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Fourier transform technique in variational treatment of two-electron parabolic quantum dot*

S. Şakiroğlu[a)†], A. Yıldız[a)], Ü. Doğan[a)], K. Akgüngör[a)], H. Epik[a)], Y. Ergün[b)], H. Sarı[c)] and İ. Sökmen[a)]

[a)] *Physics Department, Dokuz Eylül University, Buca - İzmir* 35160, *Turkey*
[b)] *Physics Department, Anadolu University, Eskişehir* 26470, *Turkey*
[c)] *Physics Department, Cumhuriyet University, Sivas* 58140, *Turkey*

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In this work, we propose an efficient method of reducing the computational effort of variational calculation with a Hylleraas-like trial wavefunction. The method consists of introducing integral transforms for the terms as $r_{12}^k \exp(-\lambda r_{12})$ which provide the calculation of the expectation value of energy and the relevant matrix elements to be done analytically over single-electron coordinates instead of Hylleraas coordinates. We have used this method to calculate the ground state energy of a two-electron system in a spherical dot and a disk-like quantum dot separately. Under parabolic confinement potential and within effective mass approximation size and shape effects of quantum dots on the ground state energy of two electrons have been investigated. The calculation shows that our results even with a small number of basis states are in good agreement with previous theoretical results.

Keywords: two-electron quantum dot, parabolic confinement, variational method, Hylleraas coordinates
PACC: 7115P, 7320D

1. Introduction

The progress in nanofabrication technology makes it possible to fabricate low-dimensional nanostructures with controllable chemical composition and geometric structure. Quantum dots (QDs) and quasi-zero-dimensional systems, have nanostructures where the strong confinement is imposed in all three spatial dimensions.[1] In these systems, a finite number of electrons are confined in a small spatial region whose size is comparable with the de Broglie wavelength of carriers.[2−4] Due to the nanoscale extensions in all spatial dimensions, QDs possess discrete energy levels that can be tuned.[5] As a consequence of reduced dimensionality with design flexibility, the singular nature (δ-function-like) of the density of states, and the presence of several comparable energies and length scales, QDs show new physical phenomena quite different from those of their bulk counterparts.[6,7]

There is an increasing interest in this extremely fascinating field in the last two decades, which is aroused by the physical effects and potential novel device applications of QDs,[7] such as electronic memories, single-electron transistors, quantum dot lasers and ultrafast computers.[5,8] The capability of control over the properties of QDs in semiconductors has attracted great attention both for experimental[9−12] and theoretical studies.[1,13−21] Various theoretical approaches have been employed to study the energy spectra and the correlation effects of interacting electrons confined in QDs. Widely used methods include numerical diagonalization,[14,17,22] the variational method,[23−25] Monte Carlo simulations,[26,27] the shifted $1/N$ method,[1,8] the series expansion method[16] and the configuration interaction method.[28−30] Most of these theoretical studies have assumed the model electron confinement usually described by a parabolic potential due to the fact that the pronounced shell structure measured in the additional energy spectra of QDs is a direct consequence of it.[10,31,32]

Experimental investigations have allowed the characterization of the energy spectra of a few-electron QDs where interesting phenomena like singlet-triplet

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†Corresponding author. E-mail: serpil.sakiroglu@deu.edu.tr

transitions, charge quantization and the Coulomb blockade have been observed.[33,34] However, from a theoretical point of view these few-body systems represent a challenging problem. Inability of exact analytical solution of this problem leads the study to resort to numerical methods or approximation schemes.[35] However, a fully quantum mechanical treatment requires numerical calculations which could be computationally expensive and time-consuming as the number of electrons grows. The simplest example of a few-electron QDs is a system consisting of two electrons, interacting via Coulomb force, where carriers are trapped by a parabolic confinement potential. But an exact analytical solution of this two-electron problem is not attainable.[8] The insights provided by the studies of this minimal system may be the first step toward the understanding of the many fundamental properties of systems with a larger number of particles.

In the present paper, we introduce a computationally efficient approach to the variational treatment of ground state energy by means of the integral representations obtained for the terms like $r_{12}^k \exp(-\lambda r_{12})$. This approach provides the calculation of most of the integrals to be performed over single-particle coordinates instead of Hylleraas coordinates. To reveal the validity of our method, we calculate the ground state energy of a two-electron quantum dot confined by two-dimensional (2D) and three-dimensional (3D) isotropic harmonic potentials using the variational method with a Hylleraas-like trial wavefunction.

