

## Variational study of two-electron quantum dots

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Low-lying energy levels of two interacting electrons confined in a two-dimensional parabolic quantum dot and subjected to an external uniform magnetic field have been calculated by using a variational method based on a direct construction of trial wave functions from the quasi-exact analytic solution of the problem. This nonperturbative method not only allows us to obtain accurate results, valid for the whole range of both spatial confinement length and the strength of the magnetic field, but also enables us to compare its analytical results with those previously found in the literature, which are crucial because of testing its reliability. It is found that our results are in excellent agreement with those of the particular exact analytical results, and are convincingly better than those found by using the uncorrelated Landau level wave functions. In fact, the approximate analytical scheme proposed here covers these results in a self-consistent manner; in other words, those can be easily reproduced by just attributing some certain values to the parameters included in the formulation. Furthermore, we have compared our results for the ground-state energy with those obtained by using conventional techniques such as Hartree, Hartree-Fock, exact diagonalization, and quantum Monte Carlo methods. We show that, in addition to its satisfactory internal consistency, our approach yields significant improvement over the Hartree, Hartree-Fock, exact diagonalization treatments, and its results are in agreement with those of the Monte Carlo analysis. Therefore, the approach and its results proposed here would be more helpful to discuss the size dependent properties of low-lying energy levels of two-dimensional parabolic quantum dots with two and specifically several electrons.

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The experimental realization<sup>1-4</sup> of quasi-two-dimensional (2D) disklike quantum dots (QDs) has stimulated great theoretical efforts towards interpretation of their various physical properties arising from the reduced dimensionality. Among these studies, attention has been focused in particular on understanding the quantum mechanical behavior of two interacting electrons confined in various 2D dot geometries under the influence of an external magnetic field, due to the fact that electron-electron interactions which are known to be quite important<sup>5</sup> in such quasi-zero-dimensional structures are enhanced by the presence of an additional confinement arising from the magnetic field. Moreover, it is commonly accepted that, since there is some direct experimental evidence that indicates QDs with just a few electrons are well described by the harmonic well potential, the 2D parabolic potential for the simulation of spatial confinement is ideally suited to study the quantum mechanical problem of two interacting electrons under the influence of a uniform magnetic field in two space dimensions. Consequently, several analytical studies in this model, as well as numerical ones, such as Hartree, Hartree-Fock (HF), exact diagonalization (ED), oscillator representation, exact numerical diagonalization, local spin density approximation (LSDA), and quantum Monte Carlo (QMC) methods, have been developed in the literature.<sup>6-16</sup>

It is well known that a system of two interacting electrons confined in a 2D parabolic potential and subjected to a uniform magnetic field is a quasi-exactly solvable quantum mechanical problem due to having a hidden  $sl_2$  algebraic structure.<sup>17</sup> In other words, the complicated nature of the recursion relations appeared in solving the associated radial part of the relevant Schrödinger equation does not allow in general an exact solution, except for the case that some cer-

tain relations between the Coulomb repulsion strength and the strength of the magnetic field and/or spatial confinement exist. As a result, the studies on exact treatments<sup>18-23</sup> so far have been content with just obtaining a few eigenvalues and their related eigenstates. There exists, however, a study<sup>24</sup> being capable of determining the general closed form solution for these states together with their associated eigenvalues, which has been very recently introduced. A full description of the quasi-exact analytical solutions to the problem, together with a comparative analysis and references to some of the relevant studies can also be found in Ref. 24.

These exact results, even for certain values of confinement potential and/or magnetic field strengths, provide to perform some tests for approaches schemed for the full problem, and are always appropriate to have an opinion in more complex circumstances, e.g., in the case of more than two electrons. For these reasons, in this paper we analyze the problem of two interacting electrons confined in a 2D parabolic QD potential and subjected to a magnetic field by means of a variational scheme based on the construction of trial wave functions from those obtained along with quasi-exact analytical procedure, in which the size dependence and the magnetic field evolution of the ground-state and excited-state energies of the system can be obtained analytically, without further restriction on spatial confinement and magnetic field strengths. We find that our calculated results agree quite excellent with those obtained by the quasi-exact analytical procedure, and give estimates for the energies lower than those found by using the wave functions of the uncorrelated Landau levels (LLs) and Hartree, Hartree-Fock (HF), and exact diagonalization schemes, as well. In other words, by assigning certain values to the variational parameters included in the present approach, one can easily reproduce

both the particular analytical results and the well-known spectrum of a system of two independent harmonic oscillators in 2D plus the expectation value of the Coulomb repulsion term calculated by means of the wave functions of these oscillators. In fact, the latter yields the first-order perturbation results whose validity are limited to very high magnetic fields, and also to QDs whose sizes are much smaller than the effective Bohr radius.

