Calculation of the energy spectrum of a two-electron spherical quantum dot

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Abstract

We study the energy spectrum of the two-electron spherical parabolic quantum dot using the exact Schrödinger, the Hartree-Fock, and the Kohn-Sham equations. The results obtained by applying the shifted-1/N method are compared with those obtained by using an accurate numerical technique, showing that the relative error is reasonably small, although the first method consistently underestimates the correct values. The approximate ground-state Hartree-Fock and local-density Kohn-Sham energies, estimated using the shifted-1/N method, are compared with accurate numerical self-consistent solutions. We make some perturbative analyses of the exact energy in terms of the confinement strength, and we propose some interpolation formulae. Similar analysis is made for both mean-field approximations and interpolation formulae are also proposed for these exchange-only ground-state cases.

I. INTRODUCTION

Progress in nanotechnology has allowed the development of small devices like quantum dots. The confinement potential can be safely approximated by a harmonic one [1,2], which has boosted the study of quantum dots with parabolic confinement during the last years (see e.g. Refs. 3 and 4, and references therein). The presence of many interacting electrons render the computation of the electronic states and properties a very complicated many-body problem. The first non-trivial exactly solvable problem of many-electrons is the one of two electrons confined in a parabolic potential, which made it a very attractive workbench for testing all kind of approximations (see e.g. [5–10]).

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The Hamiltonian describing the pair of interacting electrons in a parabolic quantum dot in the effective mass approximation can be written as

\[
\hat{H} = -\frac{\hbar^2}{2m^*}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}m^*\omega^2(r_1^2 + r_2^2) + \frac{e^2}{\epsilon|\vec{r}_1 - \vec{r}_2|}
\]  

(1)

where \(m^*\) is the effective mass, \(\omega\) the confinement strength, and \(\epsilon\) the dielectric constant of the host material and \(\nabla^2\) is the Laplacian operator.

Equation (1) can be separated into a centre-of-mass and a relative motion component. Furthermore, due to the radial symmetry of the components, only those parts of the corresponding Schrödinger equations have to be solved. The centre-of-mass part will give the well-known harmonic oscillator problem. In three dimensions, the relative motion part may admit exact solutions for special choices of the parameters (see e.g. [4]). For the two-dimensional case, similar separation and substitution can be made, and again there are no general solutions expressible in terms of special functions. Nevertheless, in Ref. [12] and more recently in Ref. [13] it was shown that there exist analytic solutions for special choices of the confinement constant.

Many-body effects are usually divided into exchange and correlation components [14]. Exchange-only effects are considered in Hartree-Fock (HF) and differently, in Kohn-Sham (KS) approaches (although in KS, the correlation effects can be included), which typically amounts for around 10% of the total energy. Correlation is about one order of magnitude smaller. Nevertheless, it has been shown that in two dimensions for two electrons in a harmonic field, correlation may play a bigger role specially for singlet states (see e.g. [15]).

The shifted-1/N method [16,17] has been applied to various condensed matter problems. Also, the two-dimensional relative motion Schrödinger problem have been solved using this technique in Refs. [9,18].

The article has been structured as follows: in Sect II we describe the Schrödinger, Hartree-Fock, and Kohn-Sham approaches we use. In Sect. III we solve the exact, HF, and KS-LDA equations using an accurate numerical technique and the shifted-1/N method. We also apply perturbation theory up to first order in both limits of confinement for the exact and mean field cases, and we propose some interpolation formulae for the energy. We discuss the accuracy of the mean field approaches, and of the shifted-1/N method for the present case.

II. METHOD

Throughout the paper the units of energy will be given in terms of the effective Rydberg constant \(R^* = \hbar^2/(2m^*a^*)\) and the effective Bohr radius \(a^* = \hbar^2/\epsilon m^*e^2\), respectively.

