

## Two-dimensional quantum-dot helium in a magnetic field: Variational theory

Orion Ciftja

Department of Physics, Prairie View A&M University, Prairie View, Texas 77446, USA

M. Golam Faruk

Department of Electrical Engineering and Department of Physics, Prairie View A&M University, Prairie View, Texas 77446, USA

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A trial wave function for two-dimensional quantum-dot helium in an arbitrary perpendicular magnetic field (a system of two interacting electrons in a two-dimensional parabolic confinement potential) is introduced. A key ingredient of this trial wave function is a Jastrow pair correlation factor that has a displaced Gaussian form. The above choice of the pair correlation factor is instrumental in assuring the overall quality of the wave function at all values of the magnetic field. Exact numerical diagonalization results are used to gauge the quality of the proposed trial wave function. We find out that this trial wave function is an excellent representation of the true ground state at all values of the magnetic field including weak (or zero) and strong magnetic fields.

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### I. INTRODUCTION

Among the variety of two-dimensional (2D) few-electron quantum dots,<sup>1-14</sup> the two-electron ( $N=2$ ) quantum dot stands out as a truly remarkable system that, despite its simplicity, shows very rich phenomena and possesses characteristic features that persist to larger systems. Such a system, often referred to as 2D *quantum-dot helium*, exhibits a highly complex behavior in the presence of a perpendicular magnetic field. Its ground-state energetics is unusually complicated and intricate singlet-to-triplet spin state transitions occur as the magnetic field is varied.<sup>15,16</sup>

The Hamiltonian of 2D quantum-dot helium in a perpendicular magnetic field can be written as

$$\hat{H}(\vec{\rho}_1, \vec{\rho}_2) = \sum_{i=1}^2 \left\{ \frac{p_i^2}{2m} + \frac{\omega_c}{2} \hat{L}_{iz} + \frac{m}{2} \left[ \omega_0^2 + \left( \frac{\omega_c}{2} \right)^2 \right] \rho_i^2 \right\} + \frac{1}{4\pi\epsilon_0\epsilon_r} \frac{e^2}{|\vec{\rho}_1 - \vec{\rho}_2|} + g_e \mu_B B_z S_z, \quad (1)$$

where  $\hat{p}_i = (\hat{p}_{ix}, \hat{p}_{iy})$  and  $\vec{\rho}_i = (\rho_{ix}, \rho_{iy})$  are, respectively, the 2D momentum and position of the  $i$ th electron,  $m$  is the electron mass,  $-e$  ( $e > 0$ ) is the electron charge,  $g_e$  is the electron  $g$  factor,  $\mu_B$  is the Bohr magneton,  $\epsilon_r$  is the dielectric constant,  $\hbar\omega_0$  is the parabolic confinement energy,  $S_z$  is the  $z$  component of the total spin,  $B_z$  is the perpendicular magnetic field,  $\hat{L}_{iz}$  is the  $z$ -component angular momentum operator for the  $i$ th electron, and  $\omega_c = eB_z/m > 0$  is the cyclotron frequency.

There have been several studies of 2D quantum-dot helium with or without magnetic field employing a variety of techniques. For example, Merkt *et al.*<sup>17</sup> studied the energy spectra of two interacting electrons in a parabolic potential in the absence and the presence of a perpendicular magnetic field employing the exact numerical diagonalization technique. Wagner *et al.*<sup>15</sup> used the exact numerical diagonalization technique to study 2D quantum-dot helium in a perpendicular magnetic field and to predict oscillations between

spin-singlet and spin-triplet states as a function of the magnetic field strength. Pfannkuche *et al.*<sup>18</sup> compared energies, pair correlation functions, and particle densities obtained from the Hartree, Hartree-Fock (HF), and exact numerical diagonalization methods and pointed out the unsuitability of the HF approach at weak magnetic fields. Pfannkuche *et al.*<sup>19</sup> used the diagonalization data to formulate a theory of 2D quantum-dot helium in a perpendicular magnetic field, explaining how the competition between the Coulomb interaction and the binding forces due to confinement and the magnetic field induces ground-state transitions. Harju *et al.*<sup>20</sup> introduced a recipe of how to build a trial wave function for 2D quantum-dot helium in a perpendicular magnetic field and applied the variational Monte Carlo (VMC) technique. His Jastrow pair correlation factor has two variational parameters and takes into account the mixing of different Landau levels for the relative motion, though the ansatz does not have the right asymptotic behavior at large interparticle distances.

A wealth of information in 2D quantum dots in general, and 2D quantum-dot helium in particular, is provided by the rotating Wigner (or electron) molecule (RWM or REM) theory.<sup>21,22</sup> Specific RWM trial wave functions have been recently derived<sup>23</sup> for 2D quantum-dot systems in high magnetic fields. The RWM wave functions are constructed by first breaking the rotational symmetry at the unrestricted Hartree-Fock (UHF) level and, second, restoring the circular symmetry via post-HF methods and projection techniques.<sup>22</sup> The UHF-level RWM wave function describes a Wigner molecule that is considered as a rigid rotor, while the second step of restoring the circular symmetry implies rotations of such molecules. At zero and weak magnetic fields the broken-symmetry UHF orbitals need to be determined numerically while at high magnetic fields they can be well approximated by one-particle lowest-Landau-level (LLL) Gaussian functions that are centered at positions that correspond to the classical equilibrium configuration of  $N$  point charges in a harmonic trap. Yannouleas and Landman<sup>22</sup> used such RWM trial wave functions to study 2D quantum-dot

helium in a magnetic field. They calculated the ground-state energies as a function of the magnetic field for the spin-triplet states of 2D quantum-dot helium and noted that for high magnetic fields (larger than 7 T; see Fig. 1 in Ref. 22) the RWM and exact diagonalization results are practically the same.

