^2 + p_{2D}^2\right)^{-1/2}$ so that

$$\frac{1}{2\alpha_Y} = \frac{\pi}{2}a^{*2}. \tag{13}$$

For comparison we have considered surface δ-potentials, that is, a force vanishing everywhere except on a spherical shell of radius a^*, namely $v(r) = \delta(r - a^*)$, whose Fourier transform is $v(p) = (a^*/\hbar)J_0(pa^*/\hbar)$. This NLP has been found to be well suited to simulate electron potentials on long quasi-one-dimensional polymers, such as polyacetylene or polyaniline [9, 11]. Thus, in this case the coupling constant becomes

$$\frac{1}{2\alpha_\delta} = 0.533\pi a^{*2}. \tag{14}$$

5. Results and discussions

We consider QDs prepared by confining 2D electrons in a GaAs–AlGaAs heterostructure. Once the material parameters are chosen ($m_e^* = 0.067m, m_h^* = 0.090m$ and $\epsilon = 13.1$, where m is the free electron mass), the only remaining free parameter is the QD size, namely L. We have calculated the exciton energy as a function of L by means of equations (7) and (9), where the coupling constant is given by (13) and (14) for the Yamaguchi's and δ NLPs, respectively. Results are shown in figure 1 and compared to those obtained from the $1/N$ shifted expansion [3] and by direct numerical diagonalization of the Hamiltonian (1*b*). We draw attention to the small-size regime where exciton is confined (L up to $2a^*$). For large L ($>a^*$), all data approach the energy of unconfined 2D excitons (~ -12 meV), as expected. The exciton energy increases as the confinement is stronger (L decreases) and the confinement effects dominate. Note that the Yamaguchi's NLP provides excellent results over the whole range of sizes when compared to the exact calculation, while the $1/N$-shifted expansion fails in the strong confinement regime ($L < a^*$). It is worth mentioning that the NLP approach with the *naive* potential function $v(r) = \delta(r - a^*)$ yields better results than the $1/N$-shifted expansion. We have tried several simple potential functions (e.g. Lorentzians peaked at $r = 0$) but found no improvements as compared to the Yamaguchi's NLP results. However, it is clear that more elaborated functions might yield better results. Finally, let us mention that variational techniques (e.g. taking a^* as a variational parameter in the above potential functions) would surely lead to more accurate results. Study along this direction is in progress.

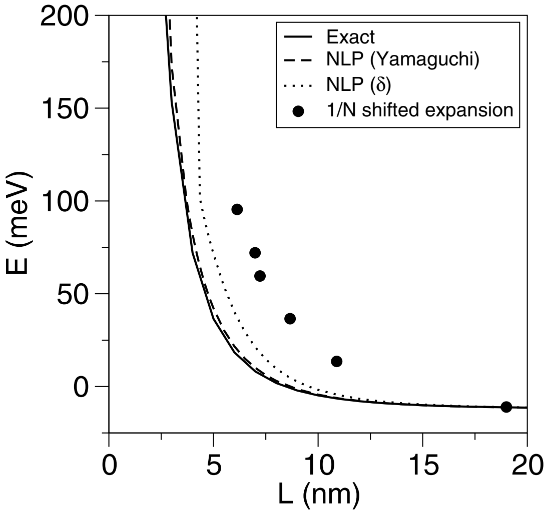

Figure 1. Exciton ground state energy as a function of the quantum dot size. Results of this work for the δ (dotted line) and Yamaguchi's (dashed line) non-local separable potential are compared to the shifted $1/N$ expansion (circles) and exact diagonalization (solid line).

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