Ground state of two-dimensional quantum-dot helium in zero magnetic field: Perturbation, diagonalization, and variational theory

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We study the ground-state properties of two-dimensional quantum-dot helium in zero external magnetic field (a system of two interacting electrons in a two-dimensional parabolic confinement potential) by using perturbation and variational theory. We introduce a family of ground-state trial wave functions with one, two, and three variational parameters. We compare the perturbation and variational energies with numerically exact diagonalization results and earlier unrestricted Hartree-Fock studies. We find that the three-parameter variational wave function is an excellent representation of the true ground state and argue on how to generalize such a wave function for larger quantum dots with arbitrary numbers of electrons.

I. INTRODUCTION

Semiconductor quantum dots are generally fabricated by applying a lateral confining potential to a two-dimensional (2D) electron system.[1–6] In these systems, the electrons move in a plane in a lateral confinement potential. The relative strength of electron-electron and electron-confinement interaction can be experimentally tuned over a wide range resulting in a peculiar electronic system with tunable physical properties. For this reason, quantum dots are sometimes refered to as "artificial atoms." In a typical quantum dot, all electrons are tightly bound, except for a few free electrons. Such artificial atoms are of immense technological value because they form the building units of larger structures. Quantum dots can contain anything from a single electron to a collection of thousands of electrons and much of the parameters that describe a quantum dot can be precisely controlled by conventional nanofabrication methods. Quantum dots are realized in several ways. One example is a quantum dot array in which the potential well at the interface is populated with very few electrons. Another example is one where a charge coupled device array operated under deep depletion may have only a few electrons in the potential well under the gate.

The standard theoretical model of a quantum dot includes the following approximations. First, the motion of the electrons is considered to be exactly 2D. Second, the confining potential is taken to be parabolic, and third the interaction between electrons is considered to be a pure Coulomb interaction. In absence of an external magnetic field, the Hamiltonian for N electrons interacting in a quantum dot is

$$\hat{H} = \sum_{i=1}^{N} \left[\frac{\hat{p}_i^2}{2m} + \frac{m}{2} \omega^2 \rho_i^2 \right] + \sum_{i>j}^{N} \frac{e^2}{|\vec{\rho}_i - \vec{\rho}_j|}, \quad (1)$$

where $\hat{\vec{p}}_i = (\hat{p}_{ix}, \hat{p}_{iy})$ and $\vec{\rho}_i = (x_i, y_i)$ are, respectively, the 2D momentum operator and position of the ith electron, m is the electron's mass, ω is the angular frequency of the parabolic

confining potential, and e is the electron's charge.

Most of the initial theoretical studies on quantum dots were done in the strong magnetic field's regime with all electrons being fully spin polarized. The goal was to study the crossover regime between microscopic quantum dots and macroscopic 2D electronic systems (2DES) of the fractional quantum Hall type.[7–10] However, in recent years, there has been a surge of interest in theoretical studies of quantum dots in zero magnetic field,[11–15] with the main focus on the Fermi-liquid–Wigner-solid crossover regime, a problem closely related with the nature of metal-insulator transition in 2D.[16] Among the variety of theoretical methods used to study quantum dots we could mention a few such as analytical calculations,[17–20] exact numerical diagonalizations,[21–27] quantum Monte Carlo (QMC) methods,[28–31] as well as density functional theory methods.[32–36]

The simplest quantum dot system consists of two electrons ($N=2$) confined in a 2D parabolic potential in zero magnetic field. The electrons repel each other with a Coulomb potential and the Hamiltonian of the system is

$$\hat{H}(\vec{\rho}_1, \vec{\rho}_2) = \frac{\hat{p}_1^2}{2m} + \frac{m}{2} \omega^2 \rho_1^2 + \frac{\hat{p}_2^2}{2m} + \frac{m}{2} \omega^2 \rho_2^2 + \frac{e^2}{|\vec{\rho}_1 - \vec{\rho}_2|}. \quad (2)$$

Because of the analogy of the system to that of helium atom (although, strictly speaking, the quantum dot is 2D, and the true helium atom is not) this system is called quantum-dot helium. It is well known that, because of the Coulomb interaction, no exact analytical solutions can be obtained for the energy spectra of an arbitrary N-electron parabolic quantum dot in zero magnetic field. However, in some cases, such as $N=2$ quantum-dot helium, exact numerical diagonalizations[22] provide useful input.

Among different quantities describing a quantum dot, the study of the ground-state properties is of fundamental importance, therefore we focus our main interest on the ground-state wave function and the ground-state energy. Even in the case of 2D quantum-dot helium in zero magnetic field, an

exact analytic solution of the problem is not available, therefore most of the methods used so far, rely on approximations or numerical calculations that some time differ considerably with each other.

