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Exact solution of the Thomas-Fermi two-dimensional *N*-electron parabolic quantum dot

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The Thomas-Fermi approach is applied to the problem of the two-dimensional parabolic quantum dot. The equation is solved exactly in conjunction with Poisson's equation for a circularly symmetric parabolic confinement. The solutions depend only on the ratio between the square of the product of the confinement constant and the dielectric constant of the host material and on the number of electrons. Asymptotic solutions for weak and strong confinement were also obtained for the chemical potential, the total energy, and the differential capacitance, reproducing the correct trends. For bounded parabolic potentials, an estimate of the maximal number of electrons that a dot can support is given. Appropiate Gaussian asymptotic behavior for the density is obtained by including a Weizsäcker-type kinetic energy term. [S0163-1829(98)07831-X]

I. INTRODUCTION

The study of quantum dots with parabolic confinement has been the object of very active research in recent years (see, e.g., Refs. 1 and 2 and references therein). Most quantum dots are structures of mesoscopic dimensions constructed on semiconductor surfaces or interfaces. While their effective dimension is usually 2, the presence of many interacting electrons renders the computation of the ground state and charge density a complicated many-body problem. For that reason only few electron dots have been treated to a fairly high degree of accuracy. Exactly solvable models have been proposed in order to gain insight into the behavior of these systems[3–5] at the exact, Hartree-Fock, or Hartree level, using simplified electron-electron interaction potentials.

When the number of electrons is large enough, the system behaves like an electron gas. It is then that the Thomas-Fermi approximation becomes useful. This approximation and its modifications[6–11] have been of frequent use in the computation of ground state properties of three-dimensional problems, e.g., in the treatment of atoms, molecules, solids, and nuclei. It has been also applied to the calculation of properties of quasi-two-dimensional systems, such as planar molecules.[12] Recently, Lieb *et al.*[13] rigorously analyzed the two-dimensional Thomas-Fermi problem in the presence of a magnetic field, with a (three-dimensional) Coulomb electron-electron interaction and parabolic confinement. The three-dimensional version of the Thomas-Fermi problem of parabolic confinement was discussed by Ballinger and March.[14]

Here we solve exactly the two-dimensional Thomas-Fermi equation coupled to Poisson's equation for a parabolic circular quantum dot. Our approach allows the analysis of the behavior of fundamental magnitudes in the limits of strong and weak confinement. For the purpose of comparison, we have also solved the corresponding classical problem. The article has been structured as follows. In Sec. II we solve exactly the two-dimensional Thomas-Fermi equation coupled to Poisson's equation and the corresponding classical problem. In Sec. III we analyze the cases of weak and strong confinement and we calculate the effective size, the chemical potential, the total energy, and the differential capacitance. An estimate of the maximal number of electrons that a bounded dot can support is given. In Sec. IV we compare our results and discuss the effect of the inclusion of a Weizsäcker-type correction to the kinetic energy.

II. EXACT SOLUTIONS

The Thomas-Fermi equation for a D-dimensional electron gas in the effective-mass approximation can be written as[15–17]

$$\frac{1}{2m^*}p_F^2+v+V_e=\mu, \tag{1}$$

where m^* is the effective mass, p_F is the Fermi momentum, v is the external potential, V_e is the electrostatic potential, satisfying Poisson's equation, and μ is the chemical potential. Since $p_F\propto\rho^{2/D}$ (D is the dimension of the space) and $V_e=\int d\vec{r}\,'\rho(\vec{r}\,')K(|\vec{r}-\vec{r}\,'|)$, where K is the kernel of the electron-electron interaction, one obtains

$$\mu=v(\vec{r}_0)+V_e(\vec{r}_0), \tag{2}$$

where $\vec{r}_0$ is the classical turning point, at which the density vanishes. This is a fundamental magnitude since it will determine the appearance of the conductance peak by the equalization of the dot's chemical potential with that of the gates.[2]