In centre-of-mass and relative coordinates and measuring in reduced units the Hamiltonian reads

\[
\hat{H} = -\left(\frac{1}{4}\nabla_{\vec{R}}^2 + \nabla_{\vec{r}}^2\right) + \gamma^2\vec{R}^2 + \frac{\gamma^2}{4}\vec{r}^2 + \frac{1}{\vec{r}}
\]  

(2)

where we have chosen the centre-of-mass \(\vec{R} = (\vec{r}_1 + \vec{r}_2)/2\) and the relative coordinate \(\vec{r} = (\vec{r}_1 - \vec{r}_2)\).
The separation leads to the harmonic oscillator problem for the centre-of-mass coordinate, with energy
\[ E_{NL} = \gamma (2N + L + 3/2) . \] (3)
and eigenfunctions
\[ \Psi_{NLM}(\vec{R}) = N_{NL} \exp(-\gamma R^2)(2\gamma)^{L/2}L^L N^{L+1/2}(2\gamma R^2) Y_{LM}(\theta_R, \phi_R) . \] (4)

For the relative coordinate equation the wavefunction can be separated into radial and angular components
\[ \Psi(r) = \frac{u(r)}{r} Y_{lm}(\theta, \phi) , \] (5)
where \( Y_{lm}(\theta, \phi) \) are the spherical harmonics which are eigenfunctions of the angular momentum operator \( L_z \), and \( L^2 \) with eigenvalues \( m \) and \( l \). This separation makes the corresponding radial Schrödinger equation the following second order ordinary differential equation
\[ \left[ -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{1}{4} \gamma^2 r^2 + \frac{1}{r} - E \right] u(r) = 0 . \] (6)

It is well known that exact solutions of equation (6) cannot be expressed in a closed form in terms of special functions. There are analytic expressions for the energy for particular values of \( \gamma \) and \( l \) as it was pointed out in Refs. [5,11], among others.

The electrons should satisfy the Fermi-Dirac statistics which means in this case that for singlet states \( (s = 0) \) the spatial part of the wavefunction should be antisymmetric and for triplet states \( (s = 1) \) symmetric. As the centre-of-mass coordinate remains the same after exchanging to electrons, the antisymmetry requirement will be in the relative part. Because of the separation in radial and angular components of the relative-coordinate wavefunction it will mean that singlet states are associated with odd \( l \) and triplet states with \( l \) even, respectively.

It is interesting to compare the results of exact calculations with independent-electron models like Hartree-Fock (HF), and Kohn-Sham (KS) [14] in order to assess the relative importance of many-body effects like exchange and correlation, and also to evaluate the performance of the local-density approximation. For two paired electrons the electronic density is \( \rho_{HF} = 2|\phi_{HF}|^2 \), where \( \phi_{HF} \) is the orbital, and the exchange potential is equal to half of the Hartree one with opposite sign. The HF equation can be written as
\[ \left[ -\frac{1}{2} \nabla^2 + v(r) + \frac{1}{2} v_H[\rho_{HF}] \right] \phi_{HF} = \varepsilon_{HF} \phi_{HF} , \] (7)
\( v(r) = \frac{1}{2} \gamma^2 r^2 \) and \( \varepsilon_{HF} \) is the HF orbital energy. The total HF energy is written as
\[ E_{HF} = 2\varepsilon_{HF} - \frac{1}{2} \int d\vec{r} \rho_{HF} v[\rho_{HF}] , \] (8)
where \( v_H \) is the Hartree potential given by
\[ v_H[\rho] = \int d\vec{r}' \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|}. \] (9)

The KS equation can be written as

\[ \left[ -\frac{1}{2} \nabla^2 + v(r) + v_H[\rho_{KS}] + v_x(\rho_{KS}) \right] \phi_{KS} = \varepsilon_{KS} \phi_{KS} \] (10)

\( \varepsilon_{KS} \) and \( \phi_{KS} \) are the KS orbital energy and eigenfunction, respectively, and again \( \rho_{KS} = 2|\phi_{KS}|^2 \). We take here the local-density approximation for which \( v_x(\rho) = \frac{4}{3}c_x \rho^{1/3} \), with \( c_x = -\frac{3}{4} \left( \frac{2}{\pi} \right)^{1/3} \) (see e.g. [14]). The total KS energy is given by

\[ E_{KS} = 2\varepsilon_{KS} - \frac{1}{2} \int d\vec{r} \rho_{KS} v_H[\rho_{KS}] - \frac{1}{3} \int d\vec{r} \rho_{KS} v_x(\rho_{KS}). \] (11)

