Two-electron quantum dot in a magnetic field: Analytical results

M. Dineykhan and R. G. Nazmitdinov
Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Russia
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Two interacting electrons in a harmonic oscillator potential under the influence of a perpendicular homogeneous magnetic field are considered. Analytic expressions are obtained for the energy spectrum of the two- and three-dimensional cases. Exact conditions for phase transitions due to the electron-electron interaction in a quantum dot as a function of the dot size and magnetic field are calculated. [S0163-1829(97)00920-X]

I. INTRODUCTION

In recent years considerable experimental and theoretical interest has been focused on the study of artificially structured atoms in semiconductors, such as quantum dots, where few electrons are confined in all three directions (see, for a review, Refs. 1–3). In experimentally realized quantum dots, the extension in the x-y plane is much larger than in the z direction. Assuming that the z extension could be effectively considered zero, the electronic properties in these nanostructures have successfully been described (see Refs. 1 and 3 and references therein) within the model of the single-electron motion in the two-dimensional harmonic oscillator potential in the presence of a magnetic field.[4] Based on a numerical solution of the Coulomb interaction between electrons, a complex ground state behavior (singlet→triplet state transitions) as a function of a magnetic field has been predicted[5,6] (see also the discussion in Ref. 2). Remarkably, these ground state transitions for $N=2$ have been observed experimentally.[7]

In the present paper we consider an analytically solvable model of two electrons in a quantum dot. The confinement potential is approximated by a harmonic oscillator potential and the problem of the Coulomb interaction is treated exactly. Though this case represents the simplest nontrivial problem with regard to the electron number, mainly the ground states of a two-dimensional quantum dot were analyzed either quantitatively[6] or analytically with some approximations.[8] The role of third dimension (z) is also investigated and the results on the analysis of the ground as well as excited states are presented.

II. MODEL: GENERAL REMARKS

Our analysis is based on the oscillator representation method (ORM) developed in Ref. 9. The ORM arisen from the ideas and methods of quantum field theory has been proposed to calculate the binding energy of different systems with fairly arbitrary potentials described by the Schrödinger equation.[10] Here, for completeness we present briefly the main ideas of the ORM.

For any potential admitting the existence of a system bound state there is always a transformation of the variables that leads to a Gaussian asymptotic form for the wave function at large distances. However, the asymptotic behavior of the Coulomb wave functions for large distances does not coincide with this behavior. Therefore, we have to modify the variables in the original Schrödinger equation so that the modified equation should have solutions with the Gaussian asymptotic behavior. In the Coulomb systems, this modification is performed by going over to the four-dimensional space, where the wave function of the Coulomb system becomes the oscillator one. In an early paper,[11] Schrödinger has noted the existence of such a transformation which transforms the three-dimensional Coulomb system into the oscillator one in the four-dimensional space. The explicit form of this transformation has been found in Ref. 12 and used to solve the classical Kepler problem.

In the next stage, it is necessary to represent the canonical variables (coordinate and momentum) of the Hamiltonian through the creation and annihilation operators $a^\dagger$ and a. From the Hamiltonian the pure oscillator part with some, yet unknown, frequency ω is extracted, i.e., $H=H_0+H_I = \omega a^\dagger a + $ *higher order terms*. The remaining part, i.e., the interaction Hamiltonian H_I, is represented in terms of normal products over $a^\dagger$ and a. In addition, it is required that the interaction Hamiltonian does not contain terms quadratic in the canonical variables. This condition is equivalent to the equation

$$\frac{d\varepsilon_0}{d\omega}=0, \tag{1}$$

which determines ω, the oscillator frequency, in the ORM and is called the *oscillator representation condition* (ORC).[9] Similar ideas are used in the Hartee-Fock-Bogoliubov theory to describe different correlations between nucleons moving in an average nuclear potential (see, for a review, Ref. 13).

Since we change our space variable $\vec{r}$ and a magnetic quantum number m will be absorbed by the dimension parameter of the auxiliary space (Ref. 9 and see below), the calculation of the wave function $\psi(\vec{r})$ would be equivalent to the calculation of the ground state function of a modified Hamiltonian in another dimension. As it has been mentioned above, the wave functions in this auxiliary space should have the oscillator Gaussian asymptotic behavior at large distances. This property is quite natural for our purposes due to physical conditions for the confined electron gas in a quantum dot. The effective confining potential (oscillator) prevents the tendency caused by the Coulomb forces to allow electrons to escape and, therefore, it should dominate in the phenomena.

