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Two-dimensional Thomas-Fermi parabolic quantum dot in a weak magnetic field

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Abstract. The Thomas-Fermi equation, in conjunction with the Poisson equation is solved exactly for the problem of the two-dimensional circular parabolic quantum dot in the presence of a weak magnetic field, in the framework of the local spin-density approximation. The total energy, chemical potential, differential capacitance, degree of polarization, and diamagnetic susceptibility were calculated. Asymptotic solutions were obtained for the limits of strong and weak confinement.

PACS. 85.30.Vw Low-dimensional quantum devices (quantum dots, quantum wires etc.) – 71.10.Ca Electron gas, Fermi gas

1 Introduction

Great advances in nanotechnology have allowed the fabrication of quasi-two-dimensional systems like quantum dots, which have been the object of very active research during the last years (see *e.g.* [1–3], and references therein). It has been shown that they have basically parabolic confinement [4,5]. The influence of an external magnetic field induces changes in their behavior, giving rise to phenomena both of academic and application interest. While their effective dimension is usually two, the many-electron nature of the problem makes the calculation of its properties a complicated task. For that reason only few-electron dots have been treated exactly or to a fairly high degree of accuracy (see *e.g.* [6–9]), or they have been studied in special geometries like in reference [10].

A few exactly solvable models have been proposed through the years in order to gain insight of the behavior of these systems of many electrons [11–13] at the exact, Hartree-Fock, and Hartree level, using model electron-electron interaction potentials.

If the number of electrons is large enough, the system can be treated approximately as an electron gas. The Thomas-Fermi approximation and its subsequent improvements [14–18] have been of great use in the calculation of the ground state properties of many-particle problems, *e.g.* atoms, molecules, solids, and nuclei. They have been also applied to the calculation of properties of quasi-two-dimensional systems, such as planar molecules [19]. Recently, Lieb *et al.* [20] have analyzed the two-dimensional Thomas-Fermi problem in the presence of a magnetic field with (three-dimensional) Coulombic electron-electron interaction for parabolic confinement. The three-dimensional Thomas-Fermi problem of parabolic confinement was studied by Ballinger and March [21]. The present author has solved exactly the Thomas-Fermi circular parabolic quantum dot of N interacting electrons through a logarithmic potential in the absence of magnetic field [22], also the corresponding classical problem, *i.e.*, neglecting the kinetic energy.

In this article we apply the local spin-density (LSD) approach to the study of a fully two-dimensional quantum dot of parabolic confinement within the Thomas-Fermi approximation. The article has been structured as follows: in Section 2 we have solved exactly the two-dimensional Thomas-Fermi equation in conjunction with the Poisson's equation for a parabolic quantum dot in the presence of a weak magnetic field; the total energy, chemical potential, differential capacitance, magnetization and diamagnetic susceptibility are also calculated. In Section 3 we obtain the strong and weak confinement limits for the dot size and all the other magnitudes calculated in the previous section. In Section 4 we briefly discuss the classical approximation in the LSD approach, and also the number of electrons that the dot could support; we also make qualitative comparisons with some results reported in literature.

2 The Thomas-Fermi solution

Let us consider a D-dimensional electron gas in the effective-mass approximation. The Thomas-Fermi

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equation can be written as [23,24]:

$$\frac{1}{2m^*}p_{\rm F}^2 + v + V_{\rm e} = \mu \tag{1}$$

where m^* is the effective mass (measured in units of electron mass), $p_{\rm F}$ is the Fermi momentum, v is the external potential, $V_{\rm e}$ is the electrostatic potential, which should satisfy the Poisson equation, and μ is the chemical potential. Throughout the whole paper we are going to use the units where $m_{\rm e} = \hbar = e = \epsilon_0 = 1$. Since $p_{\rm F} \propto \rho^{2/D}$ (D is the dimension of the space) and $V_{\rm e} = \int {\rm d}\mathbf{r}'\rho(\mathbf{r}')K(|\mathbf{r}-\mathbf{r}'|)$, where K is the kernel of the electron-electron interaction one may write

$$\mu = v(\mathbf{r}_0) + V_{\rm e}(\mathbf{r}_0) \tag{2}$$

where $\mathbf{r}_0$ is where the density vanishes (classical turning point). This magnitude will determine the appearance of the conductance peak by the equalization of the dot's and the gates' chemical potential [2].

The two dimensional Thomas-Fermi equation (1) has to be solved in conjunction with Poisson's equation:

$$\nabla^2 V_{\rm e} = -2\pi\frac{\rho(\mathbf{r})}{\epsilon}, \tag{3}$$

where ϵ is the relative dielectric constant of the host material. The solution of the above equation for the electrostatic potential is

$$V_{\rm e}(\mathbf{r}) = -\frac{1}{\epsilon}\int {\rm d}^2\mathbf{r}'\rho(\mathbf{r}')\ln(|\mathbf{r}-\mathbf{r}'|/a), \tag{4}$$

which fixes the form of the kernel of the electron-electron interaction, and where a is a constant that fixes the zero of the electrostatic potential. Other choices of the kernel (see *e.g.* [2]) do not satisfy Poisson's equation. In general, it seems a difficult task to determine the correct form of the two-dimensional electron-electron interaction kernel, since there are some effects which we have to take into account like the smearing of the wavefunction in the direction perpendicular to the plane of the electrons, and the effect of image charges on the leads [2].