The Hamiltonian for a system of two interacting electrons in the presence of both an external uniform magnetic field and a parabolic potential can be written as

$$H = \sum_{j=1}^2 \left\{ \frac{1}{2m^*} \left[ \mathbf{p}(\mathbf{r}_j) + \frac{e}{c} \mathbf{A}(\mathbf{r}_j) \right]^2 + \frac{1}{2} m^* \omega_c^2 \mathbf{r}_j^2 \right\} + \frac{e^2}{\epsilon_\infty |\mathbf{r}_1 - \mathbf{r}_2|}, \quad (1)$$

where  $\omega_c$  is the strength of spatial confinement, and  $m^*$  and  $\epsilon_\infty$  are the effective mass of each electron and the high frequency dielectric constant, respectively. For the purpose of our discussion, we introduce the relative and the center-of-mass (CM) coordinates,  $\mathbf{r} = |\mathbf{r}_1 - \mathbf{r}_2|$  and  $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ , respectively. Therefore, one can easily separate out the CM motion from Eq. (1). Consequently, the resultant Hamiltonian operator in the CM coordinate system is given by

$$H_{\text{CM}} = \frac{1}{2M} \left[ \mathbf{P}_{\mathbf{R}} + \frac{Q}{c} \mathbf{A}(\mathbf{R}) \right]^2 + \frac{1}{2} M \omega_c^2 \mathbf{R}^2, \quad (2)$$

where  $Q = 2e$  and  $M = 2m^*$ . If the symmetric gauge  $\mathbf{A}(\mathbf{R}) = \mathbf{B} \times \mathbf{R}/2$  is chosen for the vector potential of the magnetic field, Eq. (2) can then be written as a sum of two terms; the usual 2D isotropic harmonic oscillator Hamiltonian with frequency  $\omega = [\omega_c^2 + (\omega_c^2/4)]^{1/2}$  denoted by  $H_{2\text{D}}(M, \omega)$  symbolically, plus a term proportional to  $L_Z$ . Here,  $\omega_c = QB_0/Mc$  is the cyclotron frequency and  $L_Z$  is the  $Z$  component of the angular momentum operator which commutes with the first part of the Hamiltonian, i.e.,  $H_{2\text{D}}(M, \omega)$ . Since the total wave function  $\Psi(\mathbf{r}, \mathbf{R})$  of the system can be written in a simple product form  $\Psi(\mathbf{r})\Psi(\mathbf{R})$ , the normalized eigenfunctions of Eq. (2) and the corresponding eigenvalues are well-known,<sup>25,26</sup> and they are given by

$$\Psi_{n_2, m_2}(\mathbf{R}) = (-1)^{n_2} \frac{\beta^{|m_2|+1}}{\sqrt{\pi}} \left[ \frac{n_2!}{(n_2 + |m_2|)!} \right]^{1/2} e^{-\beta^2 \mathbf{R}^2/2} R^{|m_2|} L_{n_2}^{|m_2|} \times (\beta^2 \mathbf{R}^2) e^{im_2 \phi}, \quad (3)$$

and

$$E_{n_2, m_2} = (2n_2 + |m_2| + 1) \hbar \omega + m_2 \frac{\hbar \omega_c}{2}, \quad (4)$$

with  $\beta^2 = M\omega/\hbar$ , respectively. It should be noted that Eq. (4) reduces to the familiar Landau levels  $E_{n_2, m_2}(\omega_c = 0) = (2n_2 + |m_2| + m_2 + 1) \hbar \omega_c/2$  and two dimensional harmonic oscillator energy levels  $E_{n_2, m_2}(\omega_c = 0) = (2n_2 + |m_2| + 1) \hbar \omega$  in the absence of the spatial confinement and the magnetic field, respectively.