The rest of the present paper is organized as follows. In section 2, we briefly describe the formalism and method used for the variational calculation of the ground state energy of a two-electron system in a quantum dot. The results for the ground state energy are presented in section 3. Finally in section 4, we summarize the main conclusions of this work.

2. Theory and method

The effective mass Hamiltonian for an interacting pair of electrons confined in a quantum dot by a parabolic potential is given as

$$\hat{H} = \sum_{i=1}^{2} \left(-\frac{\hbar^2}{2m^*} \boldsymbol{\nabla}_i^2 + \frac{1}{2} m^* \omega_0^2 r_i^2 \right) + \frac{e^2}{4\pi\varepsilon r_{12}}. \quad (1)$$

Here ω_0 is the confining frequency and ε is the dielectric constant of the medium where the particles move. The locations of the first electron and the second electron, each with effective mass m^*, relative to the centre of a QD, are labeled by $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, respectively. $\boldsymbol{r}_{12}$ represents the interelectronic distance. For simplicity, the distortion of Coulomb interaction formed due to the difference in dielectric constant between a quantum dot and matrix material has been neglected.

In order to express the Hamiltonian in the dimensionless form, we define

$$a^* = \frac{4\pi\varepsilon\hbar^2}{m^* e^2} \quad \text{and} \quad l_0 = \sqrt{\frac{\hbar}{m^*\omega_0}}, \quad (2)$$

where a^* is the effective Bohr radius and l_0 is the characteristic length of a quantum dot. The effective Rydberg $\mathrm{Ry}^* = \hbar^2/2m^*a^*$ and the effective Bohr radius a^* are taken as the energy and the length scales, respectively. The introduced dimensionless parameter $W = 2\,(a^*/l_0)^2$ describes the relative magnitude of the confinement energy and Coulombic energy scales. $W^{-1/2}$ is related to the confinement region of electrons in a QD which later will be used to investigate quantum size effects. Upon the definitions introduced above, a dimensionless Hamiltonian of a parabolic quantum dot with two electrons is written as

$$\hat{H} = \sum_{i=1}^{2} \left(-\boldsymbol{\nabla}_i^2 + \frac{1}{4} W^2 r_i^2 \right) + \frac{2}{r_{12}}. \quad (3)$$

The Hamiltonian (3) includes six independent spherical coordinates. Using a coordinate system which explicitly includes r_{12} interelectronic distance renders it possible to treat the electron-electron correlation effects. In a Hylleraas coordinate system six degrees of freedom are arranged into two groups named 'inner' and 'outer' groups. Outer coordinates are chosen as Euler angles whereas inner coordinates are r_1, r_2 and r_{12}. Taking away Euler angles reduces Schrödinger's equation to the form including only inner coordinates.[36,37] Due to the spherical symmetry of the system, the complete description of the S-states can be performed by these inner coordinates.

One of the most important points in the variational studies on a two-electron system is to choose an appropriate wavefunction. In variational treatment of three-body Coulomb systems, functions expanded in terms of a generalized Hylleraas basis set are widely used.[38] The built-in correlated characteristics of these functions render it possible to ensure accurate energies for the ground state of two-electron and three-body molecular systems over relatively low

expansions. Having this in mind, our ansatz for a wavefunction describing the ground state of a two-electron QD confined by a parabolic potential is chosen to be in the form of

$$\Phi\left(r_1, r_2, r_{12}\right) = \sum_N C_N \, \Psi^N\left(r_1, r_2, r_{12}\right), \qquad (4)$$

where

$$\Psi^N\left(r_1, r_2, r_{12}\right) = \phi\left(r_1\right)\phi\left(r_2\right) \, \mathrm{e}^{-\lambda r_{12}} \, r_1^{n_1} \, r_2^{n_2} \, r_{12}^{n_{12}}. \qquad (5)$$

Basis function $\phi\left(r_i\right)$ has been chosen to be the solution of the non-interacting system in the form of

$$\phi\left(r_i\right) = \mathrm{e}^{-\gamma W r_i^2/2}, \quad (i = 1, 2). \qquad (6)$$