In a radially symmetric configuration equation (4) can be written as

$$V_{\rm e}(r) = \frac{N}{\epsilon}\ln a - 2\frac{\pi}{\epsilon}\left[\ln r\int_0^r {\rm d}r' r'\rho(r') + \int_r^{r_0} {\rm d}r' r'\ln r'\rho(r')\right]. \tag{5}$$

Without any loss of generality, let us suppose that the sign of the magnetic field is such that there are more spin down electrons than spin up electrons. A choice of $a \geq R_-$, where R_- will be now the effective size of the dot (where the spin down electron density vanishes), may guarantee that the electron-electron interaction is always repulsive inside of the dot, for simplicity we will take $a = R_-$, which means that $V_{\rm e}(R_-) = 0$. The form of the electron-electron interaction of equation (5) is more realistic than *e.g.* the harmonic one (see *e.g.* [2,11,13]). Furthermore, the use of the three-dimensional electron-electron interaction kernel ($K(|\mathbf{r}-\mathbf{r}'|) = |\mathbf{r}-\mathbf{r}'|^{-1}$) leads to an unphysical behavior of the derivative of the density around the origin (it is positive instead of being zero or negative) [25], probably because it is a too singular interaction potential for two dimensions, at least for the Thomas-Fermi theory.

The analysis based in equations (1–4) will be valid for zero magnetic field. The generalization to a non-zero field is done by using the local spin-density approach (LSD) (see *e.g.* [26–28]), considering only the interaction between the spin and the external magnetic field and neglecting the changes in the kinetic energy term [29]. For this purpose, we add to the spin-dependent Thomas-Fermi energy variational equation the term corresponding to the spin-field interaction

$$E[\rho_+,\rho_-;B] = E_{\rm TF}[\rho_+] + E_{\rm TF}[\rho_-] + g^*\frac{B}{2}\int {\rm d}\mathbf{r}(\rho_+ - \rho_-) + \frac{1}{2m^*}JB \tag{6}$$

where

$$E_{\rm TF}[\rho_+,\rho_-] = \int {\rm d}\mathbf{r}[\frac{\pi}{m^*}\rho_\pm^2(\mathbf{r}) + v(\mathbf{r})\rho_\pm(\mathbf{r}) + \frac{1}{2}V_{\rm e}(\rho(\mathbf{r});\mathbf{r})\rho_\pm(\mathbf{r})], \tag{7}$$

and $\rho(\mathbf{r}) = \rho_+(\mathbf{r}) + \rho_-(\mathbf{r})$ is the total density. We have changed the constant of the kinetic energy term to the spin-dependent one. We are also assuming that the magnetic field is weak enough that it will not affect the total angular-momentum state of the electrons J (because the energy of flipping one spin is small and we are neglecting the exchange energy), and it is included as the last term of equation (6). In this approximation there is no self-consistent way of determining the value of J, but with the assumptions made above, most of the properties estimated here are independent of J, at least for weak magnetic fields.

Taking the functional derivative of equation (6) we get

$$\frac{2\pi}{m^*}\rho_\pm + V_{\rm e}(r) + \frac{1}{2}m^*\omega^2 r^2 \pm \frac{1}{2}g^*B = \mu \tag{8}$$

where the + sign corresponds to the spin up electrons and the − to the spin down ones, respectively, g^* is the effective coupling constant, and μ is the chemical potential. We have included in ω the cyclotronic frequency $\omega_{\rm c} = B/m^*$ as

$$v(r) = \frac{1}{2}m^*\omega^2 r^2 = \frac{1}{2}m^*\left(\omega_0^2 + \frac{\omega_{\rm c}^2}{4}\right)r^2, \tag{9}$$

where ω_0 is the constant of confinement of the dot.

Taking the difference between the equations for the spin up and down densities (see Eq. (8)), we obtain the relation

$$\frac{2\pi}{m^*}(\rho_+ - \rho_-) = -g^*B \tag{10}$$

substituting in Poisson's equation we find

$$\frac{2\pi}{m^*}\nabla^2\rho_\pm(\mathbf{r}) - \frac{2\pi}{\epsilon}\left[2\rho_\pm(\mathbf{r}) \pm g^*\frac{m^*B}{2\pi}\right] + 2m^*\omega^2 = 0, \tag{11}$$

if equation (10) is valid.