The model is described by the Hamiltonian

$$H=\sum_{j=1}^{2}\left\{\frac{1}{2m^{\star}}\left(\vec{p}_j-\frac{e}{c}\vec{A}_j\right)^2+\frac{m^{\star}}{2}[\omega_0^2(x_j^2+y_j^2)+\omega_z^2 z_j^2]\right\}+\frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{|\vec{r}_1-\vec{r}_2|}+H_{\rm spin}, \tag{2}$$

where $H_{\rm spin}=g(\vec{s}_1+\vec{s}_2)\vec{B}$. Here $m^{\star}$ is the effective electron mass. Below, we use the units $(e=c=1)$. For the perpendicular magnetic field $(\vec{B}||z)$ we choose the gauge described by the vector $\vec{A}=[\vec{B}\times\vec{r}]/2=\frac{1}{2}\vec{B}(-y,x,0)$. Introducing the relative and center-of-mass coordinates,

$$\vec{r}=\vec{r}_2-\vec{r}_1, \quad \vec{R}=\frac{1}{2}(\vec{r}_1+\vec{r}_2), \tag{3}$$

the Hamiltonian, Eq. (3), can be separated into the center-of-mass and relative-motion terms as (see, also, Refs. 6,8)

$$H=2H_q+\frac{1}{2}H_Q+H_{\rm spin}, \tag{4}$$

$$H_q=\frac{1}{2}[\vec{p}_q+\vec{A}_q]^2+\frac{\hbar^2}{2}(\omega_q{}^2\rho_q^2+\omega_{q_z}^2 q_z^2)+\frac{k\sqrt{\hbar\omega_0}}{2q}, \tag{5}$$

$$H_Q=\frac{1}{2}[\vec{P}_Q+\vec{A}_Q]^2+\frac{\hbar^2}{2}(\omega_Q{}^2\rho_Q^2+\omega_{Q_z}^2 Q_z^2), \tag{6}$$

where $\omega_Q=2\omega_0$, $\omega_{Q_z}=2\omega_z$, $\omega_q=\frac{1}{2}\omega_0$, $\omega_{q_z}=\frac{1}{2}\omega_z$, $\vec{A}_Q=\vec{A}(q_1)+\vec{A}(q_2)$, $\vec{A}_q=\frac{1}{2}[\vec{A}(q_2)-\vec{A}(q_1)]$, and $\vec{A}(q)=(\hbar/m^{\star})[\vec{B}\times\vec{q}]$. Here we have introduced the variables $\vec{q}=(\sqrt{m^{\star}}/\hbar)\vec{r}$, $\vec{Q}=(\sqrt{m^{\star}}/\hbar)\vec{R}$, $\rho=\sqrt{x^2+y^2}$ and defined the characteristic lengths: the effective radius $a^{\star}=a_B\epsilon(m_e/m^{\star})\times[a_B=4\pi\epsilon_0(\hbar^2/m_e e^2)]$ and the oscillator length $l_0=(\hbar/m^{\star}\omega_0)^{1/2}$. These units allow one to define the dimensionless dot size $k=l_0/a^{\star}$.[6]

The separability and the conservation of the angular momentum lead to a natural ansatz for the eigenfunction of the Hamiltonian, Eq. (4),

$$\Psi=\psi(\vec{q})\phi(\vec{Q})\chi(\vec{s}_1,\vec{s}_2), \tag{7}$$

where the wave functions $\psi(\vec{q})$ and $\phi(\vec{Q})$ are[14]

$$\psi(\vec{a})=\frac{e^{im\phi}}{\sqrt{2\pi}}\psi_m(\rho_a,z) \tag{8}$$

and the eigenvalues have the form

$$E=2\epsilon_r+\frac{1}{2}E_{N,M}+E_{\rm spin}. \tag{9}$$

Here ϵ_r and $E_{N,M}$ are the eigenvalues of the Hamiltonians H_q and H_Q, respectively. According to the Pauli principle, if the spatial part of the total wave function is symmetric (antisymmetric) with respect to the inversion $r\to -r$, χ must be the singlet (triplet) spin state. We now concentrate our analysis on the relative motion Hamiltonian H_r.

III. COULOMB PROBLEM

Due to the axial symmetry of the problem, the Schrödinger equation with the Hamiltonian, Eq. (5), can be written in the form

$$\left\{-\frac{1}{2}\left[\frac{d^2}{d\rho_q^2}+\frac{1}{\rho_q}\frac{d}{d\rho_q}-\frac{m^2}{\rho_q^2}\right]-\frac{1}{2}\frac{d^2}{dq_z^2}+\frac{\hbar^2}{2}(\Omega_q{}^2\rho_q^2+\omega_{q_z}^2 q_z^2)+\frac{k\sqrt{\hbar\omega_0}}{2\sqrt{\rho_q^2+q_z^2}}\right\}\psi_m(\rho_q,q_z)=U_m\psi_m(\rho_q,q_z). \tag{10}$$

Here

$$\Omega_q=\omega_q\sqrt{1+\frac{t^2}{4}}, \tag{11}$$

where $t=\omega_c/\omega_0$, $\omega_c=B/m^{\star}$ is the cyclotron frequency, and

$$U_m=\epsilon_r-m\frac{\hbar\omega_c}{4}, \tag{12}$$

where m is a magnetic quantum number.

According to the ansatz of the ORM for the wave function, we have to change radial variables so as to obtain an oscillator asymptotic behavior for the wave functions of the transformed equation and then identify this equation with the radial Schrödinger equation in a space with a different dimension. In addition, our Hamiltonian contains a repulsive centrifugal term, and the wave function $\psi_m(\rho_q,q_z)$ must decrease at small distances. Consequently, the transformation to the higher dimensional space is realized by[9]

$$\psi_m(\rho_q,q_z)=\rho_q^{d/2-1}\Phi_m(\rho_q,q_z). \tag{13}$$

The parameter d can be chosen to compensate completely the repulsion at small distances. The calculation of the wave function $\Phi_m(\rho_q,q_z)$ is equivalent to the calculation of the ground state wave functions in a space R^d. The wave function, Eq. (13), is a regular one at short distances. Therefore, our wave function possesses necessary properties at short and large distances, i.e., it is a Gaussian one as $\rho\to\infty$ and goes to zero at $\rho\to 0$.