Here, γ and λ are adjustable variational parameters varied so as to minimize the expectation value of energy. Product $\phi\left(r_1\right)\phi\left(r_2\right)$ determines the ground state of the uncorrelated electron pair in parabolic confinement with strength W. The exponential term $\mathrm{e}^{-\lambda r_{12}}$, which determines the correlation between electrons, not only has physical meaning but also plays a crucial role in the perspective of this study. The main importance of this term is to yield the evaluation of integrals by means of integral representations obtained for the terms like $r_{12}^k \exp\left(-\lambda\, r_{12}\right)$. And finally, the $r_1^{n_1} \, r_2^{n_2} \, r_{12}^{n_{12}}$ product on the right-hand side of the expression is introduced in order to take into account the spatial correlations. The proposed wavefunction is spanned by $N \equiv \{n_1, n_2, n_{12}\}$, where integers, $n_i \, (i = 1, 2, 12)$, in the series expansion part of the wavefunction correspond to the powers of coordinates r_1, r_2 and r_{12}, respectively and are positive or equal to zero. For simplicity, in what follows we shall drop the (r_1, r_2, r_{12}) dependence of $\Psi^N\left(r_1, r_2, r_{12}\right)$.

Having the trial wavefunction (4), the standard energy eigenvalue problem arising out of Ritz's variational principle for the determination of the correlated basis Ψ_N takes the form

$$\boldsymbol{H}\,\boldsymbol{C} = E\,\boldsymbol{S}\,\boldsymbol{C}. \qquad (7)$$

Here $\boldsymbol{H}$ consists of a kinetic term, Coulomb interaction, and an interaction with confinement potential, $\boldsymbol{S}$ denotes the norm with respect to the basis function Ψ^N, and $\boldsymbol{C}$ represents the column matrix of $C_{n_1,n_2,n_{12}}$ coefficients.

Elements of $\boldsymbol{S}$ overlapping the matrix are given as

$$S_{M,N} = \left\langle \Psi^M \,\middle|\, \Psi^N \right\rangle = \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \, \Psi^{M^*} \, \Psi^N. \qquad (8)$$

In order to express the Hamiltonian of the system in Hylleraas coordinates we use the definition of vector operator del in Hylleraas-type coordinates as

$$\boldsymbol{\nabla}_i = \hat{r}_i \frac{\partial}{\partial r_i} + \sum_{j \neq i} \hat{r}_{ij} \frac{\partial}{\partial r_{ij}}. \qquad (9)$$

After a simple arrangement, the elements of the Hamiltonian matrix $\boldsymbol{H}$ can be evaluated as follows:

$$\begin{aligned}
H_{M,N} &= \left\langle \Psi^M \middle| \hat{H} \middle| \Psi^N \right\rangle \\
&= \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \left[\boldsymbol{\nabla}_{r_1} \Psi^{M^\star} \cdot \boldsymbol{\nabla}_{r_1} \Psi^N + \Psi^{M^\star} \frac{1}{4} W^2 r_1^2 \, \Psi^N \right] \\
&\quad + \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \frac{(r_1^2 - r_2^2 + r_{12}^2)}{2 r_1 r_{12}} \left(\frac{\partial \Psi^{M^\star}}{\partial r_1} \frac{\partial \Psi^N}{\partial r_{12}} + \frac{\partial \Psi^{M^\star}}{\partial r_{12}} \frac{\partial \Psi^N}{\partial r_1} \right) \\
&\quad + \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \left[\boldsymbol{\nabla}_{r_2} \Psi^{M^\star} \cdot \boldsymbol{\nabla}_{r_2} \Psi^N + \Psi^{M^\star} \frac{1}{4} W^2 r_2^2 \, \Psi^N \right] \\
&\quad + \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \frac{(r_2^2 - r_1^2 + r_{12}^2)}{2 r_2 r_{12}} \left(\frac{\partial \Psi^{M^\star}}{\partial r_2} \frac{\partial \Psi^N}{\partial r_{12}} + \frac{\partial \Psi^{M^\star}}{\partial r_{12}} \frac{\partial \Psi^N}{\partial r_2} \right) \\
&\quad + \iint \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_2 \left[2\, \boldsymbol{\nabla}_{r_{12}} \Psi^{M^\star} \cdot \boldsymbol{\nabla}_{r_{12}} + \Psi^{M^\star} \frac{2}{r_{12}} \left(r_{12}\right) \Psi^N \right]. \qquad (10)
\end{aligned}$$

The general procedure for the evaluation of integrals in matrix elements while working with wavefunctions

expressed in Hylleraas coordinates is to express integrals in the form of $I = \int F(r_1, r_2) f(r_{12}) \mathrm{d}^3 r_1 \mathrm{d}^3 r_2$ as[39]

$$I = 8\pi^2 \int F(r_1, r_2) r_1 \mathrm{d}r_1 r_2 \mathrm{d}r_2 \int_{|r_1 - r_2|}^{(r_1 + r_2)} f(r_{12}) r_{12} \mathrm{d}r_{12}.$$

In this work, unlike the general procedure mentioned above, the Fourier transforms have been used for the terms including interparticle distance r_{12}.