Now, for circular symmetry we make the substitution

$$y_\pm = \rho_\pm(r) - \frac{m^*\omega^2\epsilon}{2\pi} \pm \frac{g^*m^*B}{4\pi}, \tag{12}$$

$$\kappa^2 = \frac{2m^*}{\epsilon}, \tag{13}$$

then we obtain

$$y''_\pm + \frac{1}{r}y'_\pm - \kappa^2 y_\pm = 0 \tag{14}$$

valid in the region $r \leq R_+$, where R_+ is the classical turning point for the spin up electrons.

$$\rho_+(r) = 0 \tag{15}$$

for $r \geq R_+$. Then $\rho = \rho_-$ and equation (10) is no longer valid. Now equation (8) will be written as

$$y''_- + \frac{1}{r}y'_- - \delta^2 y_- = 0 \tag{16}$$

where $\delta^2 = \kappa^2/2$, for $R_+ \leq r \leq R_-$, where R_-, correspondingly, is the classical turning point for spin down electrons, and

$$y_- = \rho_-(r) - \frac{m^*\omega^2\epsilon}{\pi} \tag{17}$$

and finally

$$\rho_-(r) = 0 \tag{18}$$

for $r \geq R_-$.

After solving equation (11)

$$\rho_\pm(r) = A_\pm I_0(\kappa r) + A_{1\pm}K_0(\kappa r) + \frac{m^*\omega^2\epsilon}{2\pi} \mp g^*\frac{m^*B}{4\pi} \tag{19}$$

for $r \leq R^+$, and where $I_0(x)$ and $K_0(x)$ are the modified Bessel functions of first and second kind, respectively [30]. The constants $A_{1\pm}$ must be taken as zero, since the density at the origin must be bounded because there the external potential vanishes.

The total density can be written as (see Appendix A)

$$\rho_\pm(r) = \frac{m^*}{2\pi}\left[\omega^2\epsilon \mp \frac{g^*B}{2} - \left(\omega^2\epsilon - \frac{g^*B}{2}\right)\frac{I_0(\kappa r)}{I_0(\kappa R_+)}\right]. \tag{20}$$

After solving equation (16)

$$\rho_-(r) = CI_0(\delta r) + DK_0(\delta r) + \frac{m^*\omega^2\epsilon}{\pi}\cdot \tag{21}$$

The coefficients A, B, C, D, R_- and R_+ are determined in Appendix A by making use of the continuity properties of the density, the chemical potential and the normalization condition. It leads to a system of non-linear equations.

The chemical potential can be determined by using equation (2) and the choice of $a = R_-$ in equation (4), which means that the zero of the electrostatic potential is at R_-,

$$\mu = \frac{1}{2}m^*\omega^2 R_-^2. \tag{22}$$

The differential capacitance can be calculated following [31]

$$C_\mathrm{d} = \frac{1}{\mu(N) - \mu(N-1)}\cdot \tag{23}$$

As we are considering a large number of electrons, the above equation can be written as:

$$C_\mathrm{d} \approx \left(\frac{\mathrm{d}\mu}{\mathrm{d}N}\right)^{-1}. \tag{24}$$

The total energy can be calculated by taking V_e from equation (8) and substituting into the total energy expression of equations (6) and (7)

$$E = \frac{1}{2}\mu N + \frac{1}{2}\int \mathrm{d}\mathbf{r}v(r)\rho(r) + \frac{g^*B}{4}\int \mathrm{d}\mathbf{r}(\rho_+(r) - \rho_-(r)) + \frac{1}{2m^*}JB. \tag{25}$$

Substituting equations (9), (20) and (21) and integrating we get

$$\begin{aligned} E = {} & \frac{1}{2}\mu N + \frac{m^*\omega^2\pi}{2}\left[2A\left(\frac{R_+^3}{\kappa}I_1(\kappa R_+)\right.\right. \\ & \left. -2\frac{R_+^2}{\kappa^2}I_2(\kappa R_+)\right) + \frac{m^*\omega^2\epsilon R_-^2}{4\pi} \\ & +C\left(\frac{R_-^3}{\delta}I_1(\delta R_-) - 2\frac{R_-^2}{\delta^2}I_2(\delta R_-)\right. \\ & \left. -\frac{R_+^3}{\delta}I_1(\delta R_+) + 2\frac{R_+^2}{\delta^2}I_2(\delta R_+)\right) \\ & +D\left(-\frac{R_-^3}{\delta}K_1(\delta R_-) - 2\frac{R_-^2}{\delta^2}K_2(\delta R_-)\right. \\ & \left.\left. -\frac{R_+^3}{\delta}K_1(\delta R_+) + 2\frac{R_+^2}{\delta^2}K_2(\delta R_+)\right)\right] \\ & -\frac{g^*B}{4}\left\{\frac{g^*m^*B}{2}R_+^2 + m^*\omega^2\epsilon(R_-^2 - R_+^2)\right. \\ & +\frac{2\pi C}{\delta}[R_-I_1(\delta R_-) - R_+I_1(\delta R_+)] \\ & \left. -\frac{2\pi D}{\delta}[R_-K_1(\delta R_-) - R_+K_1(\delta R_+)]\right\} \\ & +\frac{1}{2m^*}JB. \end{aligned} \tag{26}$$