The main issue in the present work lies in the solution of relative motion (RM) Hamiltonian given by

$$H_{\text{RM}} = \frac{1}{2\mu} \left[ \mathbf{p}_{\mathbf{r}} + \frac{q}{c} \mathbf{A}(\mathbf{r}) \right]^2 + \frac{1}{2} \mu \omega_c^2 \mathbf{r}^2 + \frac{e^2}{\epsilon_\infty |\mathbf{r}|}, \quad (5)$$

where  $q = e/2$  and  $\mu = m^*/2$ . We solve this equation by a variational procedure based on the choice of trial wave functions given by

$$\Psi_{m_1}(\mathbf{r}) = \frac{\gamma_{|m_1|+1}^{|m_1|+1}}{\sqrt{\pi}} \sqrt{f_{m_1}^{(0)}} \left( 1 + \frac{b}{2|m_1|+1} \gamma_{|m_1|} r \right) r^{|m_1|} e^{-\gamma_{|m_1|}^2 r^2/2} e^{im_1 \phi}, \quad (6)$$

with normalization constants

$$f_{m_1}^{(0)} = \left[ \Gamma(|m_1| + 1) + 2 \frac{b}{a} \Gamma\left(|m_1| + \frac{3}{2}\right) + \left(\frac{b}{a}\right)^2 \Gamma(|m_1| + 2) \right]^{-1},$$

where we have introduced the abbreviation  $a$  to denote  $2|m_1|+1$ , in which the quantum numbers  $m_1$  can take values  $0, \pm 1, \pm 2, \dots$ . In Eq. (6),  $b$  and  $\gamma_{|m_1|}$  are the variational parameters to be determined by requiring that the energy functional calculated by means of Eq. (6) has a minimum. In fact, with a particular choice of the relevant parameters, the eigenvalues calculated with the help of Eq. (6) should reproduce the quasi-exact analytical results as mentioned before. Additionally, as it was shown by Taut<sup>19</sup> that, by constructing the total wave function of such a system as products consisting of the CM part given by Eq. (3) with  $n_2=0$  and  $m_2=0$ , and the RM part described by Eq. (6), but with  $b=0$ , one reaches the Laughlin wave functions (LWFs). There was also stated that the full states with  $m_1 = -1$  and  $m_1 = +1$  are the uncorrelated solutions of two full LLs, and hence such a total wave function comprises LWFs and the uncorrelated LLs as special cases. Therefore, one can expect that the trial wave functions given by Eq. (6) provide the lowest eigenvalues for Eq. (5). The resultant energy functional obtained by using Eq. (6) can be expressed in terms of variational parameters in the form

$$E_{m_1} = \frac{\hbar^2}{2\mu} \gamma_{|m_1|}^2 f_{m_1}^{(1)} + \frac{1}{2} \mu \omega_c^2 \frac{1}{\gamma_{|m_1|}^2} f_{m_1}^{(2)} + m_1 \frac{\hbar \omega_c}{2} + \frac{e^2}{\epsilon_\infty} \gamma_{|m_1|} f_{m_1}^{(3)}, \quad (7)$$

with

$$f_{m_1}^{(1)} = f_{m_1}^{(0)} \left\{ \left[ 2(|m_1| + 1) - (2|m_1| + 1) \left(\frac{b}{a}\right)^2 \right] \Gamma(|m_1| + 1) + (4|m_1| + 6) \left(\frac{b}{a}\right) \Gamma\left(|m_1| + \frac{3}{2}\right) + (2|m_1| + 4) \left(\frac{b}{a}\right)^2 \Gamma(|m_1| + 2) - 2 \left(\frac{b}{a}\right) \Gamma\left(|m_1| + \frac{5}{2}\right) - \left(\frac{b}{a}\right)^2 \Gamma(|m_1| + 3) - (2|m_1| + 1) \left(\frac{b}{a}\right) \Gamma\left(|m_1| + \frac{1}{2}\right) - \Gamma(|m_1| + 2) \right\},$$

$$f_{m_1}^{(2)} = f_{m_1}^{(0)} \left[ \Gamma(|m_1| + 2) + 2 \left( \frac{b}{a} \right) \Gamma \left( |m_1| + \frac{5}{2} \right) + \left( \frac{b}{a} \right)^2 \Gamma(|m_1| + 3) \right],$$

$$f_{m_1}^{(3)} = f_{m_1}^{(0)} \left[ \Gamma \left( |m_1| + \frac{1}{2} \right) + 2 \left( \frac{b}{a} \right) \Gamma(|m_1| + 1) + \left( \frac{b}{a} \right)^2 \Gamma \left( |m_1| + \frac{3}{2} \right) \right]. \quad (8)$$