The Fourier transforms for a 3D quantum dot are defined as[40,41]

$$\frac{\mathrm{e}^{-\lambda r}}{r} = \frac{1}{2\pi^2} \int \frac{\mathrm{e}^{\mathrm{i}\, \boldsymbol{q}\cdot\boldsymbol{r}}}{(\lambda^2 + q^2)} \mathrm{d}\boldsymbol{p} \tag{11}$$

and

$$\frac{1}{r_{12}} = \frac{1}{2\pi^2} \int \frac{\mathrm{e}^{\mathrm{i}\, \boldsymbol{R}\cdot(\boldsymbol{r}_1 - \boldsymbol{r}_2)}}{R^2} \mathrm{d}\boldsymbol{R}. \tag{12}$$

Utilization of these transforms leads to the general integral representations for the terms in the form of $r_{12}^k \exp(-\lambda r_{12})$, ($k \in \mathbb{Z}$ and λ is a parameter), thereby avoiding the use of a general integration technique for Hylleraas coordinates. The obtained integral representations are[42,43]

$$\int \mathrm{d}\Omega_1 \int \mathrm{d}\Omega_2 \ \mathrm{e}^{-\lambda r_{12}} \ r_{12}^{(p-1)} = 32\pi \int_0^\infty \mathrm{d}q \ \frac{\sin(qr_1)}{r_1} \ \frac{\sin(qr_2)}{r_2} \ Q_{3\mathrm{D}}[q, \lambda, p] \tag{13}$$

where

$$Q_{3\mathrm{D}}[q, \lambda, p] = (-1)^p \frac{\partial^p}{\partial \lambda^p} \left[\frac{1}{(q^2 + \lambda^2)} \right] \quad p = 0, 1, 2, \ldots,$$

and Ω_i, ($i = 1, 2$) are solid angles each describing spatial orientation of an electron. Since these integral representations separate coordinates of the electrons from each other, the integrations over r_1 and r_2 in expressions (8) and (10) lead to the integrals in similar form for each electron. These separated integrals, named $G_{3\mathrm{D}}$, are calculated analytically and have the general form in terms of hypergeometric ($_1\mathrm{F}_1$) and gamma (Γ) functions as

$$G_{3\mathrm{D}}(q, \gamma, W, m, n, k) = \frac{1}{2} q (W\gamma)^{\frac{1}{2}(-k-m-n-2)} \Gamma\left(\frac{1}{2}(k + m + n + 2) \right) \times \ {}_1\mathrm{F}_1 \left(\frac{1}{2}(k + m + n + 2); \frac{3}{2}; -\frac{q^2}{4W\gamma} \right). \tag{14}$$

Initially, integrations over r_1 and r_2 coordinates are performed analytically for H_{MN} and S_{MN}, then the numerical procedure is applied to the integrations over the q variable introduced in integral (13).

Under these definitions, integral (13) and expression (14), the elements of the $\boldsymbol{S}$ matrix for the 3D case are obtained according to the expression given below:

$$S_{M,N}^{3\mathrm{D}} = 32\pi \int_0^\infty \mathrm{d}q \, Q_{3\mathrm{D}}(q, 2\lambda, m_{12} + n_{12} + 1) \times \ G_{3\mathrm{D}}(q, \gamma, W, m_1, n_1, 1) G_{3\mathrm{D}}(q, \gamma, W, m_2, n_2, 1). \tag{15}$$

By using the lengthly definitions of A_{nd}, B_{nd}, C_{nd} and D_{nd} given in the appendix, the elements of the $\boldsymbol{H}$ matrix are calculated as follows:

$$H_{M,N}^{3\mathrm{D}} = 32\pi \int_0^\infty \mathrm{d}q \ [Q_{3\mathrm{D}}(q, 2\lambda, m_{12} + n_{12} - 1) A_{3\mathrm{D}} + Q_{3\mathrm{D}}(q, 2\lambda, m_{12} + n_{12}) B_{3\mathrm{D}} + Q_{3\mathrm{D}}(q, 2\lambda, m_{12} + n_{12} + 1) C_{3\mathrm{D}} + Q_{3\mathrm{D}}(q, 2\lambda, m_{12} + n_{12} + 2) D_{3\mathrm{D}}]. \tag{16}$$