So far, the variational treatment of 2D quantum-dot helium in presence of a magnetic field considers a wave function written as the product of a Laughlin-type wave function with a Jastrow factor

$$\Psi = J(\rho_{12}) \times (z_1 - z_2)^{|m_z|} \exp\left(-\frac{|z_1|^2 + |z_2|^2}{2l^2}\right), \quad (3)$$

where $J(\rho_{12})$ is the Jastrow factor, $z_j = x_j - iy_j$ is the 2D position in complex notation, $j = 1, 2$, and $|m_z| = 0, 1, \ldots$, is the angular momentum. In presence of an applied magnetic field in the z direction B_z we have $l = \sqrt{\hbar/(m\Omega)}$ and $\Omega^2 = \omega^2 + (\omega_c/2)^2$, where $\omega_c = eB_z/m$ is the cyclotron frequency. The only types of Jastrow factors used in the literature that we are aware of have the form $J(\rho_{ij}) \propto \exp[a\rho_{ij}/(1 + b\rho_{ij})]$, where a and b are two variational parameters,[37] a generalized version of the above form used by Pederiva *et al.*,[38] or a simpler version $J(\rho_{ij}) = 1$ used by Bolton.[29] The common property of the above Jastrow factors is that they can reproduce the many body wave function very well under a magnetic field. However, we argue that in the limit of zero magnetic field, none of the above choices represents the ground state very well. Relying on the well-known fact[29] that, in zero magnetic field, the ground state has zero angular momentum, we point out that the wave function of Eq. (3) with the above choices of Jastrow factors is no longer the very best description of the true ground state, therefore alternative scenarios need be considered. At this point we also want to mention that there are still controversies for the selection of Jastrow factors, as discussed in Ref. 29, and more recently in Ref. 38. The main motivation of the present work is to identify and demonstrate that a variational wave function with a type of Jastrow factor different from those previously considered in the literature constitutes the best choice to describe the ground state of this system.

In this work, we study the ground-state properties of 2D quantum-dot helium in zero external magnetic field by using perturbation and variational theory. Although approximative in nature, the two approaches will serve as a testing ground to build high-quality trial wave functions for quantum dot systems with arbitrary number N of electrons.

Given that a good variational wave function itself can be an excellent approximation to the true exact ground state, there is always a need to find better, yet simple enough ways to accurately describe such complicated systems as the quantum dots. After a systematic study of the ground-state properties of 2D quantum-dot helium by using perturbation and variational theory, we succesfully identify a class of trial wave functions with three variational parameters that is indeed an excellent representation of the true ground state as shown from a comparison of variational energies to respective values obtained from an exact numerical diagonalization calculation.

In Sec. II we briefly introduce the formalism and describe the single-particle states for an electron in a 2D parabolic confinement potential with no magnetic field. In Sec. III we present the results of first order perturbation theory. In Sec. IV we numerically solve the problem using exact diagonalization techniques. In Sec. V we present the results obtained with a one-parameter, two-parameter, and a three-parameter variational wave function, the last one shown to be a very good representation of the true ground state. A discussion of results and concluding remarks can be found in Sec. VI.

II. SINGLE-PARTICLE STATES

The problem of a single electron in a 2D parabolic confinement potential with no magnetic field is exactly solvable. In polar coordinates, the Hamiltonian is written as

$$\hat{H}(\vec{\rho}) = \frac{\hat{p}_\rho^2}{2m} + \frac{\hat{L}_z^2}{2m\rho^2} + \frac{m}{2}\omega^2\rho^2, \quad (4)$$

where m is electron's mass, ω is the angular frequency of the 2D parabolic confinement potential, and

$$\hat{p}_\rho^2 = -\hbar^2 \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right), \quad \hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}, \quad (5)$$

where $\vec{\rho} = (x, y)$ and φ is the polar angle. The energy eigenvalues are labeled by the quantum numbers $n_\rho = 0, 1, \ldots$, and $m_z = 0, \pm 1, \pm 2, \ldots$, and are given by

$$E_{n_\rho m_z} = \hbar\omega(2n_\rho + |m_z| + 1). \quad (6)$$

The normalized eigenfunctions are

$$\Phi_{n_\rho m_z}(\rho, \varphi) = N_{n_\rho m_z} \frac{e^{im_z\varphi}}{\sqrt{2\pi}}(\alpha\rho)^{|m_z|} e^{-\alpha^2\rho^2/2} L_{n_\rho}^{|m_z|}(\alpha^2\rho^2), \quad (7)$$

where the functions $L_{n_\rho}^{|m_z|}(\alpha^2\rho^2)$ are associated Laguerre polynomials.[39] The normalization constant $N_{n_\rho m_z}$ and the parameter α (that has the dimensionality of an inverse length) are

$$N_{n_\rho m_z} = \sqrt{\frac{2n_\rho! \, \alpha^2}{(n_\rho + |m_z|)!}}, \quad \alpha = \sqrt{\frac{m\omega}{\hbar}}. \quad (8)$$

The ground-state wave function corresponds to $n_\rho = 0$ and $m_z = 0$ and is not degenerate:

$$\Phi_{00}(\rho, \varphi) = \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2\rho^2/2}. \quad (9)$$

A complete set of single-particle solutions of the problem is the product of the orbitals in Eq. (7) and the spin functions $\chi_{sm_s}(\sigma)$, where σ is the spin variable, $s = 1/2$ is the spin quantum number of the electron, and $m_s = \pm 1/2$ is the spin angular momentum quantum number. In absence of magnetic field, the energy eigenvalues do not depend on spin.