In Eq. (7),  $\omega_c$  is again cyclotron frequency, and is equivalent to  $qB_0/\mu c = eB_0/m^*c$ , just as in the case that for the CM motion. We now introduce the standard effective atomic units so as to measure the energies in units of the effective Rydberg constant, and all the lengths in terms of the corresponding unit of length, i.e., the effective Bohr radius. They are given by the standard formulae  $R^* = m^*e^4/2\epsilon_\infty^2\hbar^2$  and  $a_0^* = \epsilon_\infty\hbar^2/m^*e^2$ , respectively. In other words, the energies and all the lengths are measured in units of  $\hbar\omega_0 = 2R^* = \hbar^2/m^*a_0^{*2}$  and  $a_0^* = (\hbar/m^*\omega_0)^{1/2}$ , respectively. Therefore, in these units, the cyclotron frequency  $\omega_c$ , the confinement frequency  $\omega_*$  and the associated confinement length  $\ell_* = (\hbar/m\omega_*)^{1/2}$  are all measured in terms of  $\omega_0$  and  $a_0^*$ , respectively, in such a way that  $\bar{\omega}_c = \omega_c/\omega_0$ ,  $\bar{\omega}_* = \omega_*/\omega_0$ , and  $\bar{\ell}_* = \ell_*/a_0^* = (1/\bar{\omega}_*)^{1/2}$ . Additionally, the variational parameters  $\gamma_{|m_1|}$  can also be made dimensionless by rescaling them with the effective Bohr radius, i.e.,  $a_0^*\gamma_{|m_1|} = 1/\bar{\gamma}_{|m_1|}$ . Then, in these units, Eq. (7) can be rewritten as

$$\bar{E}_{m_1} = \frac{1}{\bar{\gamma}_{|m_1|}^2} f_{m_1}^{(1)} + \frac{1}{4} \bar{\omega}^2 \bar{\gamma}_{|m_1|}^{-2} f_{m_1}^{(2)} + m_1 \frac{\bar{\omega}_c}{2} + \frac{1}{\bar{\gamma}_{|m_1|}} f_{m_1}^{(3)}, \quad (9)$$

where we have used the relation  $e^2/\epsilon_\infty = \hbar\omega_0 a_0^*$ . Our further considerations on Eq. (9) will be carried out in the following two ways.

The first one concerns simply the minimization of Eq. (9) with respect to  $\bar{\gamma}_{|m_1|}$ . This leads to a fourth order equation in  $\bar{\gamma}_{|m_1|}$ ,

$$\bar{\omega}^2 \bar{\gamma}_{|m_1|}^4 f_{m_1}^{(2)} - 2 \bar{\gamma}_{|m_1|} f_{m_1}^{(3)} - 4 f_{m_1}^{(1)} = 0. \quad (10)$$

As was pointed out before, with some particular choices of the relevant parameters, Eq. (9) together with Eq. (10) should reproduce correctly the uncorrelated results, and the quasi-exact results as well. To show this, we first start with the discussion of the case with  $b=0$  at high confinement limit (high spatial confinement and/or large magnetic field), namely, when  $\bar{\omega} \gg e^2/\epsilon_\infty \hbar\omega_0 a_0^*$ . In this case, one can easily check that, with  $b=0$ , Eqs. (8) yields  $f_{m_1}^{(1)} = f_{m_1}^{(2)} = |m_1| + 1$  and  $f_{m_1}^{(3)} = \Gamma(|m_1| + 1/2)/\Gamma(|m_1| + 1)$ , and hence the high confinement limit imposes the approximate solution  $\bar{\gamma}^2 = 2/\bar{\omega}$  to Eq. (10). On substituting these results back into Eq. (9) the energy expression becomes

$$\bar{E}_{m_1} = (|m_1| + 1) \bar{\omega} + m_1 \frac{\bar{\omega}_c}{2} + \sqrt{\frac{\pi}{2}} \frac{(2|m_1| - 1)!!}{(2|m_1|)!!} \sqrt{\frac{\pi}{2}}, \quad (11)$$

which is exactly the well-known first order perturbation result, and coincides with the expressions obtained by Wagner *et al.*<sup>8</sup> However, its accuracy is limited, and therefore is valid only for  $\bar{\omega} \gg 1$ , i.e., for  $\bar{\ell}_* \ll [1 + (\bar{\omega}_c/2\bar{\omega}_*)^2]^{1/4}$  from which one can deduce two obvious limitations on the energy expression, Eq. (11): one concerns the absence of the magnetic field ( $\bar{\omega}_c = 0$ ), in this case, Eq. (11) is valid only for QDs whose size are much smaller than the effective Bohr radius  $\bar{\ell}_* \ll 1$ , while the other imposes that, in the absence of spatial confinement  $\bar{\omega}_* = 0$ , Eq. (11) is valid only for magnetic fields satisfying the requirement  $\bar{\omega}_c \gg 2$ . In terms of the material parameters of GaAs,  $\hbar\omega_0 = 11.857$  meV and  $a_0^* \approx 98$  Å, these limitations define a region that Eq. (11) is valid only for sufficiently small GaAs QDs or sufficiently large magnetic fields, i.e., for  $\ell_* \ll 100$  Å and  $B \gg 13.7$  T, respectively. Secondly, if one imposes the conditions  $b^2 = 2a$  and  $\bar{\gamma}_{|m_1|} = b$  it is easy to check that  $\bar{\gamma}_{|m_1|}^2 = 2/\bar{\omega}$  is again the solution of Eq. (10), and yields eigenvalues