Using perturbation theory and retaining terms up to second order from the contribution to the energy coming from a magnetic field perpendicular to the plane of interest, Langevin's diamagnetic susceptibility can be written as [32]:

$$\chi = -\frac{N}{4}\langle 0|r^2|0\rangle = -\frac{N}{2}\pi\int_0^{R_-} \mathrm{d}r r^3\rho(r), \qquad (27)$$

substituting equations (20) and (21) into the above one we obtain that

$$\begin{aligned}\chi = -\frac{N\pi}{2}\Bigg[&2A\left(\frac{R_+^3}{\kappa}I_1(\kappa R_+) - 2\frac{R_+^2}{\kappa^2}I_2(\kappa R_+)\right)\\ &+\frac{m^*\omega^2\epsilon R_-^2}{4\pi} + C\left(\frac{R_-^3}{\delta}I_1(\delta R_-) - 2\frac{R_-^2}{\delta^2}I_2(\delta R_-)\right.\\ &\left.-\frac{R_+^3}{\delta}I_1(\delta R_+) + 2\frac{R_+^2}{\delta^2}I_2(\delta R_+)\right) + D\left(-\frac{R_-^3}{\delta}K_1(\delta R_-)\right.\\ &\left.-2\frac{R_-^2}{\delta^2}K_2(\delta R_-) + \frac{R_+^3}{\delta}K_1(\delta R_+) + 2\frac{R_+^2}{\delta^2}K_2(\delta R_+)\right)\Bigg]. \qquad (28)\end{aligned}$$

The degree of polarization ξ is the ratio of the difference between the number of spin up and down electrons, and the total number of electrons,

$$\xi = \frac{N_- - N_+}{N_- + N_+} = \frac{N_- - N_+}{N}, \qquad (29)$$

using equations (20) and (21), the above equation yields

$$\begin{aligned}\xi = \frac{1}{N}\Bigg\{&\frac{g^*m^*B}{2}R_+^2 + m^*\omega^2\epsilon(R_-^2 - R_+^2)\\ &+\frac{2\pi C}{\delta}[R_-I_1(\delta R_-) - R_+I_1(\delta R_+)]\\ &-\frac{2\pi D}{\delta}[R_-K_1(\delta R_-) - R_+K_1(\delta R_+)]\Bigg\}. \qquad (30)\end{aligned}$$

3 Asymptotic solutions

Since we are dealing with weak magnetic fields, equation (10) suggests to us that (if $\mathrm{d}\rho/\mathrm{d}r$ is not small) $\Delta = R_- - R_+$ should be small. The point where the spinless density [22] vanishes (r_0) is approximately halfway between R_+ and R_-. Thus, we can write

$$\rho_0'(r_0) \approx \frac{2\rho_0(r_0)}{\Delta}\,. \qquad (31)$$

We can assume also, that $\rho_0(r_0)$ is approximately the half of the value of $\rho_-(R_+)$, and using equation (10) we find that

$$\Delta \approx \frac{m^*g^*B}{2\pi|\rho_0'(r_0)|}\,. \qquad (32)$$

Using the form of the spinless density (Appendix B),

$$\Delta \approx \frac{g^*B}{2\omega^2\epsilon\kappa}\frac{I_0(\kappa r_0)}{I_1(\kappa r_0)}\,. \qquad (33)$$

We now consider the limiting cases of weak and strong confinement, when $\omega^2\epsilon^2 \ll N$ and $\omega^2\epsilon^2 \gg N$, respectively.

By using the asymptotics of the modified Bessel's functions [30] and the results for the unpolarized case (see Appendix B) we can see that for weak confinement

$$\Delta \approx \frac{g^*B}{2\omega^2(2m^*\epsilon)^{1/2}}\,. \qquad (34)$$

In the strong confinement limit, it is easy to see that $|\rho'(r_0)| \to \infty$, which means simply that

$$\Delta \approx \frac{m^*g^*B}{4\pi}\,. \qquad (35)$$

In both cases Δ should be small compared with r_0. For weak confinement this means that

$$N \gg \frac{1}{2}\left(\frac{g^*B}{2\omega}\right)^2 \qquad (36)$$

while for the case of strong confinement it means that

$$N^{1/2} \gg \frac{m^{*3}g^{*2}\omega B^2}{32\pi^2}\,. \qquad (37)$$

After equation (22) the chemical potential can be approximated as

$$\mu \approx \frac{1}{2}m^*\omega^2 r_0^2\left(1 + \frac{\Delta}{r_0}\right) = \mu_0 + \Delta\mu, \qquad (38)$$

where μ_0 is the chemical potential at zero magnetic field. This means that for weak confinement, using the results of reference [22] (see Appendix B)

$$\mu \approx \frac{N}{2\epsilon} + \frac{1}{4}\left(\frac{N}{2\epsilon\omega^3}\right)^{1/2} g^*B, \qquad (39)$$

and

$$\mu \approx \omega N^{1/2} + \frac{(2m^{*3}\omega^3)^{1/2}}{8\pi}N^{1/4}g^*B \qquad (40)$$

for strong confinement.