III. FIRST-ORDER PERTURBATION THEORY

If we were to ignore the Coulomb repulsion in Eq. (2), we would have a solution to the eigenvalue problem for the two-electron system, with eigenfunctions given by $\Phi_{n_{\rho_1} m_{z_1}}(\rho_1, \varphi_1)\Phi_{n_{\rho_2} m_{z_2}}(\rho_2, \varphi_2)$ and energy eigenvalues given

by $E = E_{n_{\rho_1} m_{z_1}} + E_{n_{\rho_2} m_{z_2}}$. In this idealized model, the ground-state energy is $E = 2\hbar\omega$. Since the electrons are identical fermions, the total wave function should be antisymmetric under the interchange of space and spin coordinates. Given that the space part of the wave function is symmetric, a proper description of the ground state of this idealized model is given by the normalized wave function

$$\Psi(\vec{\rho}_1, \vec{\rho}_2) = \Phi_{00}(\rho_1, \varphi_1)\Phi_{00}(\rho_2, \varphi_2)X_{\text{singlet}}$$

$$= \frac{\alpha^2}{\pi}e^{-(\alpha^2/2)(\rho_1^2 + \rho_2^2)}X_{\text{singlet}}, \qquad (10)$$

where X_{singlet} is the spin singlet state (total spin $S = 0$ and $M_s = 0$) given by

$$X_{\text{singlet}} = \frac{1}{\sqrt{2}}[\chi_+(\sigma_1)\chi_-(\sigma_2) - \chi_-(\sigma_1)\chi_+(\sigma_2)], \qquad (11)$$

where $\chi_\pm(\sigma_i) = \chi_{1/2, \pm 1/2}(\sigma_i)$ denotes the two possible spin states of the spin variable σ_i for electron $i = 1$ and 2. We treat the Coulomb repulsion as a perturbation and, given that the ground state is nondegenerate, we can then apply perturbation theory for a nondegenerate state. To first order in perturbation theory, the energy correction of the ground state is given by

$$\Delta E^{(1)} = \left\langle \Psi(\vec{\rho}_1, \vec{\rho}_2) \left| \frac{e^2}{|\vec{\rho}_1 - \vec{\rho}_2|} \right| \Psi(\vec{\rho}_1, \vec{\rho}_2) \right\rangle. \qquad (12)$$

Since the Coulomb perturbation does not involve the spin, we only need calculate the following integral:

$$\Delta E^{(1)} = \left(\frac{\alpha^2}{\pi}\right)^2 \int d^2\rho_1 \int d^2\rho_2 e^{-\alpha^2(\rho_1^2 + \rho_2^2)} \frac{e^2}{|\vec{\rho}_1 - \vec{\rho}_2|}. \qquad (13)$$

We carry out the integration by using the identity

$$\frac{1}{|\vec{\rho}_1 - \vec{\rho}_2|} = \sum_{m_z = -\infty}^{\infty} \int_0^\infty dk e^{im_z(\varphi_1 - \varphi_2)}J_{m_z}(k\rho_1)J_{m_z}(k\rho_2), \qquad (14)$$

where $J_{m_z}(k\rho_i)$ are Bessel functions. The integration over angular variables, φ_1 and φ_2 is simple, and after straightforward calculations we obtain

$$\Delta E^{(1)} = e^2 \alpha \sqrt{\frac{\pi}{2}}. \qquad (15)$$

The first-order correction of the energy is a positive contribution, since it arises from repulsive interaction, and when added to the unperturbed result gives the energy to first order of perturbation theory $E^{(1)} = 2\hbar\omega + \Delta E^{(1)}$. This can be written as

$$\epsilon^{(1)}(\lambda) = \frac{E^{(1)}}{\hbar\omega} = 2 + \lambda\sqrt{\frac{\pi}{2}}, \quad \lambda = \frac{e^2\alpha}{\hbar\omega}, \qquad (16)$$

where $\epsilon^{(1)}(\lambda)$ is a dimensionless energy (measured in units of $\hbar\omega$) and $\lambda = e^2\alpha/(\hbar\omega)$ is a dimensionless interaction parameter that gauges the strength of the Coulomb correlation relative to the confining oscillator energy.

IV. EXACT NUMERICAL DIAGONALIZATION

We gauge the accuracy of perturbation theory and, later on, variational approach, by considering exact numerical diagonalization energies as reference. In the case of 2D quantum-dot helium, the exact numerical diagonalization technique simplifies if we separate the Hamiltonian into two parts, one representing the center-of-mass (c.m.) motion and the other one representing the relative motion. The c.m. and relative coordinates are defined as

$$\vec{R} = \frac{\vec{\rho}_1 + \vec{\rho}_2}{2}, \ \vec{P} = \vec{p}_1 + \vec{p}_2, \ \vec{r} = \vec{\rho}_1 - \vec{\rho}_2, \ \vec{p} = \frac{\vec{p}_1 - \vec{p}_2}{2}. \quad (17)$$