$$\bar{E}_{m_1} = \bar{\omega} [f_{m_1}^{(1)} + f_{m_1}^{(2)} + f_{m_1}^{(3)} + m_1 \bar{\omega}_c / \bar{\omega}] / 2, \quad (12)$$

but now with the condition

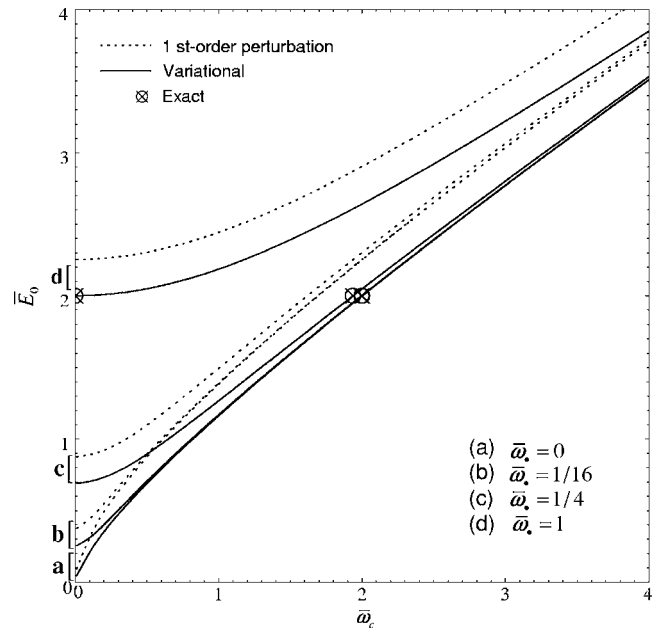


FIG. 1. The ground-state energy as a function of  $\bar{\omega}_c$  for three different approaches; (i) perturbation theory (dashed lines) obtained from Eq. (11), (ii) the present analytical approximation (solid lines) obtained from Eq. (9) together with Eq. (14), and (iii) quasi-exact results (denoted by the symbol  $\otimes$ ). By the relation between the dimensionless confinement frequency and length,  $\bar{\ell}_* = (1/\bar{\omega}_*)^{1/2}$ , while  $\bar{\omega}_* = 0$  represents the 2D bulk case,  $\bar{\omega}_* = 1/16$ ,  $1/4$ , and  $1$  corresponds to QDs whose size are  $\ell_* = 4a_0^*$ ,  $2a_0^*$ , and  $a_0^*$ , respectively.

