Two interacting electrons confined in a 3D parabolic cylindrically symmetric potential, in presence of axial magnetic field: A finite element approach

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1. Introduction

Given its potential for applications in spintronics and optoelectronic devices, the problem of two interacting electrons confined in a 0D heterostructure under axial magnetic field, is of scientific and technological importance and has been recurrently studied [1–3]. It is well known that the 3D cylindrically symmetric problem cannot be exactly reduced to a 1D problem due to the mixing of radial and axial coordinates by the Coulomb interaction, and that consequently no exact analytical solution has been found so far (except for fully 2D [4,5], and 3D spherically symmetric dots with no field [6]). Approximate solutions using a effective radial potential have been proposed but they are expected to work well mostly in the quasi-2D dot limit [5,7]. However, advances in growth techniques nowadays allow to fabricate dots with on-demand aspect ratio making this limit just a very particular case [8,9]. For the fully 3D problem an approximate estimation of the interaction in the z-direction was proposed by Nazmitdinov et al., by using semiclassical tools to separate the radial and axial variables [10].

Between the characteristics of these two electron systems, perhaps the most promising for technological implementation is the change of the total spin number of the ground state related to interaction with the external magnetic field (singlet–triplet transition), which has been well understood and experimentally observed for years [11,12]. Capitalizing this feature is obviously favored by accurate and straightforward schemes in the calculation of electron eigenenergies. Motivated on this premise, we explore reliability and precision of the finite element (FE) method to obtain electronic structure of cylindrically symmetric quantum dots modeled by a 3D parabolic confining potential. The possibility of calculating efficiently electronic states in nanostructures through a well-packed and kindly interfaced software, not only helps scientists to improve their understanding of these relevant systems, but lays bridges for engineers to become more directly engaged in boosting nanotechnology.

2. Model Hamiltonian

The studied system consists of two interacting electrons confined by a fully 3D parabolic potential axially symmetric, in the so-called Faraday configuration, i.e. under the influence of a transversal magnetic field $\mathbf{B} = (0, 0, B)$. Within the effective-mass approximation, the corresponding Hamiltonian in effective atomic units ($\hbar = e = m^* = (4\pi \varepsilon_0)^{-1} = 1$) is written

$$ H_{\text{total}} = \sum_{i=1}^{2} \left[ \frac{|\mathbf{p}_i + \mathbf{A}(r_i)|^2}{2m^*} + \frac{m^*}{2} \left[ \omega^2_1 (x_i^2 + y_i^2) + \omega^2_2 z_i^2 \right] \right] + \frac{1}{\varepsilon} |\mathbf{r}_2 - \mathbf{r}_1| + g^* \mu_B (\mathbf{s}_1 + \mathbf{s}_2) \mathbf{B}, $$

(1)
where \( m^\ast \) is the electron effective mass in units of electron mass \( m_e \), \( \varepsilon \) is the dielectric constant, \( g^\ast \) is the effective \( g \) factor, \( \mathbf{s}_1 \) (\( \mathbf{s}_2 \)) is the total spin of electron 1 (2), and \( \mathbf{A}(\mathbf{r}) = \frac{\mathbf{r}}{2}(\mathbf{y} \times \mathbf{r}) \) is the vector potential in the symmetric gauge. We adopt a cylindrically symmetric parabolic confining potential with characteristic frequencies \( \omega_{l1} \) and \( \omega_{l2} \), for the in plane and growth directions, respectively (the corresponding characteristic lengths are \( l_{11} = (1/2m^\ast \omega_{l1})^{1/2} \) and \( l_{22} = (1/2m^\ast \omega_{l2})^{1/2} \)). The choice of this unit system obeys the sake of generality, since energy results are presented in units of effective Hartree \( \text{Ha} \), making them non-dependent on any particular material (thus, lengths are to be taken in effective Bohr radius \( a^B_0 = \sqrt{\frac{\hbar^2}{m^\ast \varepsilon}} \).

The aspect ratio \( \alpha \equiv \frac{l_1}{l_2} \) is defined to describe the geometric character of the dot in such a way that \( \alpha > 0 \) refers to prolate ellipsoids (nanorod quantum dots), \( \alpha < 0 \) to oblate ellipsoids (nanodisk quantum dots), and \( \alpha = 1 \) to the particular spherical case (see Fig. 1(a)).