A procedure similar to the Fourier transforms in the 3D case can be applied to a 2D disk-like QD. Using the definition for the 2D case

$$\frac{\mathrm{e}^{-\lambda r}}{r} = \frac{1}{(2\pi)} \int_0^\infty \mathrm{d}\boldsymbol{q} \frac{\mathrm{e}^{\mathrm{i}\,\boldsymbol{q}\cdot\boldsymbol{r}}}{\sqrt{q^2+\lambda^2}} \tag{17}$$

yields

$$\int_0^\infty \mathrm{d}\theta_1 \int_0^\infty \mathrm{d}\theta_2 . \mathrm{e}^{-\lambda r_{12}} r_{12}^{(p-1)} = (2\pi)^2 \int_0^\infty \mathrm{d}q\, q\, \mathrm{J}_0(qr_1)\, \mathrm{J}_0(qr_2) Q_{2\mathrm{D}}[q,\lambda,p] \tag{18}$$

where

$$Q_{2\mathrm{D}}[q,\lambda,p] = (-1)^p \frac{\partial^p}{\partial\lambda^p}\left[\frac{1}{\sqrt{q^2+\lambda^2}}\right] \quad p = 0,1,2,\ldots,$$

and J_0 is the Bessel function.[42,43] The analytical expression for the integrals in a similar form over the separated electron coordinates is found in terms of hypergeometric ${}_1\mathrm{F}_1$ and gamma (Γ) functions as follows:

$$\begin{aligned} G_{2\mathrm{D}}(q,\gamma,W,m,n,k) = {} & \frac{1}{2}(W\gamma)^{\frac{1}{2}(-k-m-n-1)} \Gamma\left(\frac{1}{2}(k+m+n+1)\right) \\ & \times {}_1\mathrm{F}_1\left(\frac{1}{2}(k+m+n+1); 1; -\frac{q^2}{4W\gamma}\right). \end{aligned} \tag{19}$$

Evaluation of the matrix elements in the 2D case is similar to the calculation in the 3D case. Using the definitions for A_{nd}, B_{nd}, C_{nd} and D_{nd} given in the appendix, the matrix elements of $\boldsymbol{S}$ and $\boldsymbol{H}$ for the 2D case are

$$\begin{aligned} S^{2\mathrm{D}}_{M,N} = {} & (2\pi)^2 \int_0^\infty q\,\mathrm{d}q\, Q_{2\mathrm{D}}(q, 2\lambda, m_{12}+n_{12}+1) \\ & \times G_{2\mathrm{D}}(q,\gamma,W,m_1,n_1,1) G_{2\mathrm{D}}(q,\gamma,W,m_2,n_2,1), \end{aligned} \tag{20}$$

$$\begin{aligned} H^{2\mathrm{D}}_{M,N} = {} & (2\pi)^2 \int_0^\infty q\,\mathrm{d}q\, [Q_{2\mathrm{D}}(q,2\lambda,m_{12}+n_{12}-1)A_{2\mathrm{D}} + Q_{2\mathrm{D}}(q,2\lambda,m_{12}+n_{12})B_{2\mathrm{D}} \\ & + Q_{2\mathrm{D}}(q,2\lambda,m_{12}+n_{12}+1)C_{2\mathrm{D}} + Q_{2\mathrm{D}}(q,2\lambda,m_{12}+n_{12}+2)D_{2\mathrm{D}}]. \end{aligned} \tag{21}$$

3. Results and discussion

We have performed calculations for the ground state energy of a two-electron system in a parabolic quantum dot by means of a Hylleraas-like wavefunction in expression (4), which spans powers of $\{n_1, n_2, n_{12}\}$ for the corresponding coordinates r_1, r_2 and r_{12} and commensurate with the condition $(n_1+n_2+n_{12}) \leq 6$. Due to the built-in correlated characteristic of the wavefunction, relatively low expansions are sufficient to ensure a good accuracy without lengthening calculation time. We have calculated the ground state energies for the strengths of dimensionless parameter W between 0.05 and 60.0, which describes the relative magnitude of the confinement energy and Coulombic energy scales. Also the effects of parabolic confinement for the different quantum dot shapes (3D spherical and 2D disk-like) have been investigated.