According to the definition of the wave function, Eq. (13), we can transform Eq. (10) into the equation

$$\left\{-\frac{1}{2}\left[\frac{d^2}{d\rho_q^2}+\frac{d-1}{\rho_q}\frac{d}{d\rho_q}\right]-\frac{1}{2}\frac{d^2}{dq_z^2}+\frac{\hbar^2}{2}(\Omega_q{}^2\rho_q^2+\omega_{q_z}^2 q_z^2)+\frac{k\sqrt{\hbar\omega_0}}{2\sqrt{\rho_q^2+q_z^2}}\right\}\Phi_m(\rho_q,q_z)=U_m\Phi_m(\rho_q,q_z), \tag{14}$$

which can be identified with the equation in space R^d with

$$d=2+2|m|. \tag{15}$$

One can see that the magnetic quantum number m does not enter into the Schrödinger equation, Eq. (14), in the explicit form. It is absorbed by the ''dimension'' parameter d. This trick allows one effectively to avoid the problem of calcula-

tion of excited states and to perform calculations of the ground state in the auxiliary space R^d. Therefore, Eq. (14) contains the oscillator with the coordinate $\rho_q \in R^d$ and the other one with the coordinate $q_z \in R^1$, respectively.

Choosing different (fixed) values of ω_z allows us to study the dependence of the results on the slab thickness. The condition $\omega_z \gg \omega_0$ ensures that we have a genuine two-dimensional problem implying that no particles occupy a quantum mode in the z direction ($n_z=0$). From the analysis of the far-infrared frequencies in the three-dimensional oscillator potential, it follows[15] that the frequency that just forbids the occupation of a z mode is given by $\omega_z^0 \geqslant \omega_\perp(\sqrt{4N+1}-3)/2$, with $\omega_\perp$ being the average of ω_x and ω_y.

A. Two-dimensional case

Let us consider the case $z=0$, i.e., the pure two-dimensional electron gas. For the case under consideration Eq. (14) can be written as

$$H_{2d}\Phi_m(\rho_q)=U_m\Phi_m(\rho_q), \tag{16}$$

where

$$H_{2d}=-\frac{1}{2}\left[\frac{d^2}{d\rho_q^2}+\frac{d-1}{\rho_q}\frac{d}{d\rho_q}\right]+\frac{\hbar^2}{2}{\Omega_q}^2\rho_q^2+\frac{k\sqrt{\hbar\omega_0}}{2\rho_q}. \tag{17}$$

Here the wave function $\Phi_m(\rho_q)$ depends only on $\rho_q=\sqrt{\vec{\rho}_q^2}$. Therefore, we can identify the operator

$$\frac{d^2}{d\rho_q^2}+\frac{d-1}{\rho_q}\frac{d}{d\rho_q}\equiv\Delta_{\rho_q}, \tag{18}$$

with the Laplacian Δ_{ρ_q} in auxiliary space R^d if this operator acts on a function depending on the radius only. The wave function $\Phi_m(\rho_q)$ in Eq. (17) can be considered as a wave function of the ground state satisfying the Schrödinger equation

$$H\Phi_m(\rho_q)=\varepsilon(E)\Phi_m(\rho_q), \tag{19}$$

where

$$H=\frac{P_{\rho_q}^2}{2}+\frac{\hbar^2}{2}{\Omega_q}^2\rho_q^2+\frac{k\sqrt{\hbar\omega_0}}{2\rho_q}-U_m. \tag{20}$$

Taking into account Eq. (16), the desired energy E is determined by the equation

$$\varepsilon(E)=0. \tag{21}$$

Let us express the canonical variables ρ and p through the creation and annihilation operators $a^\dagger$ and a

$$\rho_j=\frac{1}{\sqrt{2\hbar\omega}}(a_j+a_j^\dagger),\quad j=1,\ldots,d,$$
$$p_j=-i\sqrt{\frac{\hbar\omega}{2}}(a_j-a_j^\dagger),\quad [a_i,a_j^\dagger]=\delta_{ij}, \tag{22}$$

where ω is a new oscillator frequency which is defined below. The vacuum state $|0\rangle$ is defined according to the standard rules,

$$\langle 0|0\rangle=1,\quad a_j|0\rangle=0. \tag{23}$$

Substituting the representation, Eqs. (22), into the definition of the Hamiltonian, Eq. (20), after some transformations

$$\frac{P_{\rho_q}^2}{2}+\frac{\hbar^2}{2}{\Omega_q}^2\rho_q^2=\frac{1}{2}(P_{\rho_q}^2+\hbar^2\omega^2\rho_q^2)+\frac{\hbar^2}{2}({\Omega_q}^2-\omega^2)\rho_q^2$$
$$\Rightarrow\hbar\omega\sum_j a_j^+a_j+\hbar\left(\frac{d\omega}{4}+\frac{d}{4}\frac{\Omega_q^2}{\omega}\right) \tag{24}$$