3. Full CI calculation

For monitoring the FE results, we perform full configuration interaction calculations for the studied dots. The implementation of the method is done following the work by Chen et al. in [13]. This kind of numerical diagonalization approach has been previously used for studying dimensionality effects, and in explaining experimental results in quantum dots [7,14–17].

The four terms of the Hamiltonian in (1), can be labeled according to

\[
H_{\text{total}} = H_1 + H_2 + H_C + H_Z,
\]

where the \( H_1 \) (\( H_2 \)) term corresponds to the kinetic and confinement energy for electron 1 (2), \( H_C \) stands for the Coulomb interaction between electron 1 and 2, and \( H_Z \) represents the Zeeman interaction between the total spin and the magnetic field. From now on, for simplicity we do not further consider this Zeeman term since its energy contribution \( E_Z = g^\ast \mu_B SB \) is not relevant for the comparison of methods in solving the coordinate dependent terms.

The two single particle terms \( H_1 \) and \( H_2 \) are exactly diagonalizable in the well-known Fock–Darwin basis [18,19]. Thus, we use this basis to write the two particle Hamiltonian and then carry out numerical diagonalization for finding eigenenergies of the system. The matrix elements corresponding to the term \( H_C \) are built up using expressions (13) and (15) of [13].

We use in our calculations basis of up to 1225 two particle states which includes s-, p-, d-, f-, and g-like single particle orbitals. This allows us to work with convergence levels of below 0.002% of relative error between subsequent runs as function of the basis number, as shown in Fig. 1(b). Additionally, for checking reliability of the code, it was tested to reproduce analytical results for the full 2D case and for the spherical 3D case [4,6], and previous similar CI calculations [13].

4. Finite element calculations

To determine the equations to be solved numerically by FE methods, it is necessary to work on the Hamiltonian (1) by using the standard procedure of introducing centre-of-mass \([\mathbf{R} = (X, Y, Z) = \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)] \) and relative \([\mathbf{r} = (x, y, z) = (\mathbf{r}_2 - \mathbf{r}_1)] \) coordinates, thus, ignoring the Zeeman term the Hamiltonian reads

\[
H_{\text{total}} = H_{\text{cm}} + H_r + H_{\text{rel}},
\]

where

\[
H_{\text{cm}} = \frac{[\mathbf{p} + \frac{2\mathbf{A}(\mathbf{R})]}{4m^\ast} + m^\ast\left[\omega_{r1}^2(X^2 + Y^2) + \omega_{r2}^2Z^2 \right]},
\]

and

\[
H_{\text{rel}} = \frac{[\mathbf{p} + \frac{2\mathbf{A}(\mathbf{r})]}{4m^\ast} + m^\ast\left[\omega_{r1}^2(x^2 + y^2) + \omega_{r2}^2 z^2 \right] - \frac{1}{\varepsilon}\sqrt{x^2 + y^2 + z^2}^2}
\]

This separability of the Hamiltonian is a peculiar property of the parabolic confinement, which allows us to decouple the system into the energy of the centre-of-mass and the energy of the relative part [6,20]. The \( H_{\text{cm}} \) part is a simple harmonic oscillator with different confinement in the plane and in the \( z \)-direction with uniform magnetic field applied normally to the plane, and its solutions are the same as the ones used for the single particle basis in the CI calculations, but for a particle with electric charge 2 and effective mass \( 2m^\ast \).

On turn, the relative part represents a much more complicated problem related to the mixing of variables due to the Coulomb interaction. Taking advantage of the axial symmetry of the problem, the Hamiltonian (3) can be written in the form

\[
H_r = -\frac{1}{m^\ast}\left[\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right) + \frac{\partial^2}{\partial z^2}\right] + \frac{B^2}{16m^\ast}\rho^2 + \frac{m^\ast}{4}\left[\omega_{r1}^2 \rho^2 + \omega_{r2}^2 z^2 \right] + \frac{1}{\varepsilon \sqrt{\rho^2 + z^2}^2} - \frac{1}{m^\ast}\left[\frac{1}{\rho^2}\frac{\partial}{\partial \rho} \frac{\partial}{\partial \varphi}\right]
\]

where clearly the angle dependence can be separated from radial and \( z \)-components, and replaced by a separation constant \( l = 0, -1, 1, -2, +2, \ldots \) associated to the quantum number of the \( z \)-component of angular momentum [6]. Then, Hamiltonian (6) becomes