Using equation (24) and equations (39) and (40) we obtain for the differential capacitance that

$$\begin{aligned}C_\mathrm{d} &\approx \left[\frac{1}{2\epsilon} + \frac{1}{8}\frac{g^*B}{(2N\epsilon\omega^3)^{1/2}}\right]^{-1}\\ &\approx 2\epsilon\left(1 - \frac{\epsilon g^*B}{4(2N\epsilon\omega)^{1/2}}\right) \qquad (41)\end{aligned}$$

for weak confinement, and

$$\begin{aligned}C_\mathrm{d} &\approx \left[\frac{1}{2}\frac{\omega}{N^{1/2}} + \frac{g^*B(2\epsilon\omega^3)^{1/2}}{32\pi N^{3/4}}\right]^{-1}\\ &\approx \frac{2N^{1/2}}{\omega}\left(1 - \frac{g^*B(2\epsilon\omega)^{1/2}}{16\pi N^{1/4}}\right) \qquad (42)\end{aligned}$$

for strong confinement.

For $r \leq r_0^+$ the difference between the total electron density (Eq. (20)) and the spinless density of equation (B.1) can be approximated by

$$\begin{aligned}\Delta\rho &= \rho_-(r) + \rho_+(r) - \rho_0(r) \\ &\approx \frac{m^*}{\pi}\left[g^*B - \omega^2\epsilon\frac{I_1(\kappa r_0)}{I_0(\kappa r_0)}\frac{\kappa\Delta}{2}\right]\frac{I_0(\kappa r)}{I_0(\kappa r_0)},\end{aligned} \tag{43}$$

which is of first order in B, since $\Delta \propto B$.

The degree of polarization can be estimated up to first order in B by

$$\xi \approx \frac{m^* g^* B r_0^2}{2N}\,. \tag{44}$$

This means that for weak confinement we have

$$\xi \approx \frac{g^* B}{2\omega^2\epsilon}, \tag{45}$$

and for strong confinement

$$\xi \approx \frac{g^* B}{N^{1/2}\omega}\,. \tag{46}$$

For the energy, after equation (25)

$$E = \frac{\mu N}{2} - \frac{g^* B\xi}{4}N + \frac{1}{2}\langle v\rangle + \frac{1}{2m^*}JB, \tag{47}$$

with

$$\langle v\rangle \approx m^*\omega^2\pi\int_0^{r_0^+}\mathrm{d}r r^3(\rho_0 + \Delta\rho) + \frac{1}{4}m^{*2}\omega^2 g^* r_0^3 B\Delta \tag{48}$$

the first term is equal to the integral from 0 to r_0 neglecting second order terms in B and the second term is of order B^2.

Thus, the total energy can be written up to first order in B as

$$E \approx E_0 + \frac{N}{2}\Delta\mu + \frac{1}{2}\Delta v + \frac{1}{2m^*}JB. \tag{49}$$

where $\Delta v = \langle v\rangle - \langle v\rangle_{B=0}$ (see Appendix A). Then,

$$\begin{aligned}E \approx E_0 &+ \frac{1}{2}m^*\omega^2 r_0\Delta + \frac{1}{8}\omega_0^2\epsilon r_0^4 B \\ &+ \frac{r_0^2\epsilon}{2m^*}\omega_0^2\left[m^{*2}\left(g^*B - \omega_0^2\epsilon\frac{I_1(\kappa r_0)}{I_0(\kappa r_0)}\frac{\kappa\Delta}{2}\right) - \frac{\epsilon B}{2}\right] \\ &\times\left(\kappa r_0\frac{I_1(\kappa r_0)}{I_0(\kappa r_0)} - 2\frac{I_2(\kappa r_0)}{I_0(\kappa r_0)}\right) + \frac{1}{2m^*}JB.\end{aligned} \tag{50}$$

This means that using the results of reference [22] for the energy, and the asymptotic series of the Bessel functions [30] in equation (50), for the weak confinement limit we have

$$\begin{aligned}E \approx &\frac{3}{8}\frac{N^2}{\epsilon} + \frac{1}{8}\left(\frac{N^3}{2\epsilon\omega^3}\right)^{1/2}g^*B + \frac{1}{8}\frac{N^2}{\omega^2 m^{*2}\epsilon}B \\ &+ \frac{2^{1/2}}{4}\frac{N^{3/2}}{\omega\epsilon m^{*2}}\left(\frac{3m^*}{2} - \frac{\epsilon}{g^*}\right)g^*B + \frac{1}{2m^*}JB\end{aligned} \tag{51}$$

and for the strong one

$$\begin{aligned}E \approx &\frac{2}{3}\omega N^{3/2} + \frac{(2m^{*3}\omega^3)^{1/2}}{16\pi}N^{5/4}g^*B + \frac{1}{2}\frac{N\epsilon}{m^{*2}}B \\ &+ \frac{2N}{m^{*2}}\left[m^{*2}\left(1 - \frac{N^{1/4}}{4\pi}\left(2m^*\omega^3\right)^{1/2}\right) - \frac{\epsilon}{2g^*}\right]g^*B \\ &+ \frac{1}{2m^*}JB,\end{aligned} \tag{52}$$

neglecting the terms of powers on B higher than one. The results of equation (51) can be read in the following way: for weak confinement the density is roughly constant which means that the confinement energy is proportional to N^2, since it is roughly $\omega^2 r_0^2 N$ and $r_0^2 \propto N/\omega^2$ after equation (B.2) of Appendix B; the electron-electron interaction energy is also proportional to N^2, since it will be proportional to the integral of the square of the density, the kinetic energy will be linear on N. For strong confinement (Eq. (52)) the leading terms are the kinetic energy and the harmonic field energy, both proportional to ωN^2, the first because it is roughly N^2/r_0^2 and the second because it is roughly $\omega^2 r_0^2 N$; from equation (B.3) of Appendix B, $r_0^2 \propto N^{1/2}/\omega$ which leads to the result that the total energy is proportional to the confinement constant and to $N^{3/2}$. The chemical potential and the capacitance could be interpreted in a similar fashion.