Accordingly, the total mass of the system is $M = 2m$ and the reduced mass is $\mu = m/2$. In this representation the Hamiltonian of the system decouples and can be written as

$$\hat{H}(\vec{R}, \vec{r}) = \hat{H}_R(\vec{R}) + \hat{H}_r(\vec{r}), \qquad (18)$$

where $\hat{H}_R(\vec{R})$ and $\hat{H}_r(\vec{r})$ are, respectively, the c.m. and relative motion Hamiltonians given by

$$\hat{H}_R(\vec{R}) = \frac{\hat{P}^2}{2M} + \frac{M}{2}\omega^2 R^2 \qquad (19)$$

and

$$\hat{H}_r(\vec{r}) = \frac{\hat{p}^2}{2\mu} + \frac{\mu}{2}\omega^2 r^2 + \frac{e^2}{r}. \qquad (20)$$

The eigenfunctions of the c.m. Hamiltonian are

$$\Phi_{n_R M_z}(R, \varphi_R) = N_{n_R M_z} \frac{e^{iM_z \varphi_R}}{\sqrt{2\pi}}(\alpha_R R)^{|M_z|}e^{-\alpha_R^2 R^2/2} \times L_{n_R}^{|M_z|}(\alpha_R^2 R^2),$$

$$(21)$$

where $n_R = 0, 1, \ldots$, $M_z = 0, \pm 1, \ldots$, and $\alpha_R = \sqrt{M\omega/\hbar} = \sqrt{2}\alpha$. The c.m. eigenenergies are of the form $E_{n_R M_z} = (2n_R + |M_z| + 1)\hbar\omega$. If we ignore the Coulomb interactions for the moment, the eigenenergies and eigenfunctions for the relative motion Hamiltonian are of the same form as Eqs. (6) and (7), with the replacement of vector $\vec{\rho}$ with $\vec{r}$, of quantum number n_ρ with n, and of α with $\alpha_r = \alpha/\sqrt{2}$, because of the reduced mass. As in any standard numerical diagonalization technique we need to calculate the matrix elements of the Hamiltonian in the basis $|n_R M_z; nm_z\rangle$. The only nondiagonal terms arise from the Coulomb potential, which is diagonal with respect to n_R, M_z, and m_z, but not n. As a result the most general nonzero Hamiltonian matrix elements have the form $\langle n_R M_z; n'm_z|\hat{H}|n_R M_z; nm_z\rangle = \langle n_R M_z|\hat{H}_R|n_R M_z\rangle\delta_{n'n} + \langle n'm_z|\hat{H}_r|nm_z\rangle$. For a given n_R, M_z, and m_z, we have $\langle n_R M_z|\hat{H}_R|n_R M_z\rangle/(\hbar\omega) = (2n_R + |M_z| + 1)$, while $h_{n'n} = \langle n'm_z|\hat{H}_r|nm_z\rangle/(\hbar\omega)$ is given by

$$h_{n'n} = (2n + |m_z| + 1)\delta_{nn'}$$

$$+ \frac{\lambda}{\sqrt{2}}\sqrt{\frac{n'!\,n!}{(n' + |m_z|)!\,(n + |m_z|)!}}I_{n'n|m_z|}, \qquad (22)$$

where

$$I_{n'n|m_z|} = \int_0^\infty dt\, t^{|m_z|} e^{-t} L_{n'}^{|m_z|}(t) L_n^{|m_z|}(t) \frac{1}{\sqrt{t}} \qquad (23)$$

and $\lambda = e^2 \alpha/(\hbar\omega)$.

For any value of the quantum number $m_z = 0, \pm 1, \ldots$, we build sufficiently large matrices with elements $h_{n'n}$ and diagonalize them by using standard numerical methods. For a given λ, the smallest of the eigenvalues represents the ground state energy for the relative motion. With the addition of the c.m. energy to the ground-state energy of the relative motion we obtain the exact numerical diagonalization value of the ground-state energy of 2D quantum dot helium at zero magnetic field.

V. VARIATIONAL THEORY

A. One-parameter variational wave function

In this section we employ variational theory and the Ritz variational principle to calculate the ground-state energy of 2D quantum dot helium. This can be done by choosing a trial variational wave function that depends on a number of parameters, calculating the expectation value of the Hamiltonian with respect to this trial wave function and then minimizing the trial energy with respect to all parameters.

We start by considering a simple normalized one-parameter variational wave function of the form

$$\Psi_a(\vec{\rho}_1, \vec{\rho}_2) = \frac{a^2}{\pi} e^{-(a^2/2)(\rho_1^2 + \rho_2^2)} X_{\text{singlet}}, \qquad (24)$$

where a is a positive variational parameter to be optimized and X_{singlet} is the spin singlet function.

The problem of determining the ground state energy reduces to the evaluation of the integral

$$E_a = \int d^2\rho_1 \int d^2\rho_2 \Psi_a(\vec{\rho}_1, \vec{\rho}_2)^* \hat{H}(\vec{\rho}_1, \vec{\rho}_2) \Psi_a(\vec{\rho}_1, \vec{\rho}_2), \qquad (25)$$

where the Hamiltonian is given in Eq. (2) and the trial wave function is normalized to 1. The variational energy as a function of the parameter a turns out to be

$$\frac{E_a(\lambda)}{\hbar\omega} = \left(\frac{a}{\alpha}\right)^2 + \left(\frac{\alpha}{a}\right)^2 + \lambda\sqrt{\frac{\pi}{2}}\left(\frac{a}{\alpha}\right), \qquad (26)$$

where $\alpha = \sqrt{m\omega/\hbar}$ and λ is the dimensionless Coulomb interaction parameter defined in Eq. (16). It is obvious that the ground-state energy will depend on the parameter λ. To simplify notation we introduce a new variable $t = a/\alpha$ and write $\epsilon(t, \lambda) = E_a(\lambda)/(\hbar\omega)$ as

$$\epsilon(t, \lambda) = t^2 + \frac{1}{t^2} + \lambda\sqrt{\frac{\pi}{2}}t. \qquad (27)$$