\[
H_r = -\frac{1}{m^\ast}\left[\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right) + \frac{\partial^2}{\partial z^2}\right] + \frac{m^\ast}{4}\left[\Omega^2 \rho^2 + \omega_{r2}^2 z^2 \right] + \frac{1}{m^\ast}\frac{l^2}{\rho^2} + \frac{\omega_{r1}}{2} + \frac{1}{\varepsilon \sqrt{\rho^2 + z^2}^2}.
\]
with \( \omega_n = B/m^* \) and \( \Omega = \sqrt{\omega_0^2 + \omega_c^2}/4 \), the cyclotron and effective in-plane frequencies, respectively.

Aiming further simplification of the relative Hamiltonian, it is possible to introduce the quantities \( l_0 = \sqrt{1/m^* \Omega} \), \( \lambda = \frac{1}{\hbar l_0 \Omega} \), and \( \kappa = \frac{\omega_{0}}{\Omega l_0} \), in such a way that changing to dimensionless coordinates \( \xi \equiv x/l_0 \) and \( \zeta \equiv z/l_0 \), the time independent Schrödinger equation for this term looks

\[
\left\{-\frac{1}{\xi^2} \frac{\partial}{\partial \xi} \left( \xi^2 \frac{\partial \psi}{\partial \xi} \right) + \frac{\partial^2}{\partial \zeta^2} \right\} + \frac{1}{2} \left( \xi^2 + \kappa^2 \zeta^2 \right) \right\} \psi(\xi, \zeta) = \epsilon \psi(\xi, \zeta),
\]

and the eigenenergy value corresponding to the relative part of the Hamiltonian reads

\[
E_i^l = \Omega \epsilon_i + \frac{\alpha l}{2}.
\]

Numerical treatment of the fully 3D problem requires to solve the partial differential equation (8) for obtaining eigenenergies. An simplified approach for this problem has been proposed by Nazmitdinov et al. [10], in which implementation of the computational solution is favored by reduction of the dimensionality of the problem, turning the partial differential equation (8) in an approximated ordinary differential eigenvalue problem (EVP) [20]. Namely, the approximation drives to the modified time independent Schrödinger equation

\[
\left\{-\frac{1}{\xi^2} \frac{\partial}{\partial \xi} \left( \xi^2 \frac{\partial \psi}{\partial \xi} \right) + \frac{\partial^2}{\partial \zeta^2} \right\} \psi(\xi) = \epsilon \psi(\xi),
\]

where \( K(\frac{\Delta \xi^2}{\xi^2 + \Delta \xi^2}) \) represents the first kind-complete elliptical integral evaluated in \( \Delta \xi^2 \equiv \frac{4 j \Omega \zeta}{\alpha \zeta} \). \( \Delta \zeta = \zeta_1 - \zeta_0 \) (with \( \zeta_0 = 0, 1, 2, \ldots \)) stands as a quantum number for excitations in the approximately separated coordinate \( \zeta \). Thus, the eigenenergy corresponding to the relative part of the Hamiltonian is

\[
E_i^l = \Omega \left( \epsilon_i + \frac{\alpha l}{2} \right).
\]

To solve (10) numerically, is obviously expected to computationally less expensive than to solve (8). Nevertheless, how less expensive and how large is the error introduced by the proposed approximation, to the best of our knowledge, remained so far as subject of speculations. Then, for solving the eigenvalue problems (8) and (10) we perform finite element calculations at different magnetic field and aspect ratio regimes.

For the FE calculations, the well-reputed finite element tool COMSOL was used [21]. Convergence tests for the obtained eigenvalues of the systems were carried out for both cases, 1D and 2D EVPs. Convergence levels below the 0.002% for subsequent runs as functions of the number of elements in the domains were achieved (see Figs. 1(c) and 1(d)).

5. Results

We fix the in plane confining frequency in a reference value of 18.33 Ha\(^*\) (which in the case of InAs dots would be equivalent to 50 meV; i.e. a characteristic length of 5.75 nm). The longitudinal frequency values are thus defined by the studied aspect ratios.

Fig. 2 shows ground and first excited eigenenergies for different aspect ratios, as functions of the external magnetic field.