For the diamagnetic susceptibility (see Eq. (27)), using the same arguments, and neglecting second and higher order terms in B, we obtain that

$$\chi \approx \chi_0 - \frac{N\pi}{2}\int_0^{r_0}\mathrm{d}r r^3\Delta\rho. \tag{53}$$

Substituting equation (43) and integrating, we obtain

$$\begin{aligned}\chi \approx \chi_0 &- \frac{N r_0^2\epsilon}{4}\left(g^*B - \omega_0^2\epsilon\frac{I_1(\kappa r_0)}{I_0(\kappa r_0)}\frac{\kappa\Delta}{2}\right) \\ &\times\left(\kappa r_0\frac{I_1(\kappa r_0)}{I_0(\kappa r_0)} - 2\frac{I_2(\kappa r_0)}{I_0(\kappa r_0)}\right),\end{aligned} \tag{54}$$

where χ_0 is the diamagnetic susceptibility for zero magnetic field [33] (see Appendix B). By using the results of equations (B.2, 35), (B.9), and (B.10), and the asymptotic expansions of the modified Bessel functions [30] of equation (54), we find that

$$\chi \approx -\frac{1}{8}\frac{N^3}{m^*\omega^2\epsilon} - \frac{3\cdot 2^{1/2}}{16}\frac{N^{5/2}}{m^*\epsilon\omega^3}g^*B \tag{55}$$

for weak confinement and

$$\chi \approx -\frac{1}{6}\frac{N^{5/2}}{m^*\omega} - \frac{N^2}{2m^*\omega^2}\left[1 - \frac{(2m^*\omega)^{3/2}N^{1/4}}{8\pi}\right]g^*B \tag{56}$$

for strong confinement, up to first order in B.

4 Discussion

The solutions obtained in Section 2 are exact in the extent we know exactly the values of R_+ and R_-, for which

we give asymptotic values in Section 3. This means that the criteria of weak magnetic field will be determined by the range of validity of the local-spin Thomas-Fermi equations. On the other hand, the validity of the results of Section 3 is limited also by the validity of the expansions used on which we retain only linear terms.

It has been shown in reference [20] that the classical limit (*i.e.* the kinetic energy term is neglected) gives the correct limit for weak confinement using three-dimensional Coulombic electron-electron interaction.

The case of zero magnetic field of a completely two-dimensional parabolic quantum dot within the classical approximation (*i.e.*, neglecting the kinetic energy) was treated in reference [22]; the result is that the density is constant in a circle of radius r_{0c},

$$\rho_c(r) = \frac{m^*\omega^2\epsilon}{\pi} \quad r \leq r_{0c}, \tag{57}$$

with

$$r_{0c} = \frac{1}{\omega}\left(\frac{N}{m^*\epsilon}\right)^{1/2}, \tag{58}$$

and is zero outside of this circle. It has been also obtained for this case that the classical limit corresponds to the limit of weak confinement.

If we try to follow the same steps for the derivation of equations (8) and (10) (but now neglecting the kinetic energy), we see that we cannot include the effects of spin since it would lead to $g^*B = 0$. This means that the consideration of the kinetic energy is crucial to get the spin effects.

In practical situations the confining potential (approximated by $\omega_0^2 r^2/2$) is always bounded and spatially finite. In the absence of magnetic field a dot with bounded potential can support a finite number of electrons and is limited by the height of the confining potential V_0 (for a more detailed discussion see Ref. [22]). In a magnetic field, the effect of (magnetic) confinement ($\omega_c^2 r^2/8$) will change the number of electrons that such a dot can support by increasing the range on which electrons can be retained in

$$\delta R \approx \frac{\omega_c^2}{8\omega_0^2} R_0 \tag{59}$$

where $R_0 = (2V_0/m^*)^{1/2}/\omega_0$. The condition for confinement will be

$$R = R_0 + \delta R \geq R_-, \tag{60}$$

which means that the sign of the variation will depend on the ratio between Δ and δR. This ratio depends on the characteristics of the material and the height of the potential of confinement. Using the asymptotic results of equations (B.2) and (34), we find that for strong confinement

$$N \leq \frac{V_0^2}{\omega^2}(1 + \delta x_s)^4 \tag{61}$$

where

$$\delta x_s = \frac{B}{8m^*\omega^3} - \frac{Bm^*g^*\omega}{4\pi}\left(\frac{m^*}{2V_0}\right)^{1/2}. \tag{62}$$

For weak confinement we get

$$N \leq 2\epsilon V_0(1 + \delta x_w)^2 \tag{63}$$

where

$$\delta x_w = \frac{B}{8m^*\omega^3} - \frac{Bg^*}{2\omega(2m^*\epsilon)^{1/2}}\left(\frac{m^*}{2V_0}\right)^{1/2}. \tag{64}$$

The signs of δx_s and δx_w will determine whether the number of electrons that the dot can support increases or decreases in respect to the unpolarized dot. Both δx_s and δx_w goes to zero as the magnetic field goes to zero, recovering the zero magnetic field cases [22].