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

$$\nabla^2V_e=-2\pi\frac{\rho(\vec{r})}{\epsilon}, \tag{3}$$

where ϵ is the dielectric constant of the host material. Solving the above equation for the electrostatic potential we get

$$V_e(\vec{r})=-\frac{1}{\epsilon}\int d^2\vec{r}\,'\rho(\vec{r}\,')\ln(|\vec{r}-\vec{r}\,'|/a). \tag{4}$$

Equation (4) fixes the form of the kernel of the electron-electron interaction. Obviously, any other choice of the kernel (see, e.g., Ref. 5) will not satisfy Poisson's equation. In a circularly symmetric configuration, Eq. (4) can be written as

$$V_e(r) = -2\pi\left[\ln r\int_0^r dr'r'\rho(r') + \int_r^{r_0} dr'r'\ln r'\rho(r')\right] + N\ln a, \tag{5}$$

where a is a constant that fixes the zero of the electrostatic potential. A choice of $a \geqslant r_0$ will guarantee that the electron-electron interaction is always repulsive inside the dot ($r_0 = |\vec{r}_0|$). For simplicity we will take $a = r_0$, which means that $V_e(r_0) = 0$. This form of the electron-electron interaction is more realistic than, e.g., the harmonic one (see, e.g., Refs. 2–5).

From Eq. (1)

$$\nabla^2 V_e = -2\pi\frac{\rho(\vec{r})}{\epsilon} = \nabla^2\left(\mu - \frac{\pi}{m^*}\rho(\vec{r}) - \frac{m^*\omega^2}{2}r^2\right) \tag{6}$$

using that in two dimensions $p_F^2 = 2\pi\rho$ and taking

$$v(\vec{r}) = \frac{m^*\omega^2}{2}r^2 \tag{7}$$

as the confining potential (throughout the whole paper we are going to use the units of $m_e = e = \epsilon_0 = \hbar = 1$), where ω is the strength parameter of the potential (confinement constant). For circular symmetry and making the change of variables

$$y = \rho - m^*\omega^2\epsilon/\pi, \tag{8}$$

with $x = r/r_0$, and defining

$$\kappa = (2m^*/\epsilon)^{1/2}r_0, \tag{9}$$

we obtain the differential equation

$$y'' + \frac{y'}{x} - \kappa^2 y = 0 \tag{10}$$

for $x \leqslant 1$ and we take

$$\rho(x) = 0 \tag{11}$$

for $x \geqslant 1$, as usual in the Thomas-Fermi approximation. The solution of Eq. (10) for ρ is

$$\rho(x) = AI_0(\kappa x) + BK_0(\kappa x) + \frac{m^*\omega^2\epsilon}{\pi}, \tag{12}$$

where $I_0(x)$ and $K_0(x)$ are the modified Bessel functions of the first and second kind, respectively,[18] and A and B are constants. Taking into account that for $x \to 0$, $I_0(x) \to 1$, and $K_0(x) \to -(\ln x/2 + C)$,[18] we see that $B = 0$, since close to the origin the external potential is zero.

The continuity condition of $\rho(1) = 0$ gives us that

$$A = -\frac{m^*\omega^2\epsilon}{\pi I_0(\kappa)}. \tag{13}$$

Note that in this case, as the external potential is bounded at the origin, the density does not diverge, like in the two-dimensional atom.[17] Instead, the density is constant close to the origin and then decays to zero at the classical turning point

$$\rho(x) = \begin{cases} \dfrac{m^*\omega^2\epsilon}{\pi}\left[1 - \dfrac{I_0(\kappa x)}{I_0(\kappa)}\right], & x \leqslant 1 \quad (14) \\ 0, & x \geqslant 1. \quad (15) \end{cases}$$

It can be seen that there is no need of having an infinite confining parabola since the density vanishes beyond a certain value of the radius. In practical situations the confining potential is always bounded. Let us assume that the maximal value of the confining potential is V_0. From Eq. (7) there is a radius $R = (2V_0/m^*)^{1/2}/\omega$, such that for $r \leqslant R$ the parabolic potential is valid, and then we assume that the Thomas-Fermi approximation will work for $r_0 \leqslant R$ since any electron outside the confining potential will be free. This means that the constraint that fixes the maximal number of electrons that the dot can support will be

$$\kappa \leqslant \frac{2}{\omega}\left(\frac{V_0}{\epsilon}\right)^{1/2}. \tag{16}$$