and

$$\frac{1}{\rho_q}=\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}e^{-\tau^2\rho_q^2}=\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\int\left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2}e^{-2i\tau(\rho_q\eta)}$$
$$\Rightarrow\sqrt{\hbar\omega}\left(\frac{\Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)}+\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\int\left(\frac{d\eta}{\sqrt{\pi}}\right)^d\right.$$
$$\left.\times e^{-\eta^2(1+\tau^2)}:e_2^{-2i\tau\sqrt{\hbar\omega}(\rho_q\eta)}:\right), \tag{25}$$

we obtain

$$H=H_0+H_I+\varepsilon_0, \tag{26}$$

where

$$H_0=\hbar\omega\sum_j a_j^+a_j, \tag{27}$$

$$\varepsilon_0=\hbar\left(\frac{d}{4}\omega+\frac{d}{4}\frac{\Omega_q^2}{\omega}\right)-U_m+\frac{\hbar}{2}\sqrt{\omega\omega_0}k\frac{\Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)}, \tag{28}$$

$$H_I=\frac{\hbar}{2}\sqrt{\omega\omega_0}kh_I, \tag{29}$$

$$h_I=\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\int\left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2(1+\tau^2)}:e_2^{-2i\tau\sqrt{\hbar\omega}(\rho_q\eta)}:. \tag{30}$$

Here : . . . : means a normal product, and we have introduced the notation $e_2^x=e^x-1-x-\frac{1}{2}x^2$. According to the ORM,[9]

the interaction Hamiltonian H_I does not contain terms quadratic in the canonical variables, i.e., proportional to $:\rho_q^2:$.

The ORC requirement, Eq. (1), determines the oscillator frequency ω which is defined in the following way:

$$\omega = x^2 \Omega_q . \tag{31}$$

The quantity x is determined with the following equation which is derived from Eqs. (28), (1):

$$x^4 + \frac{x^3}{\sqrt{2}} \frac{k}{\left(1+\frac{t^2}{4}\right)^{1/4}} \frac{\Gamma(\frac{1}{2}+|m|)}{\Gamma(2+|m|)} - 1 = 0. \tag{32}$$

It is clear that at zero Coulomb field ($k=0$) $x \equiv x_0 = 1$, while for $k \neq 0$ Eq. (32) defines the effective dependence on the Coulomb interaction of the oscillator frequency ($k \ll 1$). Considering the quantity x expanded as a Taylor series in the variable k and keeping only first order terms $x = x_0 + k x_1 + \cdots$, we obtain, according to Eqs. (11), (31), and (32),

$$\omega = (1 + k x_1)\omega_q \sqrt{1+\frac{t^2}{4}} = \widetilde{\omega}_q \sqrt{1+\frac{t^2}{4}}, \tag{33}$$

where

$$\widetilde{\omega}_q = \omega_q \cdot \left(1 - \frac{1}{2\sqrt{2}} \frac{l/a^\star}{\left(1+\frac{1}{4}t^2\right)^{1/4}} \frac{\Gamma(\frac{1}{2}+|m|)}{\Gamma(2+|m|)} \right). \tag{34}$$

When the Coloumb forces are absent ($l/a^\star = 0$) it follows that $\widetilde{\omega}_q = \omega_q$ and $\omega = \Omega_q$.

According to the ORM, the quantum number n defines the radial excitation (see Ref. 9), i.e., the highest oscillator states,

$$|n\rangle = C_n (a_j^\dagger a_j^\dagger)^n |0\rangle,$$

$$C_n = \left[\frac{\Gamma\left(\frac{d}{2}\right)}{2^{2n} n! \Gamma\left(\frac{d}{2}+n\right)} \right]^{1/2}. \tag{35}$$

Correspondingly, the energy spectrum with radial excitations is defined as

$$\epsilon^{[n]}(U) \equiv \langle n|H|n\rangle = \alpha_1 + \alpha_2, \tag{36}$$

with

$$\alpha_1 = \left(\frac{d}{4}+2n\right)\hbar\omega + \frac{d\hbar\Omega_q^2}{4\ \omega} - U_m, \tag{37}$$

$$\alpha_2 = \frac{\hbar}{2}\sqrt{\omega\omega_0}k \left(\langle n|h_I|n\rangle + \frac{\Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)} \right).$$

Taking into account Eqs. (11), (32), (36) from Eq. (21), we obtain

$$E_{nm}^{2d} = 2\epsilon_r = \varepsilon_{nm}^0 + \varepsilon_{nm}^c,$$

$$\varepsilon_{nm}^0 = \frac{\hbar\omega_0}{2}\left[\frac{m}{2}t + (1+|m|+2n)x^2 \left(1+\frac{t^2}{4}\right)^{1/2} \right], \tag{38}$$

$$\varepsilon_{nm}^c = \frac{\hbar\omega_0}{2} \frac{xk}{2\sqrt{2}} \left(1+\frac{t^2}{4}\right)^{1/4} \left[3\frac{\Gamma(\frac{1}{2}+|m|)}{\Gamma(1+|m|)} + 2\langle n|h_I|n\rangle \right],$$

where the matrix $\langle n|h_I|n\rangle$ is defined in Appendix A. In perturbation theory the effect of Coulomb forces is taken into account by the second term ε_{nm}^c. In our approach the main term ε_{nm}^0 depends on the Coulomb forces as well. In standard schemes this term corresponds to the noninteracting electrons moving in the external confining potential.[8] Here, within our model, the interaction modifies the external potential and results in the effective mean field potential of the relative motion.