In reference [31], the authors calculated the total energy, chemical potential and differential capacitance for quantum dots with up to 12 electrons within the unrestricted Hartree-Fock approximation. Their numerical results for the energy show nonlinear increase in function of the number of electrons, in qualitative agreement with our estimates. From their numerical results, a change can be observed in the behavior of the chemical potential, from nonlinear to linear variation with the increase of the number of electrons, also in agreement with our results (see Eqs. (39) and (40)). Furthermore, the calculated capacitance for strong confinement is much smaller than the capacitance for weak confinement, result that is qualitatively reproduced by equations (41) and (42), which can be seen from the strong confinement condition that leads to $\epsilon \gg N^{1/2}/\omega$.

In reference [34] the authors present density-functional calculations of circular parabolic quantum dots for zero magnetic field using the local and spin density approximations and also the current-spin density functional approximation. Based in their published results, the behavior of the total energy in function of the number of electrons can be well approximated by a function proportional to a power of N, where the value of the exponent is approximately 1.75 which is halfway between the estimates of equations (51) and (52) (2 and 3/2, respectively). Furthermore, the plot of the chemical potential (estimated as $E(N+1) - E(N)$), shows a behavior which is roughly sublinear for less electrons and becomes linear for more electrons, in qualitative agreement with our findings.

Only continuous changes in the physical magnitudes can be expected in our results, since the Thomas-Fermi approximation is unable to reproduce one-electron properties as shell structure [26,27]. Nevertheless, the results are asymptotically correct and they could serve as good starting point for more elaborated calculations.

In conclusion, we have solved exactly the Thomas-Fermi equation in conjunction with Poisson's equation for the problem of the two-dimensional circular parabolic quantum dot in the presence of a weak magnetic field within the framework of the local spin-density approximation. We have written the exact expressions for

the total energy, chemical potential, differential capacitance, degree of polarization, and diamagnetic susceptibility. We obtained asymptotic solutions for the limits of strong and weak confinement. In all expansions we have retained the terms linear in the magnetic field since we are assuming that this field is weak enough to neglect higher orders. We have also shown that in the classical limit the spin effects cannot be taken into account, at least within the LSD approach, and we have given an estimate of the number of electrons that the dot could support.

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Appendix A: Coefficients of the density

Here we derive the expressions of the coefficients.

By continuity and using equations (10), (15) and (19)

$$A_+ = A_- = A = -\left(\frac{m^*\omega^2\epsilon}{2\pi} - \frac{g^*m^*B}{4\pi}\right)\frac{1}{I_0(\kappa R_+)}\cdot \tag{A.1}$$

By continuity at R_+, and using equation (10) we get that

$$CI_0(\kappa R_+) + DK_0(\kappa R_+) + \frac{m^*\omega^2\epsilon}{\pi} = \frac{g^*m^*B}{2\pi} \tag{A.2}$$

and by continuity at R_-

$$CI_0(\delta R_-) + DK_0(\delta R_-) + \frac{m^*\omega^2\epsilon}{\pi} = 0 \tag{A.3}$$

and then

$$C = \frac{m^*}{2\pi}\frac{2\omega^2\epsilon[K_0(\kappa R_+) - K_0(\delta R_-)] + g^*BK_0(\delta R_-)}{K_0(\delta R_-)I_0(\kappa R_+) - I_0(\delta R_-)K_0(\kappa R_+)} \tag{A.4}$$

$$D = \frac{m^*}{2\pi}\frac{2\omega^2\epsilon[I_0(\delta R_-) - I_0(\kappa R_+)] - g^*BI_0(\delta R_-)}{K_0(\delta R_-)I_0(\kappa R_+) - I_0(\delta R_-)K_0(\kappa R_+)}\cdot \tag{A.5}$$

Evaluating equation (8) at R_+ and R_- we find

$$\frac{m^*\omega^2}{2}R_-^2 - \frac{m^*\omega^2}{2}R_+^2 - g^*B = V_{\rm e}(R_+) \tag{A.6}$$

and using equation (5), the above equation becomes

$$\begin{aligned} &-\frac{N}{\epsilon}\ln R_- - g^*B + \frac{2\pi}{\epsilon}\{2A\frac{R_+}{\kappa}\ln R_+ I_1(\kappa R_+) \\ &+ \frac{m^*\omega^2\epsilon}{2\pi}R_-^2\ln R^- \\ &+ \frac{C}{\delta^2}[\delta R_-\ln\delta R_- I_1(\delta R_-) - I_0(\delta R_-) \\ &- \delta R_+\ln\delta R_+ I_1(\delta R_+) + I_0(\delta R_+)] \\ &- \frac{D}{\delta^2}[\delta R_-\ln\delta R_- K_1(\delta R_-) - K_0(\delta R_-) \\ &- \delta R_+\ln\delta R_+ K_1(\delta R_+) + K_0(\delta R_+)]\} = 0. \end{aligned} \tag{A.7}$$