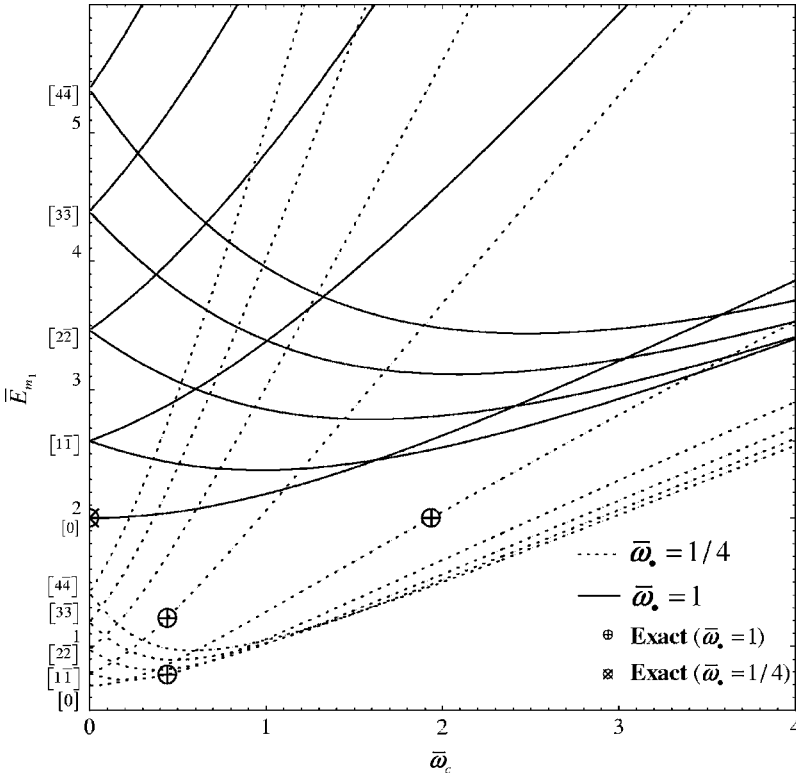


FIG. 2. The energy levels  $\bar{E}_{m_1}$  of two interacting electrons in a 2D parabolic QD with two different confinement lengths as a function of a magnetic field. Here, the curves are labeled by parenthesized numbers  $[m_1 \bar{m}_1]$  that denotes energy levels with positive and negative  $m_1$  values. The curves having lower energies correspond to energy levels with negative  $m_1$  values.

$$\bar{\omega}^{-1} = 2|m_1| + 1. \quad (13)$$

Equation (12) together with Eq. (13) leads to the same analytical expressions as those found in Refs. 18, 19, and 24. In other words, it is straightforward to show that, by using the definitions of  $f_{m_1}^{(i)}$ 's in Eq. (8), quasi-exact energy eigenvalues are found to be  $\bar{E}_{m_1} = \bar{\omega}[|m_1| + 2 + m_1 \bar{\omega}_c / 2\bar{\omega}]$ . However, of these eigenvalues, only those which satisfy the condition in Eq. (13) are allowed. Thirdly and finally, to find analytical results being valid for the whole range of  $\bar{\omega}$  one needs to find the roots of Eq. (10). This can be done by solving Eq. (10) analytically in terms of the parameters included. It can be easily shown that the real root of Eq. (10) minimizing Eq. (9) can be found as

$$\bar{\gamma}_{|m_1|} = \frac{1}{2} \{ [h_{|m_1|}^{(2)} - h_{|m_1|}^{(3)}]^{1/2} + [h_{|m_1|}^{(3)} - h_{|m_1|}^{(2)} + 4f_{|m_1|}^{(3)} / (\bar{\omega}^2 f_{|m_1|}^{(2)}) [h_{|m_1|}^{(2)} - h_{|m_1|}^{(3)}]^{1/2} \}, \quad (14)$$

with

$$h_{|m_1|}^{(1)} = \{ 9\bar{\omega}^2 f_{|m_1|}^{(2)} [f_{|m_1|}^{(3)}]^2 + 3^{1/2} (1024\bar{\omega}^6 [f_{|m_1|}^{(1)}]^3 [f_{|m_1|}^{(2)}]^3 + 27\bar{\omega}^4 [f_{|m_1|}^{(2)}]^2 [f_{|m_1|}^{(3)}]^4)^{1/2} \}^{1/3}, \quad (15)$$

and  $h_{|m_1|}^{(2)} = 2^{1/3} h_{|m_1|}^{(1)} / 3^{2/3} \bar{\omega}^2 f_{|m_1|}^{(2)}$ ,  $h_{|m_1|}^{(3)} = 2^{2/3} 8 f_{|m_1|}^{(1)} / 3^{1/3} h_{|m_1|}^{(1)}$ . Figure 1 compares our results for various confinement lengths with those obtained by using both perturbation and quasi-exact analytical treatments. From the figure, it can be easily seen that our analytical results obtained above provides better results than those found in the perturbation theory, and substantially agree with the results from the exact treatments,

performed in Refs. 18, 19, and 24, indicating that our approximation is reasonable. It should be emphasized here that, even in the case of strong confinement, i.e.,  $\bar{\omega} \gg 1$ , the perturbation calculation cannot accurately describe very small QDs. In Fig. 2, we plot our analytical results for  $\bar{E}_{m_1}$  for two different confinement lengths as a function of the dimensionless magnetic field  $\bar{\omega}_c$ . To further check the sensitivity of our approximation to the exact ones, we also included exact values in this figure for comparison. There is again seen a clear consistency between the quasi-exact and variational results.

The other way of treating Eq. (9) is to consider both  $b$  and  $\bar{\gamma}_{|m_1|}$  as variational parameters. In this case, the low-lying energy levels of two electron quantum dots can be found by minimizing Eq. (9) with respect to  $b$  and  $\bar{\gamma}_{|m_1|}$  numerically. The computed  $b_{m_1}^2$  and  $\bar{\gamma}_{m_1}$  and the associated energy levels for  $m=0, \pm 1$  are presented in Fig. 3 as a function of the dimensionless magnetic field  $\bar{\omega}_c$  for  $\bar{\omega} = 1/16$ . Here,  $\bar{\omega} = 1/16$  represents a QD with radius  $\ell \ll 4a_0^*$ .  $\bar{E}_{|m_1|}$  curves in Fig. 3 show a similar behavior to those obtained in Fig. 1, and are again in agreement with the exact results. We also compare the computed  $b_{m_1}^2$  and  $\bar{\gamma}_{m_1}$  curves with their exact values, and found close agreement between them. We note that the two pairs of curves are much closer to each other as  $\bar{\omega}_c$  goes to higher values, implying that, for perturbational description of the problem,  $\bar{\gamma}^2 = 2/\bar{\omega}$  is a reasonable solution for all  $m_1$  values in this region.