Eqs. (7) and (10) have asymptotae controlled by the harmonic potential, so the asymptotic density looks like

\[ \rho_a(\vec{r}) \propto \exp(-\gamma r^2). \] (12)

### III. RESULTS AND DISCUSSION

First we make an analysis of the solution of the exact case using the 1/N approximation. For details in the derivation of the formulae related to the shifted-1/N method, we refer to the literature (see e.g. [9,16–18]).

In order to establish the accuracy of the results obtained by the application of the shifted 1/N method we compare them with those obtained by using the Schwartz’s numeric method [19]. The method is based in a numerical approximation of functions on a mesh and gives very accurate results [20,21]. There are only empirical estimates of the error [19] which turns out to be exponentially decaying with the number of points given the mesh step. The interpolation function is chosen as

\[ f(r) = \sum_m f_m \frac{u(r)}{(r - r_m)a_m}, \] (13)

where

\[ u(r) = \sin[\pi(r/h)^{1/2}]. \] (14)

Here \( r_m \) is a zero of \( u(r) \), \( a_m \) is a zero of its derivative, and \( h \) is the step of the mesh which turns out to be quadratically spaced. The choice of the step \( h \) was made after estimating the characteristic length of the effective potential, and then multiplying the obtained estimate by five and dividing it by the square of the number of points in the mesh, usually around 300. This guarantees that \( h \) is minimal for a given \( \omega \), and also that the function value at the last mesh point is practically zero.

In figure 1 we show the behavior of the error of the energy of few lowest eigenvalues calculated using the shifted-1/N method, compared with the accurate results obtained using
the Schwartz’s method. We plotted the relative error defined as \( \delta E = E_{\text{approx}}/E_{\text{exact}} - 1 \), as function of the reduced variable \( \gamma' = \gamma/(\gamma + 1) \). The \( 0s, 0p \), and \( 0d \) states are the three lowest energy states of the relative motion with angular momentum \( l = 0, 1, \) and \( 2 \), respectively. It can be seen that the error remains bounded in 0.5\% for the first eigenvalue, in 0.075\% for the second one and 0.022\% for the third one. It is noticeable that the method always underestimates the correct values of the energy, and that the error decreases with the increase of the angular quantum number \( l \), as it should be expected. Furthermore, the error has some maximum between the two limiting cases, after which it decreases as expected, since the shifted-1/N method reproduces exactly the oscillator case.

Figure 2 shows the behavior of the total energy (the sum of the centre-of-mass and relative motion energies) as a function of \( \gamma' \), as calculated using the shifted-1/N method. The first two symbols are the indices of the centre-of-mass component of the energy, and the last two correspond to the relative motion. The lowest six states are depicted. The inset is a magnification for \( \gamma' \) from 0.01 to 0.15. Here, an apparent linear behavior can be observed, but a more careful analysis indicates that, for instance, for the ground-state first six-eight points, the effective power in terms of \( \gamma' \) is about 0.8. In the last few points the curve can be fitted well with a function of the type \( \gamma'/(1 - \gamma') \) which is the expected behavior for electrons in a harmonic field. The relative error is not shown, but it is estimated in roughly one half of the one shown in figure 1, since the centre-of-mass energy can be calculated exactly and it is typically of the size of the relative motion energy.