Starting from the minimum condition $d\epsilon(t, \lambda)/dt = 0$, we search for the real (positive) root of equation $t_0 + \lambda\sqrt{\pi/8} = 1/t_0^3$, which represents the optimal value of parameter t_0 (therefore the optimal variational parameter a_0) that minimizes the energy for any given λ.

B. Two-parameter variational wave function

Let us now consider a second family of variational wave functions with two variational parameters. The special form of the Hamiltonian in Eq. (18) allows a product ansatz for the wave function in a factorized form

$$\Psi(\vec{R}, \vec{r}) = \Phi_R(\vec{R})\Phi_r(\vec{r})X_{\text{singlet}}, \qquad (28)$$

where $\Phi_R(\vec{R})$ are the eigenstates of the c.m. Hamiltonian and $\Phi_r(\vec{r})$ is a function of the relative coordinate. The ground-state wave function for the c.m. motion (corresponding to the energy, $\hbar\omega$) is found from Eq. (21) and is

$$\Phi_{00}(R, \varphi_R) = \frac{\alpha_R}{\sqrt{\pi}} e^{-\alpha_R^2 R^2/2}. \qquad (29)$$

The eigenvalue equation $\hat{H}_r(\vec{r})\Phi_r(\vec{r}) = E_r\Phi_r(\vec{r})$ is more complicated and requires the solution of the stationary Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{\hat{L}_z^2}{2\mu r^2} + \frac{\mu}{2}\omega^2 r^2 + \frac{e^2}{r} \right]\Phi_r(\vec{r}) = E_r\Phi_r(\vec{r}), \qquad (30)$$

where $\hat{L}_z$ is the relative coordinate angular momentum operator and E_r are the energy eigenvalues for the relative motion. There are no exact analytic solutions to the above problem and almost all treatments envolve some form of approximation to derive useful results.

In view of this and in consideration to the fact that our main interest is on ground-state properties, we write a two-parameter variational wave function as a product of two terms, one depending on the c.m. coordinate and the other one depending on the relative motion coordinate. We choose a normalized two-parameter variational wave function of the form

$$\Psi_{\alpha_R, b}(\vec{R}, \vec{r}) = \Phi_{\alpha_R}(\vec{R})\Phi_b(\vec{r})X_{\text{singlet}}, \qquad (31)$$

where $\Phi_{\alpha_R}(\vec{R}) = \Phi_{00}(R, \varphi_R)$ is given from Eq. (29) and corresponds to the exact ground-state wave function for the c.m. motion. As a result, there is no need to determine an optimal value for the parameter α_R already known to be $\alpha_R/\alpha = \sqrt{2}$. On the other hand, we write the relative motion trial wave function as

$$\Phi_b(\vec{r}) = \frac{b}{\sqrt{\pi}} e^{-(b^2/2)r^2}. \qquad (32)$$

The function, $\Phi_b(\vec{r})$ is normalized to one, describes the ground state of the relative motion and need be optimized by choosing the optimal value of b via standard variational procedures. The function X_{singlet} is the spin singlet function.

The expectation value of the two-body Hamiltonian for the wave function of Eq. (31) can be reduced to the expression

$$E_b = \hbar\omega + \int d^2 r \Phi_b(\vec{r}) * \hat{H}_r(\vec{r}) \Phi_b(\vec{r}), \tag{33}$$

where the first term comes from the c.m. motion and the second integral results from the relative motion. After performing the integrals we obtain

$$\frac{E_b(\lambda)}{\hbar\omega} = 1 + \left(\frac{b}{\alpha}\right)^2 + \frac{1}{4}\left(\frac{\alpha}{b}\right)^2 + \lambda\sqrt{\pi}\left(\frac{b}{\alpha}\right). \tag{34}$$

As previously done, we introduce the dimensionless variables $t = b/\alpha$ and $\epsilon(t,\lambda) = E_b(\lambda)/(\hbar\omega)$ to obtain

$$\epsilon(t,\lambda) = 1 + t^2 + \frac{1}{4t^2} + \lambda\sqrt{\pi}t. \tag{35}$$

We minimize $\epsilon(t,\lambda)$ with respect to t in order to obtain the optimal value of parameter t_0 (therefore b_0) for any given λ.