The determination of κ will be done with the help of the normalization condition

$$N = 2\pi r_0^2\int_0^1 dx\; x\rho(x) = \omega^2\epsilon^2\kappa^2\left[1 - \frac{I_1(\kappa)}{\kappa I_0(\kappa)}\right], \tag{17}$$

i.e.,

$$\frac{N}{\omega^2\epsilon^2} = \frac{\kappa^2}{2} - \frac{\kappa I_1(\kappa)}{I_0(\kappa)}, \tag{18}$$

from which we can determine κ, A, r_0, and μ. The above equation means that κ (and the rest of the magnitudes of interest) is a function only of $\Omega = \omega^2\epsilon^2/N$.

It has been shown in Ref. 13 that the classical limit (i.e., the kinetic energy term is neglected) gives the correct limit for weak confinement. Here we are going to do the same calculation, but requiring that Poisson's equation be satisfied, i.e.,

$$\frac{m^*\omega^2 r^2}{2} + V_e(r) = \mu. \tag{19}$$

Using Eq. (3) we obtain

$$\rho_c(r) = \begin{cases} \dfrac{m^*\omega^2\epsilon}{\pi}, & r \leqslant r_{0c} \\ 0, & r \leqslant r_{0c}, \end{cases} \tag{20}$$

$$\tag{21}$$

where the c stands for classical. The turning point r_{0c} can now be determined from the normalization condition, which gives

$$r_{0c}^2 = \frac{N}{m^*\omega^2\epsilon}. \tag{22}$$

Figure 1 shows the behavior of the density for a choice of $\Omega = 1$, for which [solving numerically Eq. (18)] we get that $\kappa = 2.346\,738$. The density has been measured in units of $m^*\omega^2\epsilon/\pi$ and r in units of $(\epsilon/m^*)^{1/2}$.

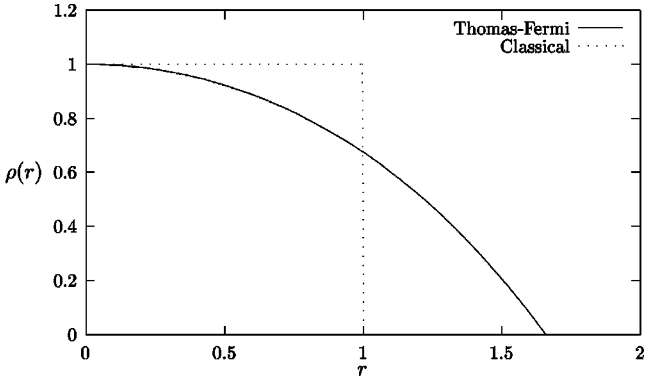

FIG. 1. Density of a parabolic two-dimensional quantum dot in the Thomas-Fermi and classical approximations for $\Omega=1$. $\rho(r)$ is in units of $m^*\omega^2\epsilon/\pi$ and r is in units of $(\epsilon/m^*)^{1/2}$.

The total energy can be calculated by taking V_e from Eq. (1) and substituting it into the total energy expression, where we also see that the kinetic energy is eliminated,

$$E=\frac{1}{2}\mu N+\pi m^*\omega^2\int_0^{r_0}dr\ r^3\rho(r). \tag{23}$$

Substituting and solving the integrals we get

$$E=\frac{1}{8}\omega^2\kappa^2\epsilon N+\frac{1}{8}\omega^4\kappa^4\epsilon^3\left[\frac{1}{4}-\frac{I_1(\kappa)}{I_0(\kappa)\kappa}+2\frac{I_2(\kappa)}{I_0(\kappa)\kappa^2}\right]. \tag{24}$$