In order to reveal the difference of the above numerical calculation from the previous analytical one, the computed ground-state energies of a 2D QD with two electrons for a range of magnetic field (varying from zero to 5 T) by using the experimental parameters for GaAs QD with confining energy  $\hbar\omega_c = 3.32$  meV given in Ref. 16 are listed in Table I.

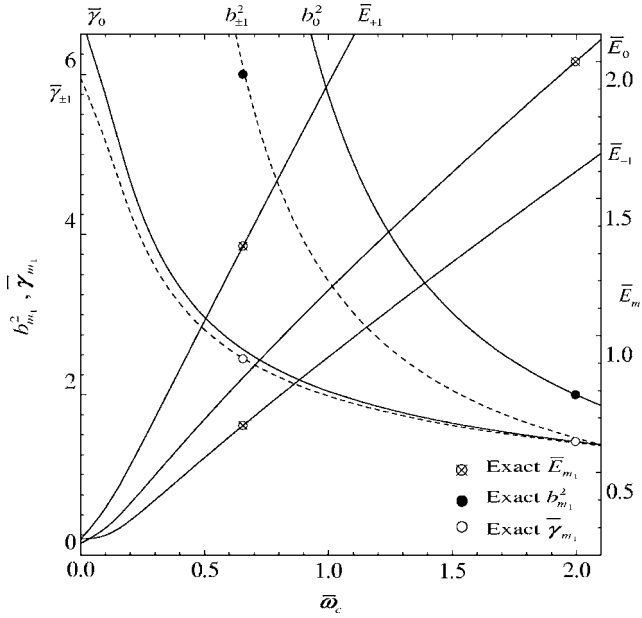


FIG. 3. The energy levels  $\bar{E}_{m_1}$  obtained from the numerical solution of Eq. (9), and dimensionless variational parameters  $b_{m_1}^2$  and  $\bar{\gamma}_{m_1}$  as a function of a magnetic field for  $\bar{\omega}_z=1/16$ . The left-handed scale is for variational parameters, while the right-handed one is for  $\bar{E}_{m_1}$ .

This provides not only some insight into how much energy is gained by using two-parameter numerical minimization as compared to the analytical one in practice, but also enables us to discuss the differences to the approaches used previously in the literature. Of these, the QMC analysis, which yields the exact energy within only a statistical error for the two-electron spin-singlet system, is a powerful tool for calculating the ground-state and excited-state energies for QDs with several electrons. Pederiva *et al.*<sup>16</sup> have performed calculations for the ground-state and excited-state energies for

TABLE I. The ground-state energies (in units of  $\hbar\omega_0$ ) for three different approaches. The results of these approaches are presented as a function of the magnetic field (in Tesla) up to  $5T$ . Here,  $E_0^P, E_0^A$ , and  $E_0^N$  refer, respectively to, perturbation, analytical, and numerical results of the present study. By  $\Delta E_0$ , we indicate the difference between our numerical and analytical energy results.

$B$ (T)	$E_0^P$	$E_0^A$	$E_0^N$	$\Delta E_0$
0.0	1.22319	1.03223	1.02214	0.01009
0.5	1.23071	1.03930	1.02928	0.01002
1.0	1.25281	1.06012	1.05029	0.00983
1.5	1.28831	1.09361	1.08408	0.00953
2.0	1.33551	1.13821	1.12909	0.00912
2.5	1.39252	1.19223	1.18360	0.00863
3.0	1.45753	1.25396	1.24589	0.00807
3.5	1.52890	1.32193	1.31446	0.00747
4.0	1.60526	1.39485	1.38800	0.00685
4.5	1.68551	1.47168	1.46547	0.00621
5.0	1.76876	1.55158	1.54601	0.00557

TABLE II. The ground-state energy (in units  $H^*$ ) results of the present study are compared with those of HF, LSDA, VMC, and DMC analyses.