C. Three-parameter variational wave function

We can further improve the two-parameter variational wave function and build a better wave function once we note that the main effect of the Coulomb repulsion is to push the two electrons further apart. In absence of Coulomb repulsion, the component of the ground-state wave function that depends on the relative coordinate is expected to be centered at $|\vec{\rho}_1 - \vec{\rho}_2| = 0$, but in presence of the Coulomb repulsion between electrons, the center of the relative motion wave function would shift towards nonzero relative coordinates ($|\vec{\rho}_1 - \vec{\rho}_2| \neq 0$). A variational wave function of the form

$$\Psi_{a,b,c}(\vec{\rho}_1, \vec{\rho}_2) = \exp\left[-\frac{a^2}{2}(\rho_1^2 + \rho_2^2) - \frac{b^2}{2}(\vec{\rho}_1 - \vec{\rho}_2)^2\right]$$
$$\times \exp[cb|\vec{\rho}_1 - \vec{\rho}_2|]X_{singlet} \tag{36}$$

has all the key ingredients to satisfy the above scenario and contains only three variational prameters to optimize. The three parameters a, b, and c are considered to be nonnegative. On physical grounds we may expect to have $a/\alpha = 1$, since the two electron equation can be separated by the variables R and r and this choice gives the exact lowest c.m. energy. Although this argument applies to the three parameter wave function (because of its special form), it is not always correct and should be treated with some care. This is because $(\rho_1^2 + \rho_2^2)$ depends on both R and r, therefore, for an arbitrary generic wave function, the optimal value of a may not always be the value that gives the exact lowest c.m. energy. For the sake of generality and as a numerical check of the minimization procedure we prefer to consider a as a variational parameter. (We later verify that the numerical minimization procedure always gives the anticipated value for parameter a.) When $b = 0$, the three-parameter wave function reduces to the one-parameter wave function (that would give the exact solution of the problem if we were to ignore the Coulomb repulsion). When $b > 0$, we would then expect the parameter c to play a significant role on improving the variational energy, because the main effect of the c-dependent term is to push the pair of electrons further apart, therefore optimizing their Coulomb correlations.

A calculation of the expectation value of the Hamiltonian with respect to the above three-parameter trial wave function gives

$$\epsilon = \frac{E}{\hbar\omega} = \frac{-B^2 f_1(A,B,c) + \frac{f_2(A,B,c)}{(4B^2)} + \lambda B f_3(A,B,c)}{f(A,B,c)}$$
$$+ \frac{A^2}{2} + \frac{1}{2A^2}, \tag{37}$$

where $A = a/\alpha$, $B = b/\alpha$, and $\lambda = e^2\alpha/(\hbar\omega)$. The four functions $f_{1,2,3}$ and f depend on the variables specified on their arguments. In an integral form they are given by

$$f_1(A,B,c) = \int_0^\infty dt\, t\, e^{-(A^2/2B^2)t^2 - t^2 + 2ct} \times \left[\left(1 + \frac{A^2}{2B^2}\right)^2 t^2\right.$$
$$\left. - 2ct\left(1 + \frac{A^2}{2B^2}\right) + c^2 - 2 - \frac{A^2}{B^2} + \frac{c}{t}\right],$$

$$f_2(A,B,c) = \int_0^\infty dt\, t^3 e^{-(A^2/2B^2)t^2 - t^2 + 2ct},$$

$$f_3(A,B,c) = \int_0^\infty dt\, e^{-(A^2/2B^2)t^2 - t^2 + 2ct},$$

$$f(A,B,c) = \int_0^\infty dt\, t\, e^{-(A^2/2B^2)t^2 - t^2 + 2ct}, \tag{38}$$

where $t = b|\vec{\rho}_1 - \vec{\rho}_2|$ is an auxiliary variable introduced to simplify the calculation of integrals. For any given value of parameter λ, we minimize the expression in Eq. (37) with respect to the variational parameters A, B, and c and as a result obtain the best variational energy and the optimal values of variational parameters, as well.

VI. RESULTS AND DISCUSSION

The optimal values of variational parameters for the one-, two-, and three-parameter variational wave functions at different λ's are given in Table I. The optimal value of parameter A for the three-parameter variational wave function was always found to be $A = a/\alpha = 1$, a value that guarantees the lowest possible c.m. energy.

In Table II we show the ground-state energies $\epsilon = E/(\hbar\omega)$ for given values of λ (first column) obtained from a variety of different methods: first order perturbation theory, variational theory, exact numerical diagonalization, and unrestricted Hartree-Fock (HF) technique,[40] as well. From the results of Table II we note that, even the energies obtained from the one-parameter variational wave function are lower than the first-order perturbation theory values, for all λ's under consideration. As expected, we find out that for a wide range of Coulomb correlation strengths, the ground-state energy obtained from first-order perturbation theory is too high. The results suggest that perturbation theory is not very accurate and may be used with some reliability only when 0

TABLE I. A display of the optimal variational parameters for different values of λ (first column) corresponding to the different types of variational wave functions for 2D quantum dot helium. For the one-parameter variational wave function (var. 1), the optimal values a/α are listed in the second column. For the two-parameter variational wave function (var. 2), the optimal values b/α are listed in the third column and $\alpha_R/\alpha = \sqrt{2}$ irrespective of λ. For the three-parameter variational wave function (var. 3), the optimal values of $B = b/\alpha$ and c are listed, respectively, in the fourth and fifth columns, while we always have $A = a/\alpha = 1$. The parameter $\alpha = \sqrt{m\omega/\hbar}$ has the dimensionality of an inverse length.