Some of the main theoretical methods used to study quantum dots are analytical calculations,<sup>24–27</sup> exact numerical diagonalizations,<sup>28–31</sup> quantum Monte Carlo (QMC) methods,<sup>32–35</sup> density functional theory methods,<sup>36–40</sup> and Hartree-Fock mean-field theory.<sup>41–44</sup> These methods have advantages and disadvantages, most notably some methods that deliver good results for the ground-state properties may be inadequate in describing excited-state properties, and vice versa. Here we are limiting our discussion to the calculation of ground-state properties only. Considering the limitations of several methods on obtaining ground-state properties (for example, exact numerical diagonalization methods are applicable only for few electrons, Hartree-Fock and perturbation theory lack the desired accuracy, etc.), the use of QMC methods, such as the VMC technique, seems to be the best strategy in the long run. Therefore the quest for better, yet simple, trial ground-state wave functions is always timely. A high-quality trial ground-state wave function is essential not only for the VMC method, but also for the more sophisticated diffusion Monte Carlo (DMC) method which relies on a guiding trial wave function. Compared to other methods, QMC methods have the greatest advantage of all, since they can be extended to a larger number of electrons in a straightforward manner and are very accurate.

In this work we introduce a trial wave function to describe the ground state of 2D quantum-dot helium in a perpendicular magnetic field. This wave function is written as a product of a Laughlin-type wave function<sup>45–47</sup> with a Jastrow pair correlation factor and has the form

$$\Psi(\vec{\rho}_1, \vec{\rho}_2) = J(\rho_{12})(z_1 - z_2)^{|m_z|} \exp\left(-\frac{\rho_1^2 + \rho_2^2}{4l_\Omega^2}\right), \quad (2)$$

where the Jastrow factor  $J(\rho_{12})$  is

$$J(\rho_{12}) = \exp\left(-\frac{b^2}{2}\rho_{12}^2 + c\rho_{12}\right). \quad (3)$$

The 2D position coordinate  $z_j = x_j - iy_j$  of the Laughlin component of the wave function is given in complex notation,  $\rho_{12} = |\vec{\rho}_1 - \vec{\rho}_2|$  is the interelectron distance,  $m_z = |m_z| = 0, 1, \dots$  is the angular momentum number, and  $b$  and  $c$  are non-negative variational parameters to be optimized. We have  $l_\Omega = \sqrt{\hbar/(2m\Omega)}$  and  $\Omega^2 = \omega_0^2 + (\omega_c/2)^2$ . The effective magnetic length  $l_\Omega$  reduces to the electronic magnetic length  $l_0 = \sqrt{\hbar/eB_z}$  when there is no confinement ( $\omega_0 = 0$ ) or when the magnetic field is very large ( $\omega_c/\omega_0 \rightarrow \infty$ ). The effective magnetic length  $l_\Omega$  can be written in terms of the inverse oscillator length  $\alpha = \sqrt{m\omega_0/\hbar}$  as

$$\frac{1}{l_\Omega^2} = 2\alpha^2 \sqrt{1 + \frac{1}{4}\left(\frac{\omega_c}{\omega_0}\right)^2}. \quad (4)$$

In this way it is easy to recover the 2D harmonic oscillator states in the limit of zero magnetic field ( $\omega_c/\omega_0 \rightarrow 0$ ). The parity of the ground-state space wave function depends on the value of angular momentum  $|m_z|$ . For even values  $|m_z| = 0, 2, 4, \dots$  the space wave function is symmetric and the spin function corresponds to a spin-singlet state ( $S=0$ ), while for odd values  $|m_z| = 1, 3, 5, \dots$  the space wave function is antisymmetric and the spin function becomes a spin triplet ( $S=1$ ).

What makes this trial wave function rather unusual is its displaced Gaussian Jastrow pair correlation factor  $J(\rho_{12})$ , which is different from earlier choices in the literature.<sup>20,33,48</sup> The rationale behind the displaced Gaussian choice of correlation factor can be better understood if one considers a pair of electrons in zero magnetic field. In the absence of an electronic repulsion between the electrons the relative coordinate ground-state wave function will be a Gaussian centered at coordinate  $\rho_{12} = 0$ , will have zero angular momentum, and will correspond to a spin-singlet state. With the Coulomb repulsion the ground state will still have zero angular momentum,<sup>33</sup> therefore it is plausible to expect that the main effect of the Coulomb correlation is simply to further separate the electrons resulting in a new relative coordinate ground-state wave function which will resemble a Gaussian centered at  $\rho_{12} \neq 0$  values. The choice in Eq. (3) mimics this physical effect.

Trial wave functions such as the RWM wave functions (for  $N=2$  and  $N>2$  electrons) also take into consideration the relative separation of electrons and have led to a rich physics regarding Wigner crystallization and the rotation of the electron molecules formed in high magnetic fields.<sup>22,49</sup> Within the framework of the RWM wave functions, which by construction are crystalline in character, the separation between electrons is achieved at the one-particle level right at the start. For instance, in the high-magnetic-field regime, the RWM wave function's Slater determinants contain LLL one-particle Gaussian orbitals which are centered at different positions  $Z_j$  (in complex notation) and have the form

$$u(z, Z_j) = \frac{1}{\sqrt{2\pi}l_0} \exp\left(-\frac{|z - Z_j|^2}{4l_0^2} - \frac{i}{2l_0^2}(xY_j - yX_j)\right), \quad (5)$$

where  $Z_j$  coincide with the equilibrium positions of classical point charges and  $l_0$  is the electronic magnetic length. In the case of our variational wave function, the separation between electrons is achieved at the two-particle (pair) level through the displaced Gaussian pair correlation factor. Despite the same idea of optimizing the separation between electrons, the displaced Gaussian pair correlation factors considered in this work have a two-body structure which make them different from the one-particle (displaced) Gaussian functions that approximate the one-particle UHF orbitals of the RWM wave functions at high magnetic fields.<sup>23</sup>

Despite the usual controversies involved in the selection of a Jastrow correlation factor it appears clearly that the displaced Gaussian pair correlation factor has all the attributes

to capture effectively most of the electronic correlations present in the ground state of this system. Some indication of the eventual high quality of the trial wave function also comes from a previous study of 2D quantum-dot helium at zero magnetic field<sup>50</sup> where the same Jastrow pair correlation factor was used.