In figure 1 we present our variational calculation results for the ground state energy of two electrons in 2D and 3D parabolic quantum dots. In order to show the quantum-size effects and compare them with the previous results, we have plotted energies normalized by W as a function of $W^{-1/2}$.

The prominent feature of the variational parameters for the 2D QD is that in the weak confinement region, the λ parameter takes the same value 0.01, whereas the γ changes in a range of 0.33–0.48. For the intermediate and the strong regimes the situation is opposite, i.e. γ takes the same value 0.5, whereas the parameter λ varies in the range 0.01–0.56. A similar situation is observed also for the 3D system. In the weak confinement regime, λ is fixed to be 0.01 whereas the range for the γ is 0.40–0.50. When the value of W increases from 1.0 to 60.0, the γ is fixed to be 0.5 though λ varies in a range of 0.02–0.40. The values of the parameters γ and λ versus confinement strength

W are presented in table 1. Another important indication of the calculation is that for the intermediate and the strong confinement cases, the convergencies are achieved for the small number of expansions both for the 2D and 3D QDs.

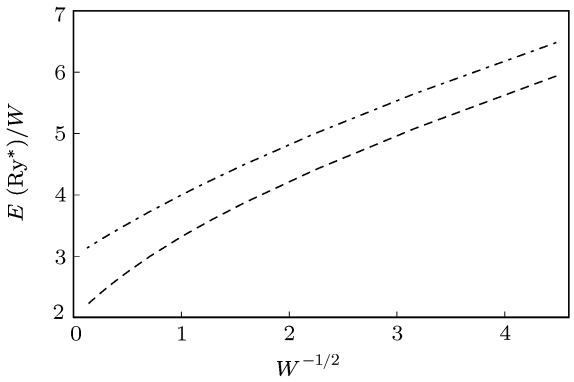


Fig.1. Ground state energy, E, normalized by W, as a function of $W^{-1/2}$, where the dashed curve represents the results of the 2D system while the dot-dashed curve describes the results of the 3D system.

Figure 1 shows that the qualitative properties of the ground state energy level for the 2D and 3D systems, i.e., the variation of ground state energy with the confinement region of the system, are similar. However, the quantitative differences are also discernable: the normalized ground state energies for the two electrons in a 2D QD are located slightly below the corresponding energies for those in a 3D QD. This is due to the enhanced effective confinement of electrons in the 2D nanostructure. Also the energies dramatically changes as the $W^{-1/2}$ changes from 0 to 4.4721. It means that the ground state energy depends not only on the dot size but also on the dot shape. Adamowski *et al*[19] studied two electrons confined in 2D and 3D quantum dots under the assumption of the Gaussian confining potential and its parabolic approximation. They needed 55 basis elements in a trial wavefunction which explicitly included interparticle distance to achieve the required accuracy. In order to investigate the energy spectra of two electrons in a 2D harmonic QD, Merkt *et al*[13] applied the numerical diagonalization by using a two-particle wavefunction. They reported that with fixing angular momentum, a matrix of size 50×50 is needed to obtain convergent eigenenergy. It is readily seen that our results, obtained with a relatively low number of expansions, are in good agreement with those in Refs.[13], [16] and [44]. This indicates that the chosen trial wavefunction (4) is suitable to accurately describe two-electron states confined in parabolic QDs.

To demonstrate the efficacy of our method with respect to the QD dimensionality and to investigate the details of size effect, it is interesting to study the electron-electron interaction energy, $E_{\mathrm{e-e}} = \langle 2/r_{12} \rangle$. The electron-electron interaction energy, calculated at a particular confinement frequency W, may be obtained simply by extracting out the energies of noninteracting electrons in the parabolic potential from the total energy of the system.

Figure 2 shows the behaviours of the Coulomb energy of the ground state for the two-electron system in a spherical and disk-like QDs as W increases. Figure 2 also indicates that the Coulomb energy is in good agreement with the energies predicted by the calculations in references [16], [18] and [44].

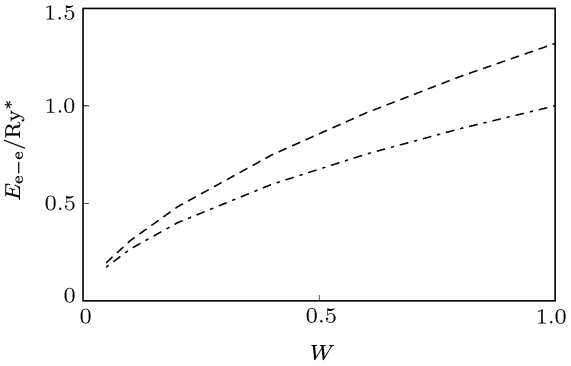


Fig.2. Comparisons between the dependences of electron-electron interaction energy, $E_{\mathrm{e-e}}$, on W for 2D and 3D quantum dots. The dashed curve indicates the two-electron system in the 2D case while the dot-dash curve shows the 3D system.