$E_{\text{HF}}$	$E_{\text{LSDA}}$	$E_{\text{VMC}}$	$E_{\text{DMC}}$	$\bar{E}_0^A$	$\bar{E}_0^N$
1.1420 <sup>a</sup>	1.04684 <sup>a</sup>	1.02165 <sup>a</sup>	1.02164 <sup>a</sup>	1.03223 <sup>b</sup>	1.02214 <sup>b</sup>

<sup>a</sup>From Table II of Ref. 16.

<sup>b</sup>From Table I of the present study.

circular GaAs QDs with  $N \leq 13$  electrons by using both the variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC) methods at zero magnetic field, and they compared their results with those obtained from HF and LSDA calculations. A comparison of our numerical calculation for the ground-state energy with corresponding QMC calculations of Pederiva *et al.* and LSDA results is given in Table II. Here, for the sake of comparison, we follow the same convention of Ref. 16. Hence, the units of energies listed in Table II are the same as for the Table II of Ref. 16, i.e., in Hartree ( $H^*$ ). Namely, the confining energy  $\hbar\omega_c=3.32$  meV corresponds  $\hbar\omega_c=0.28H^*$ , or alternatively it can be expressed in terms of dimensionless confinement frequency as  $\bar{\omega}_c=0.28$  in our dimensionless units. By a straightforward inspection of this table, our numerical result agrees to the corresponding QMC results within  $0.6mH^*$ , whereas HF and LSDA energies are  $200mH^*$  and  $25mH^*$  higher than our numerical energies.

To further check the predictions of Eq. (7), we compare our calculation for the ground-state energy with those found by using the conventional HF theory, and also by an exact numerical method.<sup>9</sup> Pfankuche *et al.*<sup>9</sup> have studied the ground-state energy of two electron QD in a magnetic field by using a Hartree, HF and exact numerical treatments. These authors have concluded that (i) the results of Hartree approximation are poor, and show strong deviations as compared to those of HF and exact numerical ones due to the problem connected with an unphysical term entered in this approximation, and (ii) due to the fact that the basis used for exact diagonalization was not the same as that used in the HF calculation, only the close agreement between HF solutions and the results of exact numerical calculations was observed at some certain values of angular momentum. In their numerical simulations for material parameters of GaAs, calculations based on the choice of at least 15 radial quantum numbers for exact results and five Landau levels for HF approximation have been realized at a confining energy  $\hbar\omega_c=3.37$  meV, which corresponds to a dimensionless confinement length  $\bar{\ell}_c=1.876$ , and at a magnetic field  $B=1.0$  T. Besides, to demonstrate that wave functions with larger angular momenta tend to decrease the interaction energy because of their larger spatial extend, they performed energy estimates obtained with the use of only a few basis sets listed in Table I of Ref. 9. It should be noted that the value of the confining energy used in Ref. 9 is slightly different from the previous case. Therefore, we will use this value here for comparison, rather than 3.32 meV. Their corresponding calculated numerical values are  $E^{\text{HF}}=14.033$  meV, (13.863 meV), and  $E^{\text{ED}}=12.605$  meV (12.733 meV), re-

spectively. Here, the energy estimates obtained with the use of only a few basis sets listed in Table I of Ref. 9 are quoted in parentheses. By using the same parameters as they did, one can easily obtain relatively lower energies by using our numerical and analytical approaches, i.e.,  $E_0^N=12.598$  meV and  $E_0^A=12.714$  meV, respectively. Accordingly, our calculations provide better results compared with those obtained by Hartree, HF, and ED schemes, and are in agreement with those obtained in Ref. 16 for a two electron case, by using the QMC method. This is because of the fact that the trial wave functions we choose include inherently the quasi-exact solutions, and thus include the correct electron-electron correlations.

In summary, we have introduced two individual self-consistent approaches to the calculation of energy levels of two interacting electrons in 2D parabolic QDs, by proposing approximate wave functions with correct electron-electron correlations. While the first gives analytical expressions for the low-lying energy levels of two interacting electrons confined in a 2D parabolic potential and subjected to an external uniform magnetic field, the next is the numerical one, and provides results relatively better than the first one. We have

performed our calculations only for the low-lying energy levels, the others can, in principle, also be included by using the same procedure. Within these approximations, one takes advantages of both their theoretical simplicity and their apparent ability to obtain more accurate results as compared with those obtained by using conventional techniques such as Hartree, HF, and exact diagonalization approaches. We believe that every quantum mechanical treatment of the problem with nonperturbative methods help to provide an adequate description of 2D parabolic QDs to understand their electronic properties, and suggests a realistic theoretical discussion of the numerical treatments of QDs with several electrons.

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