Motivated by these arguments, it is the objective of this work to perform a complete study of 2D quantum-dot helium in an arbitrary perpendicular magnetic field that ranges from very weak (or zero) to very strong, using the trial wave function introduced in Eqs. (2) and (3). In the process we will test how effective the displaced Gaussian pair correlation factor is in representing the effect of electronic correlations at arbitrary magnetic fields. Exact numerical diagonalization calculations will be used as a gauge of accuracy of the variational results.

The paper is organized as follows. In Sec. II we introduce the variational method and the trial wave function and calculate various quantities corresponding to such a wave function. In Sec. III we show the results obtained from the variational wave function and compare them to the exact diagonalization method. A discussion of the results is given in Sec. IV and concluding remarks can be found in Sec. V.

## II. VARIATIONAL THEORY

In this section we apply the variational method to study 2D quantum-dot helium in a perpendicular magnetic field using the trial wave function of Eq. (2) with the Jastrow pair correlation factor having the displaced Gaussian form given in Eq. (3). We will show that, after optimization, the proposed trial wave function is an excellent representation of the true ground state at any value of the magnetic field and compares very favorably to the exact numerical diagonalization results.

There are two dimensionless parameters that determine the behavior and properties of the system under consideration:

$$\lambda = \frac{1}{4\pi\epsilon_0\epsilon_r} \frac{e^2\alpha}{\hbar\omega_0}, \quad \gamma = \frac{\omega_c}{\omega_0}, \quad (6)$$

where  $\lambda$  gauges the strength of the Coulomb correlation relative to the confinement energy and  $\gamma$  measures the strength

of the magnetic field relative to confinement. One can immediately see that  $\lambda = l/a_B$ , where  $l = 1/\alpha$  is the harmonic oscillator length and  $a_B = 4\pi\epsilon_0\epsilon_r\hbar^2/(me^2)$  is the effective Bohr radius.

Since the parity of the space wave function is determined by the value of the angular momentum  $|m_z|$ , the ground-state angular momentum value determines whether the ground state corresponds to a spin-singlet or spin-triplet state. Therefore, a stringent test of quality for this trial wave function is to check whether the lowest-variational-energy state has always the correct angular momentum number as calculated from numerical diagonalizations under different combinations of Coulomb correlation, confinement, and magnetic field.

In a general situation where both Coulomb correlation and magnetic field are present, there is no way to anticipate the correct value of the ground-state angular momentum number. Exceptions are the simple cases of (i) absence of Coulomb correlations or (ii) absence of a perpendicular magnetic field, where it is straightforward to prove that the ground state is expected to have zero angular momentum.

Obviously, such behavior should be reflected by the trial wave function under investigation. With no Coulomb correlation ( $\lambda=0$ ), the ground state has zero angular momentum ( $|m_z|=0$ ) in both the presence and absence of the perpendicular magnetic field. Under these conditions, the corresponding trial wave function becomes that of Eq. (2) with Jastrow correlation  $J(\rho_{12})=1$  and angular momentum  $|m_z|=0$  as expected. In the absence of a perpendicular magnetic field, the ground state still has zero angular momentum ( $|m_z|=0$ ) with or without the Coulomb correlation; therefore a trial wave function with  $J(\rho_{12}) \neq 1$  and angular momentum  $|m_z|=0$  is again consistent with the expected scenario.

However, when both Coulomb correlation and magnetic field are present, the situation changes drastically. As the magnetic field increases, a ground state with nonzero angular momentum ( $|m_z| \neq 0$ ) may arise; therefore in addition to the Jastrow pair correlation factor also the Laughlin factor starts contributing to keeping the electrons apart in a more effective way.

A calculation of the expectation value of the Hamiltonian with respect to the trial wave function  $E = \langle \Psi | \hat{H} | \Psi \rangle / \langle \Psi | \Psi \rangle$  gives

$$\epsilon(B, c, \gamma, m_z, \lambda) = \frac{E}{\hbar\omega_0} = -\frac{|m_z|}{2} \gamma + \frac{-B^2 f_1(B, c, \gamma, m_z) + (1 + \gamma^2/4) f_2(B, c, \gamma, m_z)/(4B^2) + \lambda B f_3(B, c, \gamma, m_z)}{f(B, c, \gamma, m_z)} + \sqrt{1 + \frac{\gamma^2}{4}}, \quad (7)$$

where  $B = b/\alpha$  and  $c$  are variational parameters,  $\gamma = \omega_c/\omega_0$  is linearly proportional to the magnetic field ( $\propto B_z$ ), and  $\lambda = e^2\alpha/(4\pi\epsilon_0\epsilon_r\hbar\omega_0)$  is the Coulomb correlation parameter. All the above quantities are dimensionless and the ground-state energy is given in units of  $\hbar\omega_0$ . Note that the Zeeman energy

term is not specifically included in the expression for the variational energy.

The functions  $f_{1,2,3}$  and  $f$ , as well as the function  $g$ , depend on the variables specified in their arguments and in integral form are given by

TABLE I. The exact numerical diagonalization ground-state energies  $\epsilon = E/(\hbar\omega_0)$  for 2D quantum-dot helium subject to a perpendicular magnetic field as a function of dimensionless Coulomb coupling parameter  $\lambda = e^2\alpha/(4\pi\epsilon_0\epsilon_r\hbar\omega_0) = 0, 1, \dots, 6$  and values of magnetic field  $\gamma = \omega_c/\omega_0 = 0, 1, \dots, 5$ . The angular momentum  $m_z$  of the ground state is also specified. The parameter  $\alpha = \sqrt{m\omega_0}/\hbar$  has the dimensionality of an inverse length.