We show comparisons of the ground state energies as well as the Coulomb energies at various confinement strengths of two electrons in 2D QDs with those in 3D QDs in table 1. It is important to pay attention to the results for $W = 0.05$ and $W = 1.0$ that are frequently given in the literature. The case, $W = 1.0$ is an intermediate regime where neither the confinement energy nor the Coulombic energy scale dominates the other, whereas the case $W = 0.05$, is the weak confinement regime. For both cases our results are in good agreement with the cited results given in table 1. In addition, as the confinement strength strongly increases, i.e. $W \to \infty$ ($W^{-1/2} \to 0$), the energy values approach the exact harmonic oscillator energies: $E/W = 2.0$ and 3.0, in 2D and 3D, respectively. Thus we can say that our method and variational wavefunction are applicable to the entire range of W. Another important conclusion seen from table 1 is that the energies are enhanced as the dimensionality of the quantum dot increases.

Table 1. Electron-electron interaction energies calculated by using the wavefunction given in expression (4) compared with results given in the literature. Energies are in units of effective Rydbergs, Ry*.

2D					3D			
W	γ	λ	E	$E_{\mathrm{e-e}}$	γ	λ	E	$E_{\mathrm{e-e}}$
0.05	0.33	0.01	0.2966[a]	0.1966[a]	0.40	0.01	0.3239[a]	0.1739[a]
			0.2952[b]	0.1951[b]				0.1732[b]
			0.2962[c]					
0.1	0.38	0.01	0.5082[a]	0.3082[a]	0.43	0.01	0.5650[a]	0.2650[a]
				0.3048[b]				0.2634[b]
0.2	0.42	0.01	0.8816[a]	0.4816[a]	0.46	0.01	1.0000[a]	0.4000[a]
				0.4732[b]				0.3969[b]
0.4	0.45	0.01	1.5479[a]	0.7479[a]	0.48	0.01	1.7975[a]	0.5975[a]
				0.7290[b]				0.5921[b]
0.6	0.47	0.01	2.1637[a]	0.9637[a]	0.49	0.01	2.5521[a]	0.7521[a]
				0.9345[b]				0.7447[b]
0.8	0.48	0.01	2.7511[a]	1.1511[a]	0.50	0.01	3.2835[a]	0.8835[a]
1.0	0.49	0.01	3.3195[a]	1.3195[a]	0.50	0.02	4.0000[a]	1.0000[a]
			3.2703[b]	1.2715[b]			3.9896[b]	0.9896[b]
			3.3196[c]					
2.0	0.50	0.01	6.0000[a]	2.0000[a]	0.50	0.04	7.4602[a]	1.4602[a]
4.0	0.50	0.06	10.9930[a]	2.9930[a]	0.50	0.08	14.1157[a]	2.1157[a]
6.0	0.50	0.11	15.7675[a]	3.7675[a]	0.50	0.12	20.6204[a]	2.6204[a]
8.0	0.50	0.15	20.4252[a]	4.4252[a]	0.50	0.15	27.0464[a]	3.0464[a]
10.0	0.50	0.18	25.0071[a]	5.0071[a]	0.50	0.17	33.4220[a]	3.4220[a]
			24.744[b]				33.385[b]	
20.0	0.50	0.31	47.3033[a]	7.3033[a]	0.50	0.25	64.8973[a]	4.8973[a]
40.0	0.50	0.45	90.5677[a]	10.5677[a]	0.50	0.34	126.9856[a]	6.9856[a]
60.0	0.50	0.56	133.0785[a]	13.0785[a]	0.50	0.40	188.5886[a]	8.5886[a]

[a] Present work, [b] Ref.[44], [c] Ref.[16].