B. Three-dimensional case

Despite that $\omega_z \gg \omega_0$, in real samples the effect of the third direction should be taken into account, and the prediction based on the pure two-dimensional case is expected to be modified.

Taking into account the definition Eq. (17), Eq. (14) can be written in the following form:

$$[(H_{2d} - U_m) + h_z + h_{\rm res}]\Phi_m(\rho_q, q_z) = 0, \tag{39}$$

where

$$h_z = -\frac{1}{2}\frac{d^2}{dq_z^2} + \frac{\hbar^2}{2}\omega_{q_z}^2 q_z^2, \tag{40}$$

$$h_{\rm res} = \frac{k\sqrt{\hbar\omega_0}}{2}\left(\frac{1}{\sqrt{\rho_q^2+q_z^2}} - \frac{1}{\sqrt{\rho_q^2}} \right). \tag{41}$$

Since the terms H_{2d} and h_z give the main contribution to the total Hamiltonian, the term $h_{\rm res}$ is related to a dimension of the problem and can be considered as a correction term. Let us introduce a transformation for the one-dimensional oscillator h_z similar to the two-dimensional case [see Eq. (22)],

$$q_z = \frac{1}{\sqrt{2\hbar\omega_z}}(A^\dagger + A), \quad p_z = i\sqrt{\frac{\hbar\omega_z}{2}}(A^\dagger - A). \tag{42}$$

After some transformation of the Hamiltonian, Eq. (39), we obtain

$$H = H_0 + \varepsilon_0 + \frac{\hbar}{2}\sqrt{\omega\omega_0}k h_I. \tag{43}$$

Here

$$H_0 = \hbar\omega_{q_z} A^\dagger A + \hbar\omega \sum_j a_j^\dagger a_j, \tag{44}$$

$$\varepsilon_0(U)=\hbar\left(\frac{d}{4}\omega+\frac{d}{4}\frac{\Omega_q^2}{\omega}+\frac{\omega_z}{2}\right)-U_m + \frac{\hbar}{2\sqrt{\pi}}\sqrt{\omega\omega_0}k\int_{-\infty}^{\infty}d\tau(1+\tau^2)^{-d/2}(1+\gamma\tau^2)^{-1/2}, \tag{45}$$

and h_I consists of four terms (see Appendix B). Here ω is defined by Eq. (31) and $\gamma=\omega/\omega_{q_z}\ll 1$. Finally, applying the definition of the radial excitations [see Eq. (36)] for the three-dimensional case, Eq. (43), from the condition, Eq. (21), we obtain the following expression for the lowest energy level with $n_z=0$,

$$E_{nm0}=E_{nm}^{2d}+\frac{\hbar xk}{2\sqrt{2}}\left[\left(1+\frac{t^2}{4}\right)^{1/4}Q(\gamma)+2\frac{\Gamma(\frac{1}{2}+|m|)}{\Gamma(1+|m|)}S_n(\gamma)\right], \tag{46}$$

where the quantities $Q(\gamma)$, $S_n(\gamma)$ are defined in Appendix B.

IV. DISCUSSION

The solution to the Hamiltonian of the center-of-mass motion H_Q is well known[4] and the energy can be written as

$$E_{N,M}=2\hbar\omega_0\left[(2N+|M|+1)\sqrt{1+\frac{t^2}{4}}+\left(2n_z+\frac{1}{2}\right)\frac{\omega_z}{2\omega_0}+\frac{1}{2}Mt\right], \tag{47}$$

where $N=0,1,\ldots$ and $M=0,\pm1,\ldots$ are radial and azimuthal quantum numbers, respectively. The spin of the two electrons leads to an additional Zeeman energy,

$$E_S=g^\star\mu_B S_z=\frac{1}{4}[1-(-1)^m]g^\star\frac{m^\star}{m_e}\frac{\omega_c}{\omega_0}\hbar\omega_0. \tag{48}$$

m is a magnetic quantum number corresponding to the relative motion and $g^\star$ is an effective Lande factor ($q^*=-0.44$).

Summing Eqs. (47), (48), (38) [or Eq. (46) in the three-dimensional case, respectively] we are able to investigate different ground states as a function of the dot size $k=l_0/a^\star$ and relative strength of the magnetic field ω_c/ω_0. Since the center-of-mass quantum numbers N,M and the quantum number m are conserved by the Coulomb interaction, the ground state has the quantum numbers $N=0$, $M=0$, $n=0$. Comparing the energy with different $m\leqslant 0$ we can define the ground state energy for a given dot size k at different strength of a magnetic field ω_c/ω_0.