$\lambda$	$\gamma$					
	0	1	2	3	4	5
0	2.00000 $m_z=0$	2.23607 $m_z=0$	2.82843 $m_z=0$	3.60555 $m_z=0$	4.47214 $m_z=0$	5.38516 $m_z=0$
1	3.00097 $m_z=0$	3.30508 $m_z=0$	3.95732 $m_z=1$	4.71894 $m_z=1$	5.61430 $m_z=1$	6.53067 $m_z=2$
2	3.72143 $m_z=0$	4.06684 $m_z=1$	4.61879 $m_z=1$	5.43123 $m_z=2$	6.30766 $m_z=2$	7.22681 $m_z=3$
3	4.31872 $m_z=0$	4.60594 $m_z=1$	5.23689 $m_z=1$	6.01256 $m_z=2$	6.89002 $m_z=3$	7.81384 $m_z=4$
4	4.84780 $m_z=0$	5.11165 $m_z=1$	5.73642 $m_z=2$	6.53522 $m_z=3$	7.41600 $m_z=4$	8.33874 $m_z=5$
5	5.33224 $m_z=0$	5.58995 $m_z=1$	6.21499 $m_z=2$	7.01716 $m_z=3$	7.90109 $m_z=4$	8.82281 $m_z=6$
6	5.78429 $m_z=0$	6.04534 $m_z=1$	6.67999 $m_z=2$	7.46782 $m_z=4$	8.34530 $m_z=5$	9.27057 $m_z=6$

$$f_1(B, c, \gamma, m_z) = \int_0^\infty dt t g(t, B, c, \gamma, m_z) \times \left\{ \left[ \frac{|m_z|}{t} + c - t \left( 1 + \frac{1}{2B^2} \sqrt{1 + \frac{\gamma^2}{4}} \right) \right]^2 - \frac{1}{B^2} \sqrt{1 + \frac{\gamma^2}{4}} - 2 + \frac{c}{t} - \frac{|m_z|^2}{t^2} \right\},$$

$$f_2(B, c, \gamma, m_z) = \int_0^\infty dt t^3 g(t, B, c, \gamma, m_z),$$

$$f_3(B, c, \gamma, m_z) = \int_0^\infty dt g(t, B, c, \gamma, m_z),$$

$$f(B, c, \gamma, m_z) = \int_0^\infty dt t g(t, B, c, \gamma, m_z),$$

$$g(t, B, c, \gamma, m_z) = t^{|m_z|} \exp[-(t^2/2B^2)\sqrt{1 + \gamma^2/4} - t^2 + 2ct], \quad (8)$$

where  $t = b\rho_{12}$  is an auxiliary variable introduced to simplify the calculation of integrals. The optimization procedure is straightforward: given the values of Coulomb and magnetic field parameters  $\lambda$  and  $\gamma$  we calculate the lowest energies for a set of integer values of  $m_z$  by optimizing the variational parameters  $B$  and  $c$  through standard numerical procedures.

### III. RESULTS

The best way to gauge the accuracy of the trial wave function is to directly compare the variational results to exact numerical diagonalization values. Table I displays the diagonalization ground-state energies  $\epsilon = E/(\hbar\omega_0)$  for 2D quantum-dot helium in a perpendicular magnetic field for values of Coulomb correlation  $\lambda = 1, \dots, 6$ , and values of magnetic field  $\gamma = 0, 1, \dots, 5$ . The ground-state angular momentum  $m_z$  is also specified.

In Table II we show the variational ground-state energies and optimal values of parameters  $B$  and  $c$  for 2D quantum-dot helium in a perpendicular magnetic field at different  $\lambda$ 's and  $\gamma$ 's. The results are rounded in the last digit. The variational energies shown in Table II are in excellent agreement with numerical diagonalization results reported in Table I. This agreement holds for the whole range of Coulomb correlations and perpendicular magnetic fields considered in this work.

In the strong-magnetic-field limit, the variational energies are practically identical (within the range of very small statistical errors) to the exact numerical diagonalization values, indicating the overall excellent quality of the trial wave function. Even more remarkable is the fact that for any combination of  $\lambda$ 's and  $\gamma$ 's the angular momentum of the lowest-variational-energy state is always reached at the exact value obtained from the exact numerical diagonalizations. We note there are cases, such as  $\lambda = 5$  and  $\gamma = 4$ , where the energy difference between ground state and higher states with different angular momentum is extremely small. (For  $\lambda = 5$  and  $\gamma = 4$  the diagonalization method gives a ground state with energy  $\epsilon = 7.90109$  and angular momentum  $|m_z| = 4$ , while the first excited state has an energy slightly higher,  $\epsilon$

TABLE II. The variational ground-state energies  $\epsilon=E/(\hbar\omega_0)$ , angular momentum values  $m_z$ , as well as optimal parameter values  $B=b/\alpha$  and  $c$  for 2D quantum-dot helium subject to a perpendicular magnetic field as a function of dimensionless Coulomb coupling parameter  $\lambda=e^2\alpha/(4\pi\epsilon_0\epsilon_r\hbar\omega_0)=0, 1, \dots, 6$  and values of magnetic field  $\gamma=\omega_c/\omega_0=0, 1, \dots, 5$ . The parameter  $\alpha=\sqrt{m\omega_0/\hbar}$  has the dimensionality of an inverse length.