Although we are able to solve the Schrödinger equation very accurately for this system, perturbation analysis can give some more insight of the behavior of the electrons under weak and strong confinement. For weak confinement (\( \gamma \to 0 \)) we have that the kinetic energy term can be neglected (see e.g. [32]), which corresponds to the strong interaction limit (Wigner crystallization). Then, the energy is approximately taken as the minimum of the effective potential (this is the zeroth order approximation to the energy),

\[
V_l(r) = l(l + 1)\left(\frac{1}{r^2} + \frac{1}{4}\gamma^2r^2 + \frac{1}{r}\right),
\]

the minimum is reached for \( r_0^l \) that satisfies the equation

\[
\gamma^2r_0^l - 2r_0^l - 4l(l + 1) = 0 .
\]

For \( l = 0 \) \( r_0^0 = (2/\gamma^2)^{1/3} \) and for \( l \gg \gamma/2 \) \( r_0^l \approx (2l/\gamma)^{1/2} \). The minimum of the potential is then

\[
U_0^l = l(l + 1)\left(\frac{1}{r_0^l} + \frac{1}{4}\gamma^2r_0^l + \frac{1}{r_0^l}\right),
\]

which is \( 2^{-1/3}2^{2/3}/\gamma^{2/3} \) for \( l = 0 \) and \( \gamma(2l + 1)/2 + \gamma^{1/2}/(2l)^{1/2} \) for large enough values of \( l \).

The next order in the approximation is to get the effective frequency \( \gamma_0^2 = \frac{1}{2}d^2V_l(r)/dr^2|_{r=r_0^l} \),

\[
\gamma_0^2 = 4\gamma^2 + \frac{3(l + 1)}{r_0^l},
\]

which is \( \gamma_0^2 = 3/4\gamma^2 \) and \( \gamma_0^2 = \gamma^2 + 3/4\gamma^2/l + 2^{1/2}/4(\gamma/l)^{3/2} \) for large \( l \). Now we can estimate the energy levels of this effective harmonic field. So the total energy in the weak confinement limit is
\[ E_{nl} \approx l(l+1)\frac{1}{r_0^2} + \frac{1}{4}\gamma^2 r_0^2 + \frac{1}{r_0^2} + 2n(n+1/2), \]

where \( n = 0, 1, \ldots \) For \( l = 0 \)

\[ E_{n0} \approx \frac{3}{2} 2^{-1/3} \gamma^{2/3} + \frac{3^{1/2}}{2} \gamma(n+1/2). \]

For \( l \) large enough

\[ E_{nl} \approx \frac{1}{2} \gamma(2l+1) + \left(\frac{\gamma}{2l}\right)^{1/2} + 2\left[ \gamma^2 + \frac{3\gamma^2}{4l} + \frac{2l^{1/2}}{4} \left(\frac{\gamma}{l}\right)^{3/2} \right]^{1/2}(n+1/2). \]

Equation (20) gives the explanation why the effective power of the ground-state energy for small \( \gamma' \) is approximately 0.8: it is between 2/3 and 1, the effective powers for the weak field limit for the relative motion and the centre-of-mass energies in terms of \( \gamma' \approx \gamma \).

In the strong confinement regime, the zeroth order approximation amounts to neglect the electron-electron interaction, so it corresponds to the oscillator’s energy. Application of the first order of the perturbation theory [23] for strong confinement (\( \gamma \rightarrow \infty \)) for the relative coordinate equation leads to

\[ E_{nl} \approx E_{nl}^{osc} + \langle \phi_{nl}^{osc} | r^{-1} | \phi_{nl}^{osc} \rangle, \]

where \( E_{nl}^{osc} = 2\gamma(2n + l + 3/2) \) and substituting \( \phi_{nl}^{osc} \) (which is similar to equation (4)) into the above equation gives

\[ E_{nl} \approx 2\gamma(2n + l + 3/2) + \frac{\gamma^{1/2}}{2^{1/2}} \sum_{k,k'=0}^n a_{nl,2k} a_{nl,2k'} \Gamma(l + k + k' + 1) N_{nl}^2 \] (23)

where \( a_{nl,2k} \) are the coefficients of the generalized Laguerre polynomials (of Eq.(4)) that satisfy the recursion

\[ a_{nl,2k} = a_{nl,2(k-1)} \frac{k - n - 1}{k(k + l + 1/2)} \]

with \( a_{nl,0} = 1 \). Furthermore, the normalization constant is given by

\[ N_{nl}^{-2} = \sum_{k,k'=0}^n a_{nl,2k} a_{nl,2k'} \Gamma(l + k + k' + 3/2). \]