Finally, the normalization condition will give us the missing equation

$$\begin{aligned} N = \int \mathrm{d}^2\mathbf{r}\rho(\mathbf{r}) = 2\pi\Bigg\{&\int_0^{R_+}\mathrm{d}r r[\rho_+(r) + \rho_-(r)] \\ &+ \int_{R_+}^{R_-}\mathrm{d}r r\rho_-(r)\Bigg\}. \end{aligned} \tag{A.8}$$

Substituting equations (20) and (21) into equation (29), it becomes

$$\begin{aligned} N = {}& m^*\omega^2\epsilon R_-^2 + \frac{4\pi A}{\kappa}R_+ I_1(\kappa R_+) \\ &+ \frac{2\pi C}{\delta}[R_- I_1(\delta R_-) - R_+ I_1(\delta R_+)] \\ &- \frac{2\pi D}{\delta}[R_- K_1(\delta R_-) - R_+ K_1(\delta R_+)]. \end{aligned} \tag{A.9}$$

We have to solve the system of non-linear equations comprised of equations (A.1), (A.4), (A.5), (A.7), and (A.9), to get R_+, R_-, A, C, and D.

Regarding the expectation value of the potential, equation (48) can be written as

$$\langle v\rangle \approx \langle v\rangle_{B=0} + \frac{\omega_{\rm c}^2}{4}\langle r^2\rangle + m^*\omega_0^2\pi\int_0^{r_0}\mathrm{d}r r^3\Delta\rho. \tag{A.10}$$

Substituting equation (44) into equation (47) and approximating as usual, we will have up to first order in B,

$$\begin{aligned} \langle v\rangle \approx {}& \langle v\rangle_{B=0} + \frac{1}{8}\omega_0^2\epsilon r_0^4 B \\ &+ \frac{r_0^2\epsilon}{2m^*}\frac{\omega_0^2}{I_0(\kappa r_0)}\left[m^{*2}\left(g^*B - \omega_0^2\epsilon\frac{I_1(\kappa r_0)}{I_0(\kappa r_0)}\frac{\kappa\Delta}{2}\right)\right. \\ &\left.-\frac{\epsilon B}{2}\right](\kappa r_0 I_1(\kappa r_0) - 2I_2(\kappa r_0)) = \langle v\rangle_{B=0} + \Delta v, \end{aligned} \tag{A.11}$$

where $\langle v\rangle_{B=0}$ is the expectation value of the potential for zero magnetic field.

Appendix B: Unpolarized case formulae

From reference [22] the spinless density is

$$\rho_0(r) = \frac{m^*\omega^2\epsilon}{\pi}\left[1 - \frac{I_0(\kappa r)}{I_0(\kappa r_0)}\right], \tag{B.1}$$

where r_0 is the classical turning point (effective radius of the dot) which is determined by the normalization condition, that leads to a nonlinear equation. The effective radius of the dot is

$$r_0 \approx \frac{N^{1/2}}{\omega(m^*\epsilon)^{1/2}} \tag{B.2}$$

for weak confinement, and

$$r_0 \approx N^{1/4} \left(\frac{2}{m^* \omega} \right)^{1/2} \tag{B.3}$$

for strong confinement.

The chemical potential at zero magnetic field [22] can be written as

$$\mu_0 \approx \frac{N}{2\epsilon} \tag{B.4}$$

for weak confinement and

$$\mu_0 \approx \omega N^{1/2} \tag{B.5}$$

for strong confinement.

Correspondingly, the differential capacitance can be written as

$$C_{\mathrm{d}}^0 \approx 2\epsilon \tag{B.6}$$

for weak confinement, and

$$C_{\mathrm{d}}^0 \approx \frac{2N^{1/2}}{\omega} \tag{B.7}$$

for strong confinement.

The diamagnetic susceptibility for zero magnetic field limit [33] is equal to

$$\chi_0 = -\frac{N\omega^2 \epsilon m^*}{2} r_0^2 \left[\frac{r_0^2}{4} - \frac{r_0}{\kappa} \frac{I_1(\kappa r_0)}{I_0(\kappa r_0)} + 2 \frac{I_2(\kappa r_0)}{I_0(\kappa r_0)} \frac{1}{\kappa^2} \right]. \tag{B.8}$$

In the weak confinement limit this becomes

$$\chi_0 \approx -\frac{1}{8} \frac{N^3}{m^* \omega^2 \epsilon} \tag{B.9}$$

and

$$\chi_0 \approx -\frac{1}{6} \frac{N^{5/2}}{m^* \omega} \tag{B.10}$$

in the strong one.

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