	$\gamma$					
	0	1	2	3	4	5
$\lambda=0$	2.00000	2.23607	2.82843	3.60555	4.47214	5.38516
$m_z$	0	0	0	0	0	0
$B$	0	0	0	0	0	0
$c$	0	0	0	0	0	0
$\lambda=1$	3.00174	3.30578	3.95737	4.71899	5.61435	6.53068
$m_z$	0	0	1	1	1	2
$B$	0.40185	0.41627	0.22809	0.24247	0.25600	0.18816
$c$	1.67676	1.63743	1.11252	1.05000	0.99691	0.81641
$\lambda=2$	3.72565	4.06704	4.61899	5.43127	6.30769	7.22683
$m_z$	0	1	1	2	2	3
$B$	0.49791	0.29039	0.30813	0.24041	0.25184	0.20584
$c$	2.21655	1.64297	1.55874	1.26233	1.20167	1.04900
$\lambda=3$	4.32576	4.60635	5.23732	6.01263	6.89004	7.81385
$m_z$	0	1	1	2	3	4
$B$	0.54243	0.34137	0.36669	0.28354	0.23794	0.21288
$c$	2.57492	1.98559	1.88097	1.54922	1.34215	1.18987
$\lambda=4$	4.85637	5.11233	5.73655	6.53525	7.41601	8.33875
$m_z$	0	1	2	3	4	5
$B$	0.56603	0.37934	0.30103	0.25770	0.22591	0.20806
$c$	2.85052	2.26315	1.88523	1.62705	1.45132	1.30691
$\lambda=5$	5.34141	5.59088	6.21518	7.01722	7.90111	8.82282
$m_z$	0	1	2	3	4	6
$B$	0.57976	0.40862	0.33005	0.28447	0.25575	0.20855
$c$	3.07820	2.49976	2.09758	1.81530	1.60855	1.38742
$\lambda=6$	5.79354	6.04652	6.68025	7.46785	8.34532	9.27058
$m_z$	0	1	2	4	5	6
$B$	0.58818	0.43192	0.35512	0.26257	0.24321	0.22777
$c$	3.27473	2.70721	2.28554	1.85449	1.66757	1.52332

=7.906 40, and angular momentum  $|m_z|=5$ .) Nevertheless, on all occasions the trial wave function with lowest energy has an angular momentum that corresponds to the exact diagonalization value.

Both diagonalization and variational results are in full agreement and confirm the expected outcome that (i) in the absence of Coulomb correlations ( $\lambda=0$ ) or (ii) in the absence of a perpendicular magnetic field ( $\gamma=0$ ), the ground state has zero angular momentum. However, when both  $\lambda \neq 0$  and  $\gamma \neq 0$ , ground states with nonzero angular momentum arise. For very large values of the perpendicular magnetic field the ground state has increasingly large angular momentum values where each change of  $|m_z|$  indicates a singlet-to-triplet spin state transition, a phenomenon that has been observed in recent experiments<sup>16</sup> with ultrasmall quantum dots. Since the ground-state spin of 2D quantum-dot helium can be either singlet ( $S=0$ ) or triplet ( $S=1$ ) it is plausible to expect that this quantum dot has the potential to serve as a qubit of a

quantum computer, with the magnetic field tuning the transition between the two spin states, an idea suggested by Burkard *et al.*<sup>51</sup>

Because the change of angular momentum indicates a spin state transition, it is the mean square distance between the two electrons (which is directly related to the angular momentum number) that should indicate jumps or nonmonotonic behavior, contrary to the dependence of energy on  $\lambda$  which is monotonic. Therefore, in addition to ground-state energies, we also calculated the mean square distance between two electrons  $\langle |\vec{\rho}_1 - \vec{\rho}_2|^2 \rangle$  for a wide range of  $\lambda$ 's and  $\gamma$ 's. The results are displayed in Table III where we show  $\alpha^2 \langle |\vec{\rho}_1 - \vec{\rho}_2|^2 \rangle$  for values of  $\lambda=0, 1, \dots, 10$  and  $\gamma=0, 1, \dots, 5$ . In the absence of Coulomb correlations, the increase of the magnetic field brings electrons closer to each other resulting in a reduced mean square distance. However, in the presence of Coulomb correlations there are values of  $\lambda$  and  $\gamma$  where electrons find it energetically favorable to jump to outer or-

TABLE III. The optimal variational value of  $\alpha^2 \langle |\vec{\rho}_1 - \vec{\rho}_2|^2 \rangle$  for 2D quantum-dot helium subject to a magnetic field as a function of dimensionless Coulomb coupling parameter,  $\lambda = e^2 \alpha / (4\pi\epsilon_0 \epsilon_r \hbar \omega_0) = 0, 1, \dots, 10$  and values of magnetic field,  $\gamma = \omega_c / \omega_0 = 0, 1, \dots, 5$ . The parameter  $\alpha = \sqrt{m\omega_0 / \hbar}$  has the dimensionality of an inverse length.

$\lambda$	$\gamma$					
	0	1	2	3	4	5
0	2.00000	1.78885	1.41421	1.10940	0.894427	0.742781
1	3.18193	2.79350	3.19963	2.47708	1.97594	2.33444
2	4.15428	4.62431	3.56731	3.71459	2.96353	3.14825
3	4.97151	5.12920	3.92383	3.90825	3.92870	3.94601
4	5.69236	5.61781	5.35004	5.08275	4.88226	4.73529
5	6.34774	6.09048	5.62186	5.24316	4.98332	5.51752
6	6.95629	6.54753	5.89000	6.39368	5.91907	5.58307
7	7.52912	6.98994	7.27192	6.53384	6.85216	6.35681
8	8.07359	7.41855	7.49712	7.67346	6.93629	7.12900
9	8.59467	8.80371	7.72156	7.79918	7.86399	7.18439
10	9.09607	9.16053	9.08988	7.92518	7.94189	7.95454

bits (increasing the angular momentum and their mean square distance, as well) despite the effect of the magnetic field. A manifestation of this behavior comes in the form of jumps of  $\alpha^2 \langle |\vec{\rho}_1 - \vec{\rho}_2|^2 \rangle$  for magnetic field  $\gamma=1$  relative to the zero-magnetic-field case ( $\gamma=0$ ) as seen in Fig. 1. For instance, for Coulomb correlation values  $\lambda=0$  and 1 electrons are squeezed closer to each other in the presence of a magnetic field (the values of  $\alpha^2 \langle |\vec{\rho}_1 - \vec{\rho}_2|^2 \rangle$  at  $\gamma=1$  represented by empty circles are below the corresponding values at  $\gamma=0$  represented by filled circles); however, for a larger correlation, such as  $\lambda=2$ , this is not the case any more.