	Var. 1	Var. 2	Var. 3	
λ	a/α	b/α	b/α	c
0.0	1.000000	0.707107	0.000000	0.00000
1.0	0.873542	0.557394	0.401849	1.67676
2.0	0.788274	0.480537	0.497908	2.21655
3.0	0.726623	0.432455	0.542433	2.57492
4.0	0.679582	0.398732	0.566026	2.85052
5.0	0.642208	0.373335	0.579761	3.07820
6.0	0.611583	0.353267	0.588185	3.27473
7.0	0.585880	0.336856	0.593558	3.44916
8.0	0.563892	0.323085	0.597084	3.60699
9.0	0.544787	0.311297	0.599450	3.75177
10.0	0.527975	0.301043	0.601063	3.88599

$\leq \lambda < 1$. Comparing the third and fourth columns of Table II, we see that the two-parameter variational wave function is a clear improvement upon the one-parameter variational wave function, however, the data clearly show that the three-

TABLE II. Ground-state energies $\epsilon = E/(\hbar\omega)$ of 2D quantum dot helium as a function of dimensionless Coulomb coupling parameter $\lambda = e^2\alpha/(\hbar\omega)$ (first column) obtained from first order perturbation theory (second column), one-parameter variational wave function (third column), two-parameter variational wave function (fourth column), three-parameter variational wave function (fifth column) are compared with exact numerical diagonalization results (sixth column) and unrestricted Hartree-Fock (HF) results (Ref. 40), where available (seventh column). The parameter $\alpha = \sqrt{m\omega/\hbar}$ has the dimensionality of an inverse length.

| λ	$\epsilon^{(1)}(\lambda)$	ϵ (var. 1)	ϵ (var. 2)	ϵ (var. 3)	ϵ (diag.)	ϵ (HF)
0.0	2.00000	2.00000	2.00000	2.00000	2.00000	
1.0	3.25331	3.16838	3.10331	3.00174	3.00097	
2.0	4.50663	4.20662	4.01702	3.72565	3.72143	4.034
3.0	5.75994	5.15405	4.82331	4.32576	4.31872	
4.0	7.01326	6.03404	5.55838	4.85637	4.84780	5.182
5.0	8.26657	6.86152	6.24164	5.34141	5.33224	
6.0	9.51988	7.64662	6.88494	5.79354	5.78429	6.107
7.0	10.7732	8.39658	7.49609	6.22032	6.21129	
8.0	12.0265	9.11675	8.08061	6.62674	6.61804	6.930
9.0	13.2798	9.81125	8.64257	7.01626	7.00795	
10.0	14.5331	10.48330	9.18504	7.39141	7.38351	7.686
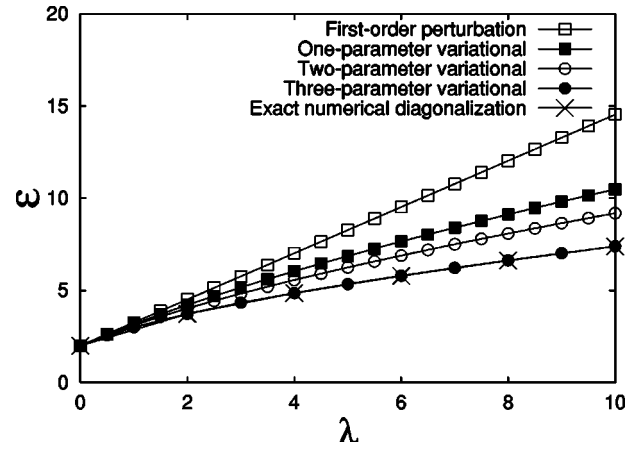
FIG. 1. Plot of the dimensionless ground-state energy $\epsilon = E/(\hbar\omega)$ of 2D quantum dot helium as a function of the dimensionless Coulomb interaction parameter $\lambda = e^2\alpha/(\hbar\omega)$ for values of λ from 0 to 10. The ground-state energies obtained from the three-parameter wave function (solid circles) are practically identical to exact numerical diagonalization results (crosses).

parameter variational wave function (fifth column) is the best choice.

One notes that the variational ground state energies obtained from the three-parameter variational wave function (fifth column) are extremely close to exact numerical diagonalization values (sixth column), and considerably better than unrestricted Hartree-Fock (HF) calculations (seventh column). Furthermore, the results in Table II show that this excellent agreement between the three-parameter variational wave function energies and numerical diagonalization results persists for all λ's under consideration (even for very large λ's, where Coulomb correlation effects are expected to be very strong). This further indicates the excellent quality of this variational wave function.

In Fig. 1 we plot the dimensionless ground-state energy $\epsilon = E/(\hbar\omega)$ as a function of the dimensionless Coulomb interaction parameter $\lambda = e^2\alpha/(\hbar\omega)$ for values of λ ranging from 0 (no Coulomb repulsion) to $\lambda = 10$. The results represent the values obtained from first-order perturbation theory (empty square), one-parameter variational theory (filled square), two-parameter variational theory (empty circle), three-parameter variational theory (filled circle), and exact numerical diagonalization results (crosses). The three-parameter variational wave function energies are practically identical to the exact numerical diagonalization values.