In our calculations, we used the effective mass $m^\star=0.067m_e$ of typical quantum dots for GaAs. In Fig. 1(a) the energy spectra without a contribution of the Coulomb forces are presented. While without the Coulomb forces the ground state is always the state with $m=0$, the Coulomb interaction [Fig. 1(b)] leads to a sequence of different ground states $m=-1,-2,\ldots$ which are an alternating sequence of singlet and triplet states.

The main mechanism, which defines the optimum quantum number m of the ground state, is the interplay between the dot size and the strength of the magnetic field. This question has been nicely discussed for the two-dimensional quantum dots in Ref. 6 (see, also, Ref. 2). A similar behavior is observed for the radial excitations with $n=1,2,\ldots$.

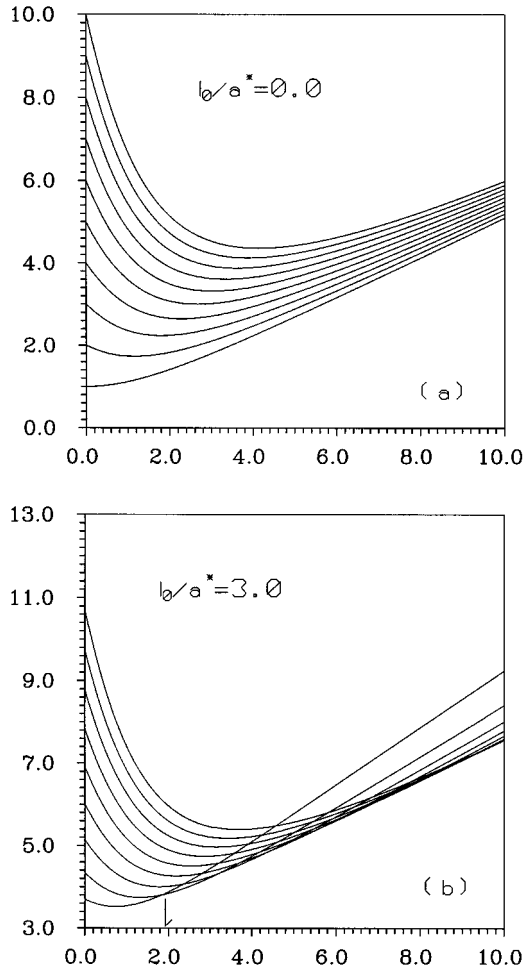

FIG. 1. The energy spectrum of a two-dimensional quantum dot in units of $\hbar\omega_0$ as a function of the magnetic field strength ω_c/ω_0. The family of states with the quantum numbers $N=0$, $M=0$, $n=0$, and $m\leqslant 0$ is shown (a) without and (b) including the Coulomb interaction between the two electrons. The arrow indicates the value of the magnetic field strength $\omega_c/\omega_0=1.91$, where the second ''crossing'' occurs between the lowest states $m=-1$ and $m=-2$.

If the third extension (z) is taken into account, the ground phase transitions are shifted to a higher magnetic field (see Fig. 2). Since the extension of the slab is inversely proportional to the confining frequency ($\omega_z\sim 1/d_z$), the thicker the slab the larger value of the magnetic field that is needed to observe the ground state transition $m\rightarrow m'$. This fact has to be taken into account in experiments.

The singlet-triplet ground phase transition occurs when the following condition is fulfilled $E_{0,m}=E_{0,m-1}(m\leqslant 0)$. For a negative Lande factor the spin-splitting energy in a magnetic field will lower the energy of the spin $S_z=+1$ component of the triplet states. In particular, the relation $E_{0,m}=E_{0,m-1}=E_{0,m-2}$ (m odd) defines the point when the singlet phase ceases to exist.[6] Beyond this point we can observe phase transitions between triplet states defined by the

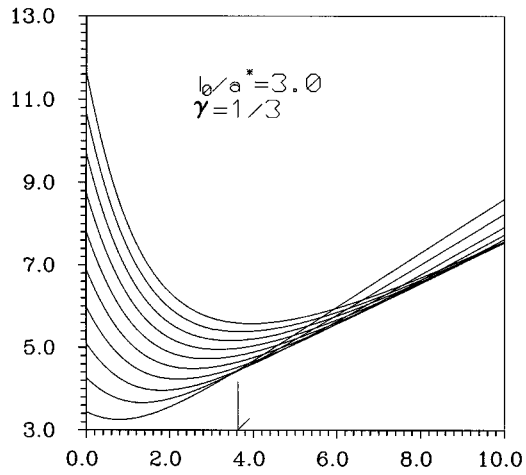

FIG. 2. Similar to Fig. 1 for the three-dimensional quantum dot $(1/\gamma=\omega_z/\omega=3)$ including the Coulomb interaction between the two electrons. Here, the second ''crossing'' occurs at $\omega_c/\omega=3.64$. The decreasing of the ratio $1/\gamma$ leads to the ''crossing'' of levels at higher magnetic field strength.