Based on the perturbative results of Eqs. (17), (19) and (23) we propose the following interpolation formula

\[ E_{nl}^{(int)}(\gamma) = \frac{\gamma^{-1} E_{nl}^{(0)} + \gamma E_{nl}^{(\infty)}}{\gamma^{-1} + \gamma}, \]

where the superscripts \((0)\) and \((\infty)\) correspond to the zero and infinite confinement limits. For \( \gamma \rightarrow 0 \) equation (26) will return approximately the weak confinement limit and for
\( \gamma \to \infty \) the strong confinement limit. For the zeroth order approximations equation (26) leads to

\[
E^{(\text{int})}_{nl}(\gamma) = \frac{\gamma^{-1}U_0^l + 2\gamma^2(2n + l + 3/2)}{\gamma^{-1} + \gamma},
\]

and for the first order perturbative results, it will be

\[
E^{(\text{int})}_{nl}(\gamma) = \frac{\gamma^{-1}[U_0^l + 2\gamma(n + 1/2)] + \gamma[2\gamma(2n + l + 3/2) + 2^{-1/2}\gamma^{1/2}\Delta_{nl}]}{\gamma^{-1} + \gamma},
\]

where \( \Delta_{nl} \) denotes the summation in the right hand side of equation (23). The interpolation scheme of equation (27) performs consistently bad, except for the very weak, and very strong fields. The error goes up to 41\% for the ground-state, underestimating the correct values. The introduction of first order corrections, corresponding to the interpolation scheme of equation (28) brings a dramatic improvement on the values: for the ground-state the relative error is never worse than 3.3\% for the energy of the relative motion, which means that the relative error of the total energy is around 1.7\%.

In the case of the mean-field approximations like Hartree-Fock and Kohn-Sham, we have considered the paired-electron ground-state case, and since the confining potential is radially symmetric, the orbitals and the density are also radially symmetric. We implemented the shifted-1/N technique for the HF and KS equations. Here, a word about accuracy is needed: although the solution of the Schrödinger-like equations using Schwartz’s method is very accurate, the estimate of the Hartree potential is not as accurate anymore, nevertheless, five to six figures are always guaranteed. The results are shown in table 1 in the first and third columns, indicated as \( HF - 1/N \) and \( KS - 1/N \), respectively. Since the resulting wavefunction from the application of the 1/N has a complicated form which makes difficult a direct evaluation of the density or of the Hartree potential, we assumed that as initial guess the non-interacting density, which is also correct asymptotically. For comparison purposes, we have used again the Schwartz technique self-consistently to solve both the HF and KS equations. Numerical results are shown in the second and fourth columns of table 1, indicated as \( HF - \text{num} \) and \( KS - \text{num} \), respectively. Also for comparison purposes, we included the results of solving the full Schrödinger equation using the shifted-1/N method and the numeric solution, which are the last two columns indicated as \( \text{Exact} - 1/N \) and \( \text{Exact} - \text{num} \), respectively.

Table 1 shows very good agreement between the results from the accurate numerical result and the ones calculated with the 1/N method. We should not be too enthusiastic about the accuracy, since the remarkable agreement is probably a result of the compensation of errors from the calculation of the Hartree potential and energy (due to its simplicity) and the intrinsic error of the 1/N method, specially for the weak field case. It can also be seen that the relative accuracy improves from typically few times \( 10^{-2} \) to \( 10^{-4} - 10^{-5} \) with the increase of the strength of the field. Also the systematic difference between the HF and KS methods is reduced with stronger confinement. Both behaviors can be understood by taking into account that the confinement potential dominates over the decaying electron-electron interaction potential, and with the increase of the strength of confinement the problem becomes just a harmonic potential problem, for which the shifted-1/N is designed to give the exact energy, although the quality of the wavefunction is not too good.
In order to better understand the behavior of the pair of electrons in strong and weak confinement within these mean-field theories, we can recourse to perturbation analysis. In the strong confinement limit ($\gamma \to \infty$) the system will behave basically as a pair of non-interacting electrons, and the electron-electron interaction (Hartree and exchange potentials) can be considered as a perturbation. The HF and KS orbitals become