The differential capacitance can be calculated following[19]

$$C_d=\frac{1}{\mu(N)-\mu(N-1)}. \tag{25}$$

III. ASYMPTOTIC BEHAVIOR

In the limit of weak confinement, where $N\gg\epsilon^2\omega^2$ ($\Omega\rightarrow 0$, $\kappa\rightarrow\infty$, and fixing the number of electrons $\omega\rightarrow 0$), using the asymptotic behavior of $xI_1(x)/I_0(x)=x-1/2+O(x^{-1})$, we get

$$\frac{N}{\omega^2\epsilon^2}\approx\frac{\kappa^2}{2}-\kappa+\frac{1}{2}, \tag{26}$$

from which we get the solution

$$\kappa\approx 1+\left(\frac{2}{\Omega}\right)^{1/2}=1+\frac{2^{1/2}N^{1/2}}{\omega\epsilon}. \tag{27}$$

In practice, the above approximation will work for $\Omega<0.1$ with a relative error better than 0.1%. The weak confinement limit would correspond to

$$\kappa\approx\left(\frac{2}{\Omega}\right)^{1/2}=\frac{2^{1/2}N^{1/2}}{\omega\epsilon}. \tag{28}$$

Making an expansion around zero of $xI_1(x)/I_0(x)=x^2/2-x^4/16+O(x^6)$, we get the solution for strong confinement ($N\ll\epsilon^2\omega^2$, $\Omega\rightarrow\infty$, and $\kappa\rightarrow 0$)

$$\kappa\approx\frac{2}{\Omega^{1/4}}=\frac{2N^{1/4}}{(\omega\epsilon)^{1/2}}, \tag{29}$$

which works with a relative error better than 0.5% for $\Omega>10^3$. The effective size of the dot can be determined using Eq. (9):

$$r_0\approx\frac{N^{1/2}}{\omega}\frac{1}{(m^*\epsilon)^{1/2}} \tag{30}$$

for weak confinement and

$$r_0\approx N^{1/4}\left(\frac{2}{m^*\omega}\right)^{1/2} \tag{31}$$

for strong confinement.

The chemical potential can be calculated after Eq. (2) as $\mu=\omega^2\epsilon\kappa^2/4$ since we have chosen the zero of the electrostatic potential at r_0. Therefore, in the strong confinement limit we have

$$\mu\approx\omega N^{1/2} \tag{32}$$

and for the weak confinement limit

$$\mu\approx\frac{N}{2\epsilon}. \tag{33}$$

Reading the asymptotics of Eqs. (32) and (33), we conclude that for fixed confinement constant, the chemical potential of the dot will change the dependence of the number of electrons from a power law with an exponent of 1/2 to 1. On the other hand, fixing the number of electrons, with the increase of the value of confinement constant, the behavior of the chemical potential will change from independent to a linear dependence on ω. From Eqs. (19) and (22) the classical result coincides with Eq. (33).

After Eq. (24) and using the corresponding asymptotics, in the strong confinement limit the total energy will be

$$E\approx\frac{2}{3}\omega N^{3/2} \tag{34}$$

and for the weak confinement limit

$$E\approx\frac{3}{8}\frac{N^2}{\epsilon}. \tag{35}$$

Again, for the energy we observe a change in the power law with N (the exponents moves from 3/2 to 2) and for the confinement constant from independent to a linear dependence. The classical total energy can be easily calculated using Eqs. (19) and (22) and gives

$$E_c=\frac{N^2}{2\epsilon}. \tag{36}$$

After Eq. (25), the differential capacitance in strong confinement will be

$$C_d\approx\frac{1}{\omega[N^{1/2}-(N-1)^{1/2}]}. \tag{37}$$

If, furthermore, $N \gg 1$, then

$$C_d \approx \left(\frac{d\mu}{dN} \right)^{-1} = \frac{2N^{1/2}}{\omega}. \tag{38}$$

For weak confinement

$$C_d \approx \left(\frac{d\mu}{dN} \right)^{-1} = 2\epsilon. \tag{39}$$

The classical result will be the same as Eq. (39).