The corresponding eigenenergies for non-interacting particles are also shown. Two important features are observed: First, the neglecting of the Coulomb interaction between electrons introduce a significant error respect to the actual eigenenergies of the system, and then it should be strongly avoided (especially for nanorod-like dots). Second, if Zeeman energy would be considered (which at principle does not depend on the geometry), the singlet–triplet ground state transition generally would require higher magnetic fields for smaller aspect ratios. This is contrary to the predicted behavior in [10], where the analysis is made assuming quasi-2D dots, but makes physical sense due to the decreasing energy spacing with the increase of the aspect ratio.

In order to determinate accuracy of the FE results respect to the CI ones, we compare for both FE approaches (2D and 1D EVPs), the relative differences for the obtained i-th eigenvalues as functions of the magnetic field and aspect ratio by defining

\[
\Delta E_i^{\text{CI,2D}} \equiv \left| 100 \times \frac{E_i^{\text{CI}} - E_i^{\text{DFE}}}{E_i^{\text{CI}}} \right|,
\]

and

\[
\Delta E_i^{\text{CI,1D}} \equiv \left| 100 \times \frac{E_i^{\text{CI}} - E_i^{\text{DFE}}}{E_i^{\text{CI}}} \right|,
\]

respectively; where \( E_i^{\text{CI}} \) represents the i-th eigenvalue obtained from the CI method while \( E_i^{\text{DFE}} \) (\( E_i^{\text{DFE}} \)) the i-th eigenvalue obtained from the 2D (1D) FE calculation.

Fig. 3 allows to compare the mismatch between each of the FE schemes and the CI results. Clearly the approximated character of the 1D EVP approach is reflected in these plots, and its increased inaccuracy for higher aspect ratios becomes evident. It is interesting to note that for strong fields the introduced error is slightly erased due to the increase of the ratio between confinement strength and Coulomb interaction magnitude, on which the approximation is exerted.

While the 2D EVP scheme fits very well to the reference values in all the different studied regimes, the reliability of the 1D scheme starts failing notably with the elongation of the dot. The approximation performance is enhanced for the first excited state as expected, considering the reduction of the Coulomb interaction associated to the charge delocalization of excited states.

Regarding calculation times. In Table 1, the elapsed time in seconds for the three different calculations (carried out in the conditions in which convergences reported in Fig. 1 are obtained), are shown. The calculations were made using a commercial "core
Fig. 3. (Color online.) Upper panel: Relative difference between the CI obtained ground state eigenvalue and the FE obtained value from the 1D EVP (left), and the FE obtained value from the 2D EVP (right). Lower panel: as in the upper panel but for the first excited state.

Table 1
<table>
<thead>
<tr>
<th>CI method</th>
<th>FE 2D EVP</th>
<th>FE 1D EVP</th>
</tr>
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<tbody>
<tr>
<td>470 s</td>
<td>8 s</td>
<td>2 s</td>
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Evidently the time consumptions for the FE schemes, beyond being shorter than that for the CI approach, confirm the efficiency of the method. Albeit longer than the time required for the 1D EVP calculation, the time for the 2D EVP seems very reasonable and not much more computationally expensive.

Two electron wave function calculations can be easily implemented in each of these three numerical approaches and they will be subject of further studies. However it is worth noting that the separation between centre-of-mass and relative part of the Hamiltonian leads to an interesting conditional nature of the relative part of the wave function which can be thoroughly investigated by using the described FE approaches.

6. Conclusions

In summary, we have shown two different ways to use the finite element method for calculating two interacting electron eigenenergies in 0D nanostructures. The so-called approach 1D EVP, where average of the interaction in $z$ is applied, presents efficiency and fairly accurate results for quantum disk-like dots, however its reliability showed fails for increased aspect ratios. This effect is clearly related to underestimation of the Coulomb interaction by the average in the approximation.

On the other hand, the results from the non-approximated FE approach exhibited highly accuracy when compared to the reference CI calculations. This optimal performance is consistent along the different field and aspect ratio regimes explored in this study.

One of the main advantages of the presented FE approaches is their versatility to describe systems of various geometries and materials. Thus, these methods allow us to study a wide range of cases. Likewise, these exact results can be used as reference data for more sophisticated methods as Density functional theory, which recently has begun to be used in describing nanostructures.

As a main conclusion we propose the presented FE based schemes (especially the so-called 1D EVP); as novel, efficient; and reliable techniques to calculate electron structures in quantum dots.

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References