$$\phi(\vec{r}) = \left(\frac{\gamma}{\pi}\right)^{3/4} \exp\left(-\frac{1}{2} \gamma r^2\right), \quad (29)$$

so, the Hartree energy will be $2(2\gamma/\pi)^{1/2}$ and the LDA exchange $3c_x^213/(3\gamma/\pi)^{1/2}/4$. Then the total HF energy will be

$$E^{(\infty)}_{HF} = 3\gamma + \left(\frac{2\gamma}{\pi}\right)^{1/2}, \quad (30)$$

and the total KS energy

$$E^{(\infty)}_{KS} = 3\gamma + \left(\frac{3}{4} \gamma^{1/3} 3^{1/2} 2c_x \right) \left(\frac{\gamma}{\pi}\right)^{1/2}. \quad (31)$$

In the weak confinement limit ($\gamma \to 0$), due to scaling arguments, we can neglect the kinetic energy, and we can assume constant density, at least within a certain radius $R$ (this is asymptotically true for the HF approximation and arguably for the KS one). Now taking Eqs. (7) and (10), and using Poisson’s equation, we get that $\rho_{HF} \approx \gamma^2/(2\pi)$ and $\rho_{KS} \approx \gamma^2/(4\pi)$. Then from normalization condition $R = \left[3/(2\pi \rho)\right]^{1/3}$. The Hartree potential will take the form

$$v_H(r) = \frac{3}{R} - \frac{r^2}{R^3}, \quad \text{if } r \leq R, \quad (32)$$

and $v_H(r) = 2/r$ if $r \geq R$. The Hartree energy will be equal to $12/(5R)$. Substituting the above result into equation (8) we get that the Hartree-Fock energy will be

$$E^{(0)}_{HF} \approx (3\gamma)^{2/3}. \quad (33)$$

Substituting the result for the Hartree energy into equation (11) we find that in this limit the Kohn-Sham energy will be equal to

$$E^{(0)}_{KS} \approx \gamma^2/3(6^{3/2} + 2c_x/(5(4\pi)^{1/3})). \quad (34)$$

Again, we can use interpolation schemes like the one of equation (26), for the HF ground-state energy we will have

$$E^{(\text{int})}_{HF}(\gamma) \approx \frac{(3\gamma)^{2/3} + \gamma^2[3\gamma + (2\gamma/\pi)^{1/2}]}{1 + \gamma^2}. \quad (35)$$

In the Kohn-Sham case we can write down

$$E^{(\text{int})}_{KS}(\gamma) \approx \frac{\gamma^{2/3}[6^{3/2} + 2c_x/5/(4\pi)^{1/3}] + \gamma^2[3\gamma + (2^{3/2} + 3 \gamma^{1/3} 3^{1/2} 2c_x/4)(\gamma/\pi)^{1/2}]}{1 + \gamma^2}. \quad (36)$$
Comparing the asymptotics of the exact equation for the ground-state in the strong confinement limit with the asymptotics of the HF equation, we observe that they coincide. In the Kohn-Sham case the zeroth order is the same, but the coefficient of the first order perturbation is slightly higher (1.62 compared to the exact $\sqrt{2} \approx 1.41$). In the low density limit (weak confinement), although the three asymptotes are proportional to $\gamma^{2/3}$ in the zeroth order, the coefficients differ substantially; the exact is 1.19, the HF 2.08, and the KS 3.17. This indicates a consistent overestimation of the energy by the independent-electron approximations, which is the expected behavior at least for the HF approximation. Our findings for this system for the weak and strong asymptotae, and the numerical results, suggest that KS-LDA energies are always higher than the HF ones, which is consistent with numerical experience on atoms and molecules [14]. From the results shown in table 1 we can estimate the correlation energies for the ground-state for different confinement strengths: for $\gamma' = 0.1$, the correlation energy is about 5.6% of the total energy, meanwhile for $\gamma' = 0.9$ (strong confinement) it is about 0.17% (for the lightest many-electron atom, Helium, it is about 1.4%, and for Argon with $Z = 18$, it is only 0.14%). This adds evidence to the suggestion that for harmonic fields correlation effects are more important, also in three dimensions, especially for weak confinement.