The increase in the mean square distance between the two electrons reflects the formation of a rotating Wigner (electron) molecule (RWM or REM). Quantum mechanically one can immediately see that  $\langle \vec{R} \rangle = 0$ , where  $\vec{R}$  is the center of

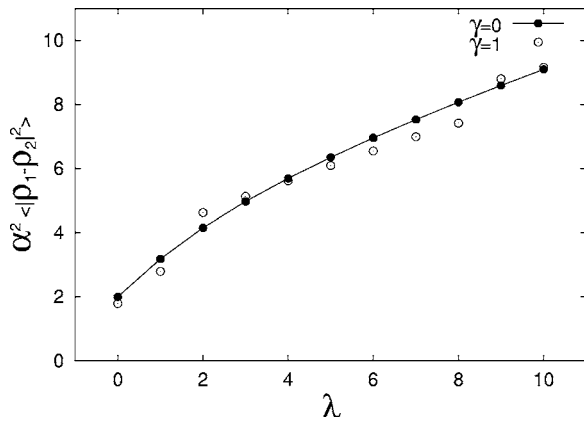


FIG. 1. Variational mean square distance between two electrons,  $\alpha^2 \langle |\vec{\rho}_1 - \vec{\rho}_2|^2 \rangle$ , for 2D quantum-dot helium system in a perpendicular magnetic field as a function of dimensionless Coulomb coupling parameter  $\lambda = e^2 \alpha / (4\pi\epsilon_0 \epsilon_r \hbar \omega_0)$  for two values of magnetic field corresponding to  $\gamma = \omega_c / \omega_0 = 0$  and 1. The line joining the data points at zero magnetic field serves as a guide to the eye.

mass (c.m.) position and  $\langle \vec{\rho}_1 \rangle = -\langle \vec{\rho}_2 \rangle$ . This represents the quantum counterpart of the classical minimum-energy configuration for two point charges in a harmonic trap which requires  $\vec{\rho}_1 = -\vec{\rho}_2$ . A plot of the electronic density will reveal that the electrons are mainly localized on a thin ring centered at the zero of the parabolic potential. The electronic density will exhibit the circular symmetry of the Hamiltonian and will only depend on distances (no angular dependence). The electronic density is insensitive to angular correlations which are very important, particularly for large values of the angular momentum. A better probe of the angular characteristics of the wave function is the conditional probability distribution (CPD) function<sup>52</sup> which for  $N$  electrons is quite generally defined as  $P(\vec{\rho}, \vec{\rho}_0) = \langle \Psi | \prod_{i=1}^N \delta(\vec{\rho}_i - \vec{\rho}) \delta(\vec{\rho}_j - \vec{\rho}_0) | \Psi \rangle / \langle \Psi | \Psi \rangle$ , where  $\Psi$  is the wave function under consideration. For the case of quantum-dot helium ( $N=2$ ) this becomes

$$P(\vec{\rho}, \vec{\rho}_0) = 2 \frac{|\Psi(\vec{\rho}, \vec{\rho}_0)|^2}{\langle \Psi | \Psi \rangle}, \quad (9)$$

where the wave function is given from Eq. (2). When calculating the CPD function the position vector of one electron,  $\vec{\rho}_0$ , is fixed, while  $\vec{\rho}$  is moved so the resulting function of  $\vec{\rho}$  measures the probability of finding one electron at  $\vec{\rho}$  given that there is one located at  $\vec{\rho}_0$ . Obviously, for any choice of  $\vec{\rho}_0 \neq 0$  the CPD function enables us to obtain the angular distribution of the second electron. Figure 2 shows the CPD function for the ground state of 2D quantum-dot helium at  $\gamma=0$  and  $\lambda=10$ . The contour plots of the CPD function shown in the present work are calculated with  $\vec{\rho}_0$  on the  $x$  axis with  $\rho_0$  corresponding to the distance at which the electronic density function (which is circular shaped) has the maximum (crudely this can be thought of as the radius of the thin ring). The black dot indicates  $\vec{\rho}_0$ . One can see clearly that the second electron is mainly localized in the opposite position of the fixed electron. This demonstrates that the

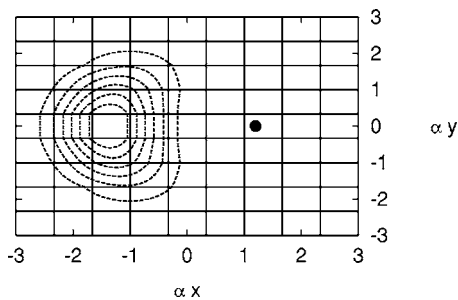


FIG. 2. Contour plots of the CPD function  $P(\vec{\rho}, \vec{\rho}_0)$  corresponding to the displaced Gaussian ground-state wave function for 2D quantum-dot helium at zero magnetic field ( $\gamma=0$ ) and  $\lambda=10$ . The black dot denotes the location of the fixed electron situated at position  $\alpha\vec{\rho}_0=(\alpha x_0 \neq 0, 0)$ . Distances are given in dimensionless units where  $\alpha$  is the inverse oscillator length  $\sqrt{m\omega_0/\hbar}$ .

quantum ground state has the same symmetry as the classical lowest-energy configuration.

#### IV. DISCUSSION

Beyond the ground-state energetics and ground-state angular momenta, we test the accuracy of the trial wave function in two well-known limits: (i) the infinite-magnetic-field limit ( $\gamma \rightarrow \infty$ ) where the ground-state energy should approach the energy of a classical system of  $N=2$  point charges in a parabolic potential (adjusted by the quantum zero-point energy when Coulomb correlations are absent), and (ii) the lowest-Landau-level limit where the ground-state energy of the trial wave function must coincide with the lowest-Landau-level Laughlin wave function for  $N=2$  electrons without the parabolic potential confinement.