Finally, let us obtain a bound for the number of electrons that a dot can support from Eq. (16). For strong confinement it will be

$$N \leqslant \frac{V_0^2}{\omega^2} \tag{40}$$

and for weak confinement

$$N \leqslant 2\epsilon V_0. \tag{41}$$

IV. DISCUSSION AND FINAL REMARKS

We would like to note the agreement of the behavior of the magnitudes calculated in the weak confinement limit and the classical one, as can be checked by comparing the results for the chemical potential for the differential capacitance and Eqs. (35) and (36) for the energy, where there is a small difference in the multiplicative constant, since in the classical limit we have not included the kinetic-energy term. This is in agreement with the results of Ref. 13 that the weak confinement limit corresponds to the classical one.

Also, we would like to note the qualitative agreement of our results with the results of Ref. 19, where the total energy, the chemical potential, and the differential capacitance for a few electrons in the unrestricted Hartree-Fock approximation were calculated. In their Fig. 1, a change can be seen in the dependence of the energy on the number of electrons upon increasing the strength of confinement, in agreement with our results. Similar changes can be seen in the chemical potential in their Fig. 2. The capacitance, as seen in their Fig. 3, increases for small confining constant a and stays almost constant for stronger confinement c [compare with the results of Eqs. (37)–(39)]. Of course, we should not expect oscillations in the chemical potential or the capacitance since we are dealing with an approximation that is not able to reproduce the shell structure.

From Eqs. (14) and (15) and Fig. 1 we see that the asymptotic behavior at infinity is not correct, but it can be checked easily that the introduction of a Weizsäcker-type correction to the kinetic-energy term would give the correct one, which is proportional to $\exp(-\omega r^2)$. For arbitrary dimensions, writing the first-order density matrix as a product of a local (purely density-dependent) factor and a nonlocal one gives a separation of the kinetic energy into Weizsäcker and a non-Weizsäcker terms[20] (see also, e.g., Ref. 21). This suggests the appearance of a Weiszäcker-type correction to the kinetic energy.

The Hamiltonian for the N-electron two-dimensional parabolic quantum dot is[2]

$$-\frac{1}{2m^*}\sum_{i=1}^{N} \nabla_i^2 + \frac{m^*\omega^2}{2}\sum_{i=1}^{N} r_i^2 + \sum_{i<j} V(|\vec{r}_i - \vec{r}_j|). \tag{42}$$

For large distances, the electron-electron interaction term can be neglected and then the corresponding Schrödinger equation decouples in a set of N harmonic oscillatorlike equations, which asymptotically behave as the Gaussian discussed above.

For large r, where we expect the density to vanish, the dominant term of the kinetic energy will be the Weizsäcker-type correction

$$\Delta T = \delta \int d\vec{r} \frac{|\vec{\nabla}\rho(\vec{r})|^2}{\rho(\vec{r})}, \tag{43}$$

where δ is some parameter. Taking the functional derivative of the above expression and taking into account that for large distances the other surviving term will be the external potential, we obtain

$$\frac{|\vec{\nabla}\rho|^2}{\rho^2} - 2\frac{\nabla^2\rho}{\rho} \approx -\frac{\omega^2}{2\delta} r^2. \tag{44}$$

Substitution of the ansatz $\rho(r) \propto \exp(-\alpha r^2)$ into the above equation leads to the result that α is proportional to ω, showing that the inclusion of a Weizsäcker-type term in the kinetic energy may correct the asympotic behavior of the density.

We have solved exactly the problem of N particles of effective mass m^* interacting through a logarithmic potential (i.e., satisfying Poisson's equation) in a medium of dielectric constant ϵ confined by a harmonic field of constant ω in the Thomas-Fermi approximation in two dimensions. For comparative purposes we have also solved the classical case. We have calculated the chemical potential, the total energy, and the differential capacitance and we have analyzed their behaviors in the limits of weak and strong confinement. From the analysis of the results we conclude that the qualitative behavior of the calculated magnitudes is the correct one and that the weak confinement limit corresponds to the classical behavior. We have also given an estimate of the maximal number of electrons that a dot can support if the confining potential is bounded. Furthermore, we have shown that the inclusion of a Weizsäcker-type correction to the kinetic energy may cure the improper behavior of the Thomas-Fermi density.

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