For all λ's under consideration, the three-parameter variational wave function energies are sizeably lower than the respective unrestricted HF values.[40] This is explained by noting that, in the absence of a magnetic field, the spin singlet state is the state of lowest energy, therefore the neglect of electronic pair correlations in the HF approach is responsible for the poor quality of the HF singlet ground state. On the contrary, the three-parameter variational wave function captures all essential electronic correlations through the parameter c-dependent term.

With the intent to generalize such a wave function to larger quantum dots, we can rewrite the three-parameter

variational wave function for 2D quantum dot helium as

$$\Psi = D_\uparrow D_\downarrow \prod_{i<j}^{N=2} J(\rho_{ij}), \qquad (39)$$

where $D_\uparrow$, $D_\downarrow$ are Slater determinants for spin "up" and spin "down" states and $J(\rho_{ij})$ is a two-body Jastrow correlation factor which in our case has the form

$$J(\rho_{ij}) = \exp\left(-\frac{b^2}{2}\rho_{ij}^2 + cb\rho_{ij}\right), \qquad (40)$$

where $\rho_{ij} = |\vec{\rho}_i - \vec{\rho}_j|$ and b, c are non-negative variational parameters to be optimized. It is obvious that the wave function in Eq. (39) is equivalent to the wave function in Eq. (36) since $D_\uparrow D_\downarrow \propto \exp[-(a^2/2)(\rho_1^2+\rho_2^2)]$ for $N=2$. To the best of our knowledge, a three-parameter trial wave function with a Jastrow factor of the form of Eq. (40) has not been previously considered neither for $N=2$, nor for arbitrary N quantum dots, with or without magnetic field. Therefore, we believe it is appropriate to compare this trial wave function to other different trial wave functions considered in the literature.

For example, Harju *et al.*[37] have studied a 2D $N=2$ quantum dot in presence of a magnetic field using a variational wave function of the form of Eq. (3) with Jastrow factor of the form

$$J(\rho_{ij}) \propto \exp\left(\frac{a\rho_{ij}}{1+b\rho_{ij}}\right), \qquad (41)$$

where a and b are two variational parameters.

Although the trial wave function of Eq. (36) cannot be directly compared to that in Eq. (3), since the first describes 2D quantum dot helium at zero magnetic field, while the second considers a nonzero magnetic field, it is evident that these two variational wave functions have very different Jastrow factors. Furthermore, as noted in Ref. 37, the Jastrow ansatz of Eq. (41) does not have the right asymptotic behavior for $\rho_{ij} \to \infty$, where the electronic correlations are expected to vanish and not saturate to a finite value. In a separate study, Bolton[29] considered systems of $N=2-4$ interacting electrons in a quantum dot, in the presence of magnetic field, using the fixed-node diffusion Monte Carlo (DMC) method. For $N=2$ electrons and a starting wave function of Laughlin form, he found out that, without Coulomb interaction, the state with angular momentum $m_z=0$ remains the ground state over the entire range of magnetic fields (nonzero and zero magnetic field). With the inclusion of the Coulomb interaction, the situation at zero magnetic field is not altered, although this is no longer the case for a nonzero magnetic field. It is obvious that, for zero magnetic field and angular

momentum $m_z=0$, the Laughlin factor of the ground-state wave function in Eq. (3) reduces to $\propto e^{-(\alpha^2/2)(\rho_1^2+\rho_2^2)}$, which corresponds to the un-normalized product of wave functions for two uncorrelated electrons. Therefore, in the limit of zero magnetic field, the wave function of Eq. (3) transforms into a wave function of the form of Eq. (36) possesing the same one-body term, but having a very different two-body Jastrow factor.

We point out that generalizations of trial wave functions as in Eq. (39) in absence[31] and in presence of weak magnetic fields[41] have always considered Jastrow correlation factors of the type of Eq. (41) so far. A generalized version of the Jastrow factor in Eq. (41) was also used in recent DMC calculations[38] to calculate ground- and excited-state properties for up to $N=13$ electrons in a 2D quantum dot. Clearly, the variational wave functions under consideration in this work have substantially different Jastrow correlation factors when compared to earlier studies.

We can readily generalize the wave function of Eq. (39) with the proposed Jastrow factor of Eq. (40) to quantum dots with arbitrary number N of electrons. By doing so, the product of Jastrow factors is now extended to all pairs of electrons and we need to consider Slater determinants of $N_\uparrow$ spin "up" and $N_\downarrow$ spin "down" electrons, with $N_\uparrow + N_\downarrow = N$. As a first scenario, one might consider the variational parameters, b and c to be the same for any pair of electrons, irrespective of their relative spin. Under a more sophisticated treatment, one would assume different variational parameters b and c for pairs of electrons with parallel and opposite spins. This is because in larger systems we have correlations between pairs of electrons not only of opposite spin (as in the case of $N=2$ quantum-dot helium), but also of pairs of electrons of parallel spins. It is reasonable to expect that pairs of electrons with parallel and opposite spins will not correlate in the same way, under the most general circumstances.

Whether we consider the first or the second scenario (with more variational parameters), standard variational Monte Carlo (VMC) techniques would be applied to get an accurate evaluation of the relevant physical properties of the system. Trial wave functions of this type could also be good starting points to implement additional DMC simulations as those performed by Bolton[29] for 2D quantum dots with few electrons. Work in this direction is in progress.

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