condition $E_{0,m}=E_{0,m-2}$ (m odd). Therefore, at strong magnetic field $\omega_c \gg \omega_0$, i.e., in the limit $t\to\infty$ and $x\to 1$, for singlet-triplet phase transitions $m\to m-1$, we obtain

$$\frac{l_0}{a^\star}=\frac{8\Gamma(2+|m|)}{3\Gamma(\frac{1}{2}+|m|)}\left[\left(\frac{\omega_0}{\omega_c}\right)^{3/2}+\frac{1}{2}\left(\frac{\omega_c}{\omega_0}\right)^{1/2}(-1)^m g^\star\frac{m^\star}{m_e}\right]f_{\rm st}(\gamma), \tag{49}$$

$$f_{\rm st}(\gamma)=1+\frac{\gamma}{6}\frac{5+2|m|}{(3-2|m|)(1-2|m|)}+O(\gamma^2), \tag{50}$$

and for triplet-triplet phase transitions $m\to m-2$ (m odd),

$$\frac{l_0}{a^\star}=\frac{8}{3}\left(\frac{\omega_0}{\omega_c}\right)^{3/2}\frac{\Gamma(3+|m|)}{\Gamma(\frac{1}{2}+|m|)}\frac{4}{(5+4|m|)}f_{tt}(\gamma), \tag{51}$$

$$f_{tt}(\gamma)=1-\frac{\gamma}{2}\frac{7+6|m|}{(5+4|m|)(3-2|m|)(1-2|m|)}+O(\gamma^2). \tag{52}$$

In these expressions the pure two-dimensional case is realized in the limit $\gamma\to 0$.

The higher the excitations in the two-electron quantum dots the lesser the influence of the Coulomb forces on the ''crossing'' of levels. For example, the value of the parameter $k=l_0/a^\star$ for singlet-triplet phase transitions decreases with increasing radial quantum number n. In particular, for the two-dimensional system we have obtained the following relation between parameters $k=l_0/a^\star$ for a singlet-triplet transition at different n,

$$\frac{(l_0/a^\star)_{n=1}}{(l_0/a^\star)_{n=0}}=\frac{2+|m|}{7+|m|}. \tag{53}$$

While the interplay between the magnetic field and the Coulomb forces determines the features of a phase transition (singlet $\to$ triplet) for the ground state $(n=0)$,[6] mainly the magnetic field leads to the phase transitions for the high-lying states $n>0$.

The model allows the calculation of the magnetization $M=-dE/dB$. Since at low energy the magnetization is closely related to the slope of the ground energy, at $T=0$ K, we obtain for $n=0$,

$$\mu=-\frac{dE_{0m}}{dB}=\frac{\hbar}{2}\Bigg[m+\frac{x^2(|m|+1)}{2}\frac{t}{\sqrt{1+\frac{1}{4}t^2}}+\frac{xk}{2\sqrt{2}}\frac{t}{\left(1+\frac{1}{4}t^2\right)^{3/4}}\frac{\Gamma(|m|+\frac{1}{2})}{\Gamma(|m|+1)}f_\mu(\gamma)+\frac{g^\star}{2m_e}[1-(-1)^m]\Bigg], \tag{54}$$

$$f_\mu(\gamma)=1+\frac{\gamma}{6}\frac{1}{1-2|m|}+O(\gamma^2). \tag{55}$$

As it was mentioned in Refs. 5 and 6, the phase ground state transitions would be reflected in sharp discontinuities in the magnetization. The above exact expression can be useful for the analysis of the experimental features related to the phase transitions. Also, it allows one to control the approximation made in the calculations in Refs. 6 and 16.

V. SUMMARY

Within the proposed model the analytical expressions for the energy levels and the magnetization of the two-electron quantum dots are obtained. The Coulomb interaction is treated exactly and from the analysis of the energy spectrum it follows that the interplay between the Coulomb forces and the magnetic field is an important ingredient for the prediction of the ground phase transitions. The Coulomb forces lead to the modification of the external potential and give rise to the effective confining potential of the relative motion. Their contribution in the properties of single-electron states decreases with the increasing of the radial quantum number n. Finally, we would like to mention that the third extension (z) modifies the value of a magnetic field needed to observe the phase transition: the thicker the slab the larger the value of a magnetic field. We hope that the results presented here will be useful for the analysis of the electron properties in two-electron quantum dots and will allow us to make a conclusion on a deviation of the real confining potential from the harmonic oscillator one.

APPENDIX A: TWO-DIMENSIONAL CASE: MATRIX $\langle n|h_I|n\rangle$

Here we describe some details of the calculations of the quantity

$$\langle n|h_I|n\rangle=\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\int\left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2(1+\tau^2)} \times\langle n|:e_2^{-2i\tau\sqrt{\hbar\omega}(\rho_q\eta)}:|n\rangle. \tag{A1}$$