To study limit (i) we calculate the lowest classical energy  $E_c$  for  $N=2$  point charges in a harmonic potential, which in dimensionless units is

$$\epsilon_c = \frac{E_c}{\hbar\omega_0} = \frac{3}{4}(2\lambda)^{2/3}. \quad (10)$$

We note that the classical energy is not affected by the presence or absence of a magnetic field. The classical ground-state configuration for  $N=2$  electrons is one in which the respective positions of the particles are exactly opposite to each other at an optimal distance,  $\vec{\rho}_1 = -\vec{\rho}_2 \neq \vec{0}$ .

Naturally, one cannot immediately compare the quantum variational energy  $\epsilon$  to its classical counterpart  $\epsilon_c$  since without Coulomb correlations ( $\lambda=0$ ) the lowest quantum energy  $\epsilon$  is nonzero while the lowest classical energy  $\epsilon_c$  is zero. This difference in energy between the two quantities represents the quantum zero-point energy (at  $\lambda=0$ ) which in dimensionless units is

$$\epsilon_0 = \frac{E_0}{\hbar\omega_0} = 2\sqrt{1 + \frac{\gamma^2}{4}}. \quad (11)$$

If we adjust the classical energy by  $\epsilon_0$  the quantities to compare are  $\epsilon$  versus  $(\epsilon_c + \epsilon_0)$ . Figure 3 shows the variational ground-state energy of 2D quantum-dot helium in a perpen-

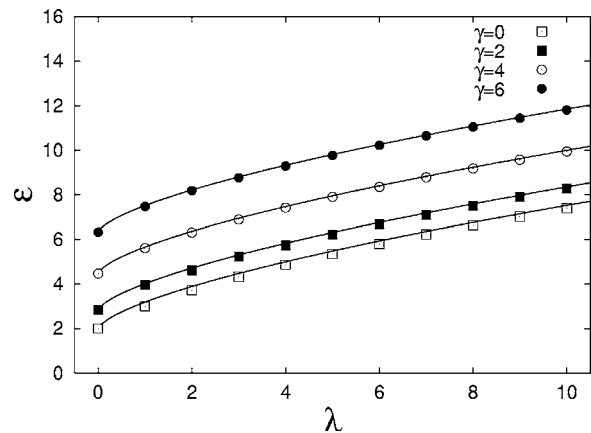


FIG. 3. Variational ground-state energy of 2D quantum-dot helium in a perpendicular magnetic field  $\epsilon=E/(\hbar\omega_0)$  as a function of dimensionless Coulomb coupling parameter  $\lambda=e^2\alpha/(4\pi\epsilon_0\epsilon\hbar\omega_0)$  for values of magnetic field corresponding to  $\gamma=\omega_c/\omega_0=0, 2, 4$ , and 6. The solid lines represents the “adjusted” classical energy  $\epsilon_c+\epsilon_0$  as a function of  $\lambda$  calculated at the given  $\gamma$  values.

dicular magnetic field  $\epsilon$  and the adjusted classical energy  $\epsilon_c + \epsilon_0$  (solid lines) as a function of Coulomb correlation parameter  $\lambda$  for selected values of the magnetic field parameter  $\gamma$ . Quite surprisingly there is very good agreement between the “quantum” ground-state energy and the “adjusted classical” ground-state energy at all magnetic fields including weak magnetic fields. As the magnetic field grows (increasing values of  $\gamma$ ) the agreement only improves as can clearly be seen from the data. We also checked that in the infinite-magnetic-field limit ( $\gamma \rightarrow \infty$ ) both  $\epsilon(\text{variational}) - \epsilon_0$  and  $\epsilon(\text{diag}) - \epsilon_0$  tend to  $\epsilon_c(\text{classical})$ . This behavior was first noted by Yannouleas and Landman<sup>22</sup> in a study in which RWM wave functions were used to describe few-electron quantum dots. They also recognized the importance of such finding in challenging the composite fermion picture of quantum dots, which instead implies that  $\epsilon - \epsilon_0 \rightarrow 0$  as  $\gamma \rightarrow \infty$ . The same result is obtained here, using not the RWM wave function, but the displaced Gaussian variational wave function.

To check limiting behavior (ii) we use the Laughlin wave function to calculate the energies for the same  $\lambda$ 's and  $\gamma$ 's in which the displaced Gaussian trial wave function was used and then compare the results. The ground-state energies obtained with the Laughlin wave function are displayed in Table IV. The angular momentum  $m_z$  for which the lowest Laughlin energy is obtained is also specified. As expected, one notes that the Laughlin wave function is not a good description of the system at weak (and zero) magnetic fields (for instance, there are several occasions in which the Laughlin ground-state energy has the wrong angular momentum, such as the cases  $\gamma=0$  and  $\lambda=2, 3, \dots$ , etc.). However, comparing the energies in Table II–IV one sees that, in the limit of strong magnetic fields (increasing  $\gamma$ 's), the ground-state energy of the displaced Gaussian variational wave function quickly approaches the Laughlin values. This is clearly seen in Fig. 4 where we plot the ground-state energy corresponding to the displaced Gaussian variational wave function and the Laughlin wave function for  $\lambda=2$  and 6 as a function of

TABLE IV. Ground-state energies  $\epsilon=E/(\hbar\omega_0)$  corresponding to the Laughlin wave function for 2D quantum-dot helium subject to a perpendicular magnetic field for given values of dimensionless parameters  $\lambda$  and  $\gamma$ . The angular momentum  $m_z$  of the ground state is also specified.