4. Conclusion

In this paper we introduce the integral representations for the terms as $r_{12}^k \exp(-\lambda r_{12})$ and calculate variationally the ground state energies of two electrons in 2D and 3D parabolic QDs by using a Hylleraas-like trial wavefunction. The structure of the present variational wavefunction, expression (4), facilitates the calculation of most of the integrations in matrix elements to be done analytically, without time-consuming numerical calculations. This process has been performed by successive use of the integral representations in expression (13) and integral (18).[42,43] An inevitable numerical procedure has been invoked at the last stage of the calculations. In the present work, to ensure the validity of our method, size and shape effects of a quantum dot on the ground state energy are investigated. The use of an explicitly correlated Hylleraas-like basis with relatively low expansions, allows the ground state energy, within a reasonable accuracy, to be calculated. Calculations for the two-electron system in 2D and 3D QDs lead to qualitatively similar but quantitatively different results for the ground state energies as well as electron-electron energies as expected. A comparison between our results and the previous theoretical results as mentioned in section 3 indicates that they are in good agreement with each other in ground state energy, confirming that the chosen trial wavefunction (4) and

the method presented in this work accurately describe the ground state of two-electron in a parabolic quantum dot.

Appendix

If the subscript nd indicates the dimension of space, 2D or 3D, definitions used for the calculation of the elements of matrix $\boldsymbol{H}$ are given below:

$$\begin{aligned} A_{nd} = \frac{1}{2} \big(& - \left(m_2 n_{12} + m_{12} n_2\right) G_{nd}(q,\gamma,W,m_1,n_1,3) G_{nd}(q,\gamma,W,m_2,n_2,-1) \\ & + \left(\left(m_1+m_2\right) n_{12} + m_{12}\left(n_1 + 4\,n_{12} + n_2\right)\right) \\ & \times G_{nd}(q,\gamma,W,m_1,n_1,1) G_{nd}(q,\gamma,W,m_2,n_2,1) \\ & - \left(m_{12} n_1 + m_1 n_{12}\right) G_{nd}(q,\gamma,W,m_1,n_1,-1) G_{nd}(q,\gamma,W,m_2,n_2,3)\big)\,, \end{aligned} \tag{A1}$$

$$\begin{aligned} B_{nd} = \frac{1}{2} \big(& \left(m_2 + n_2\right) \lambda G_{nd}(q,\gamma,W,m_1,n_1,3) G_{nd}(q,\gamma,W,m_2,n_2,-1) \\ & - \left(-4 + \left(m_1 + 4\,m_{12} + m_2 + n_1 + 4\,n_{12} + n_2\right)\lambda\right) \\ & \times G_{nd}(q,\gamma,W,m_1,n_1,1) G_{nd}(q,\gamma,W,m_2,n_2,1) \\ & + \left(m_1 + n_1\right) \lambda G_{nd}(q,\gamma,W,m_1,n_1,-1) G_{nd}(q,\gamma,W,m_2,n_2,3)\big)\,, \end{aligned} \tag{A2}$$

$$\begin{aligned} C_{nd} = \frac{1}{4} \big(& \left(2\left(m_{12} n_1 + m_1\left(2\,n_1 + n_{12}\right)\right) G_{nd}(q,\gamma,W,m_1,n_1,-1)\right. \\ & \left. + W^2\left(1 + 4\,\gamma^2\right) G_{nd}(q,\gamma,W,m_1,n_1,3)\right) \\ & \times G_{nd}(q,\gamma,W,m_2,n_2,1) + G_{nd}(q,\gamma,W,m_1,n_1,1) \\ & \times \left(2\left(m_{12} n_2 + m_2\left(n_{12} + 2\,n_2\right)\right) G_{nd}(q,\gamma,W,m_2,n_2,-1)\right. \\ & - 4\left(\left(m_1 + m_{12} + m_2 + n_1 + n_{12} + n_2\right) W\gamma - 2\,\lambda^2\right) G_{nd}(q,\gamma,W,m_2,n_2,1) \\ & \left. + W^2\left(1 + 4\,\gamma^2\right) G_{nd}(q,\gamma,W,m_2,n_2,3)\right)\big)\,, \end{aligned} \tag{A3}$$

$$\begin{aligned} D_{nd} = -\frac{1}{2}\lambda \big(& \left(m_1 + n_1\right) G_{nd}(q,\gamma,W,m_1,n_1,-1) G_{nd}(q,\gamma,W,m_2,n_2,1) \\ & + G_{nd}(q,\gamma,W,m_1,n_1,1)\left(\left(m_2 + n_2\right) G_{nd}(q,\gamma,W,m_2,n_2,-1)\right. \\ & \left. - 4\,W\,\gamma\, G_{nd}(q,\gamma,W,m_2,n_2,1)\right)\big)\,. \end{aligned} \tag{A4}$$

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