IV. CONCLUDING REMARKS

In the present article we have calculated the energy spectrum of a two-electron spherical quantum dot for the few lowest states, using the shifted-1/N method and the very accurate numerical Schwartz’s method. From the comparison of the numerical results we could assess the quality of the shifted-1/N method, which consistently underestimates the correct values, although the error is rather small, and it decreases with the increase of the relative angular momentum. We have also applied perturbation theory up to first order in both limits of confinement of the electron, and we have proposed some interpolation formulae for the energy. Inclusion of first order perturbation allowed to construct an interpolation expression that performs reasonably well. We also solved the mean-field Hartree-Fock and local-density Kohn-Sham problems for the ground-state. Using the shifted-1/N method we got from reasonable to high accuracy already in the first iteration, compared to the self-consistent numeric solution using the Schwartz’s method. We made an analysis of the strong and weak confinement limits, and proposed interpolation formulae for both the Hartree-Fock and Kohn-Sham ground-state energies. It was shown that the correlation energy is relatively big for this systems, especially for weak confinement.

V. ACKNOWLEDGMENTS

One of the authors (V.M.V.) would like to acknowledge support by CONICIT, Venezuela, under project 96000061.
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FIG. 1. Relative error ($\delta E = (E_{1/N}/E_{\text{exact}} - 1) \times 100$) of the energy of the relative motion for the lowest energy states for $l = 0, 1,$ and $2$ calculated with the $1/N$ method, as a function of the reduced frequency $\gamma' = \gamma/\gamma + 1$. 
FIG. 2. Total energy as a function of $\gamma' = \gamma/(\gamma + 1)$ for the few lowest energy states. $0S$, and $0P$ depict the lowest energy states for the centre-of-mass motion for $L = 0$, and 1, respectively, and $0s, 0p$, and $0d$ the lowest energy states for the relative motion for $l = 0, 1$, and 2, respectively. The inset shows a magnification for small $\gamma'$. 
| $\gamma'$ | $HF - 1/N$ | $HF – num$ | $KS - 1/N$ | $KS – num$ | $Exact - 1/N$ | $Exact – num$ |
|-------|-----------|----------|-----------|---------|-------------|-------------|
| 0.1   | 0.5666    | 0.5768   | 0.5960    | 0.6082  | 0.5443      | 0.54606     |
| 0.2   | 1.1163    | 1.1241   | 1.1644    | 1.1742  | 1.0858      | 1.08926     |
| 0.3   | 1.7758    | 1.7826   | 1.8408    | 1.8503  | 1.7398      | 1.74478     |
| 0.4   | 2.6200    | 2.6255   | 2.7029    | 2.7118  | 2.5791      | 2.58569     |
| 0.5   | 3.7673    | 3.7717   | 3.8711    | 3.8791  | 3.7217      | 3.73012     |
| 0.6   | 5.4477    | 5.4508   | 5.5775    | 5.5842  | 5.3972      | 5.40775     |
| 0.7   | 8.1906    | 8.1922   | 8.3558    | 8.3608  | 8.1345      | 8.14778     |
| 0.8   | 13.5693   | 13.5693  | 13.7902   | 13.7928 | 13.5057     | 13.5232     |
| 0.9   | 29.3703   | 29.3679  | 29.7094   | 29.7082 | 29.2930     | 29.3194     |

TABLE I. Three-dimensional two-electron quantum dot total energy, using the Hartree-Fock ($HF$), Kohn-Sham ($KS$), and exact Schrödinger ($Exact$) equations for selected values of the reduced confinement constant ($\gamma'$), calculated using the shifted-$1/N$ (1/N), and Schwartz’s numeric (num) methods.