$\lambda$	$\gamma$					
	0	1	2	3	4	5
0	2.00000 $m_z=0$	2.23607 $m_z=0$	2.82843 $m_z=0$	3.60555 $m_z=0$	4.47214 $m_z=0$	5.38516 $m_z=0$
1	3.25331 $m_z=0$	3.51671 $m_z=1$	3.98787 $m_z=1$	4.74972 $m_z=1$	5.64527 $m_z=1$	6.54155 $m_z=2$
2	4.25331 $m_z=1$	4.17932 $m_z=1$	4.73309 $m_z=1$	5.47320 $m_z=2$	6.34988 $m_z=2$	7.24827 $m_z=3$
3	4.87997 $m_z=1$	4.84193 $m_z=1$	5.33361 $m_z=2$	6.09150 $m_z=3$	6.93735 $m_z=3$	7.84253 $m_z=4$
4	5.50663 $m_z=1$	5.45996 $m_z=2$	5.89253 $m_z=2$	6.61737 $m_z=3$	7.46625 $m_z=4$	8.37252 $m_z=5$
5	6.13329 $m_z=1$	5.95692 $m_z=2$	6.39990 $m_z=3$	7.11735 $m_z=4$	7.95855 $m_z=5$	8.86033 $m_z=6$
6	6.75994 $m_z=1$	6.45388 $m_z=2$	6.86566 $m_z=3$	7.57749 $m_z=4$	8.41976 $m_z=5$	9.31802 $m_z=7$

the magnetic field parameter  $\gamma$ . The convergence of variational and Laughlin ground-state energies in the limit of strong magnetic field is quite general and happens at any arbitrary value of the Coulomb correlation strength  $\lambda$ , though for clarity of the plot in Fig. 4 we display only the curves corresponding to  $\lambda=2$  and 6.

Given the very good performance of the trial wave function in describing 2D quantum-dot helium in an arbitrary perpendicular magnetic field, we plan to generalize the treatment to larger quantum dots. In this case the liquid or solid (crystalline) character of larger quantum dots in a magnetic field is rather nontrivial and crucially depends on the values of  $\gamma$  and  $\lambda$  as well as the density of the system. To that effect

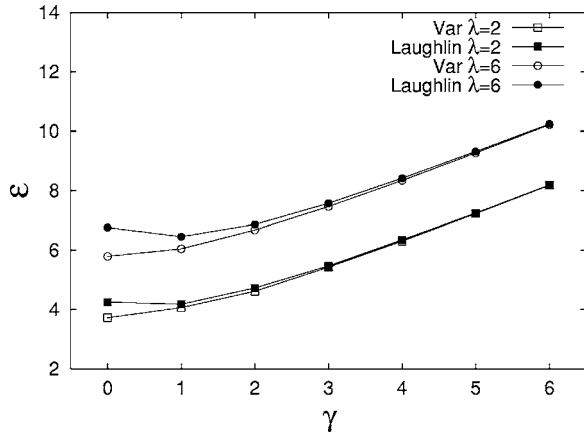


FIG. 4. The ground-state energy curves  $\epsilon=E/(\hbar\omega_0)$  as a function of the magnetic field parameter  $\gamma$  for the case of displaced Gaussian variational wave function (Var) and Laughlin's wave function (Laughlin) for two values of the Coulomb correlation strength,  $\lambda=2$  and 6. The solid lines joining the data points serve as a guide to the eye.

we would describe any 2D quantum dot in a perpendicular magnetic field with a generalized trial wave function of the form

$$\Psi_N = \prod_{i<j}^N [J(\rho_{ij}) \times (z_i - z_j)^n] D_{\uparrow}(\Phi) D_{\downarrow}(\Phi) \chi(S), \quad (12)$$

where  $N$  is the number of electrons in the dot,  $\chi(S) = \chi(s_1, s_2, \dots, s_N)$  is the spin function for  $N_{\uparrow}$  spin-up and  $N_{\downarrow} = N - N_{\uparrow}$  spin-down electrons, and the space wave function has a Jastrow-Slater form. The determinants  $D_{\uparrow}(\Phi)$  and  $D_{\downarrow}(\Phi)$  are Slater determinants for spin-up and spin-down electrons built out of (i) Fock-Darwin (FD) orbitals<sup>53,54</sup> or (ii) Gaussian localized orbitals<sup>55</sup> (for a crystalline state, only). The displaced Gaussian pair correlation factor  $J(\rho_{ij})$  as specified in Eq. (3) guarantees the quality of the wave function at all magnetic fields ranging from weak (and zero) to strong, and the integer quantum number,  $n=0, 1, 2, \dots$  which takes even (odd) values for, respectively, antisymmetric (symmetric) spin functions determines the overall parity of the space wave function as required by Pauli's principle. In such a case, a full VMC simulation would be the method of choice and the optimized trial wave function can be further used as a guiding function for DMC calculations.

## V. CONCLUSIONS

To conclude, we have introduced a very accurate trial wave function for 2D quantum-dot helium in an arbitrary perpendicular magnetic field. A key element of this description is a Jastrow pair correlation factor that has a displaced Gaussian form and contains two variational parameters to optimize. The variational energies are in excellent agreement with exact numerical diagonalization calculations at any



value of the perpendicular magnetic field including weak (and zero) or strong fields. In agreement with the RWM formalism we find that, for given values of the Coulomb correlation strength, the quantum ground-state energy of 2D quantum-dot helium at any value of the magnetic field is close to the value of the adjusted classical energy. Quantum and classical energies converge in the limit of infinite magnetic field. For a given Coulomb correlation strength and in the limit of infinite magnetic field, the energies of the displaced Gaussian trial wave function agree very well with the energies obtained from Laughlin's wave function, though we note that Laughlin's wave function is a poor description of the system for weak (zero) and intermediate magnetic fields. For weak (zero) and intermediate magnetic fields a Jastrow pair correlation factor of the nature studied in this work should be included in the total wave function in conjunction with the Laughlin or RWM component, which are most effective in high magnetic fields. A Jastrow pair correlation factor, such as the displaced Gaussian factor introduced in this study, is essential to provide an accurate description of the system at any value of the magnetic field not limited to

high magnetic fields only. Other Jastrow pair correlation factors such as those constructed through Padé approximations with several variational parameters<sup>48</sup> also provide quite an accurate description of the system and compare favorably with exact diagonalization results. However, the displaced Gaussian pair correlation factor is a very intuitive and simple physical choice that guarantees a consistent and excellent description of quantum-dot helium system at all magnetic fields ranging from weak (zero) to infinity. A generalization of this trial wave function for  $N$ -electron quantum dots in a perpendicular magnetic field is also discussed.

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