Taking into account the following equations,

$$e^{i\vec{k}\vec{a}}e^{i\vec{p}\vec{a}^+}=e^{i\vec{p}\vec{a}^+}e^{i\vec{k}\vec{a}}e^{-(\vec{k}\vec{p})},$$

$$e^{i\vec{k}\vec{a}}\vec{a}^+e^{-i\vec{k}\vec{a}}=\vec{a}^+ +i\vec{k}, \tag{A2}$$

$$e^{\alpha\vec{a}^+\vec{a}}\vec{a}e^{-\alpha\vec{a}^+\vec{a}}=\vec{a}e^{-\alpha},$$

the fact that

$$(a^\dagger a^\dagger)^n=(-1)^n\frac{d^n}{d\alpha^n}e^{-\alpha(a^\dagger a^\dagger)}\bigg|_{\alpha=0} =(-1)^n\frac{d^n}{d\alpha^n}\int\left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2-2i\sqrt{\alpha}(a^\dagger\eta)}\bigg|_{\alpha=0} \tag{A3}$$

and Eq. (35), after some transformation, we obtain

$$\langle n|:e_2^{-iB(a^\dagger\eta)-iB(a\eta)}:|n\rangle =C_n^2\frac{\partial^{2n}}{\partial\alpha^n\partial\beta^n}\sum_{j=2}^{2n}\frac{(B^2\eta^2)^j}{j!}\frac{(\alpha+\beta-4\alpha\beta)^j}{(1-4\alpha\beta)^{j+d/2}}\bigg|_{\alpha,\beta=0},$$

where $B=\tau\sqrt{2}$. Using these results, we have for Eq. (A1)

$$\langle n|h_I|n\rangle=\frac{3}{4}\frac{\Gamma(d/2-1/2)}{\Gamma(d/2)}S_n, \tag{A4}$$

where

$$S_n=\frac{4\Gamma(1+n)}{3\sqrt{\pi}}\sum_{k=2}^{2n}\frac{(-1)^k\Gamma(k+1/2)}{\Gamma(k+d/2)}N_k(n,d),$$

and

$$N_k(n,d)=\sum_{p=0}^{n}\frac{2^{2p-k}\Gamma(k+n-p+d/2)}{(n-p)!(2p-k)![(k-p)!]^2}.$$

In a particular case, $n=1$, and $n=2$ for S_n, we have

$$S_1=\frac{2}{d},\quad S_2=\frac{4}{d(d+2)}\left[d+\frac{19}{8}\right].$$

APPENDIX B: THREE-DIMENSIONAL CASE: DEFINITION OF h_I, $Q(\gamma)$, AND $S_n(\gamma)$

Using the same technique as for the two-dimensional case and omitting tedious calculations, we present the final result:

$$h_I=h_1+h_2+h_3+h_4, \tag{B1}$$

$$h_1=\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\int\left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2(1+\tau^2)}:e_2^{-2i\tau\sqrt{\hbar\omega}(\rho_q\eta)}: \times\frac{1}{\sqrt{1+\gamma\tau^2}}\left[1+\frac{\gamma\tau^2\hbar\omega_{q_z}}{(1+\gamma\tau^2)}:q_z^2:\right], \tag{B2}$$

$$h_2=\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\int_{-\infty}^{\infty}\left(\frac{dt}{\sqrt{\pi}}\right)e^{-t^2(1+\gamma\tau^2)}:e_2^{-2i\tau\sqrt{\hbar\omega_{q_z}\gamma}(q_zt)}: \times\frac{1}{(1+\tau^2)^{d/2}}\left[1+\frac{\tau^2\hbar\omega}{(1+\tau^2)}:\rho_q^2:\right], \tag{B3}$$

$$h_3=\gamma\hbar^2\omega\omega_{q_z}\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\frac{\tau^2}{(1+\gamma\tau^2)^{3/2}}\frac{\tau^2}{(1+\tau^2)^{d/2+1}}:\rho_q^2::q_z^2:, \tag{B4}$$

$$h_4=\int_{-\infty}^{\infty}\frac{dtd\tau}{\sqrt{\pi}}\int\left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2(1+\tau^2)-\tau^2(1+\gamma\tau^2)}: \times e_2^{-2i\tau\sqrt{\hbar\omega_{q_z}\gamma}(q_zt)}::e_2^{-2i\tau\sqrt{\hbar\omega}(\rho_q\eta)}:, \tag{B5}$$

$$Q(\gamma)=\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\frac{1}{(1+\tau^2)^{d/2}}\left[\frac{1}{\sqrt{1+\gamma\tau^2}}-1\right] =-\frac{\gamma}{2}\frac{\Gamma(|m|+\frac{1}{2})}{\Gamma(|m|+1)}+O(\gamma^2), \tag{B6}$$

$$S_n(\gamma)=\frac{\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{d-1}{2}\right)}\int_{-\infty}^{\infty}\frac{d\tau}{\sqrt{\pi}}\int\left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2(1+\tau^2)} \times\langle n|:e_2^{-2i\tau\sqrt{\hbar\omega}(\rho_q\eta)}:|n\rangle\left[\frac{1}{\sqrt{1+\gamma\tau^2}}-1\right] =\frac{\gamma}{2\sqrt{\pi}}\frac{\Gamma(n+1)\Gamma(|m|+1)}{\Gamma(1+|m|+n)}\sum_{l=2}^{2n}(-1)^l \times\frac{\Gamma(\frac{1}{2}+l)}{\Gamma(1+l+|m|)}N_l(n,d)\frac{1+2l}{1-2|m|}+O(\gamma^2). \tag{B7}$$

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