Orbital and spin magnetization of a confined electronic system in the transition between a quantum dot and a ring.

Gabriel Vasile, Vidar Gudmundsson, and Andrei Manolescu
Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

Abstract.
In order to understand the orbital and spin magnetization of a confined electronic system we analyze these ground state properties in the transition from a quantum dot to a quantum ring of finite thickness. The Coulomb interaction between the electrons is treated in the Hartree and Hartree-Fock approximations and special care is taken to include also the contributions of the nonlocal current to the summation of the magnetic moments of the occupied states. We identify changes in the many-body structure of the ground state and in the magnetization curves versus the magnetic field and other parameters characterizing the system. We compare the results of two models for quantum dots (or rings), one with the electrons moving continuously in the system, and one with the electrons moving on a lattice.

1. Introduction

Recently the magnetization of an electronic systems consisting of few hundred electrons confined in each dot of an array of quantum dots has been measured [1]. Researchers hope that the magnetization measurements will turn out to be an additional method to probe the ground state of small electronic systems. The temperature scales of different types of magnetization oscillations in circularly symmetric or slightly asymmetric quantum dots with many noninteracting electrons has been modeled [2]. The relation of the magnetization and the persistent currents in quantum dots and rings with many noninteracting electrons has been investigated in a model by Tan and Inkson [3], and by Aldea et al. [4]. The effects of an impurity on the magnetization of two interacting electrons in a square dot with hard walls have been reported [5]. The effects of the geometry of quantum dots on the magnetization for noninteracting or electrons interacting in the Hartree Approximation (HA) have been reported by Magnúsdóttir and Gudmundsson [6].

For few electrons, the exchange interaction and their spin configuration is important when considering the influence of the Coulomb interaction on the magnetization. Here we use the Hartree-Fock Approximation (HFA) to investigate the magnetization of confined systems with 4 - 6 electrons in the transition from dots to rings in order to understand better the connection between features in the magnetization and properties of the ground state in rather pure systems that will become the subject of experiments in close future.

2. Models

We consider a quantum dot with few electrons confined by the potential

$$V_{\text{conf}}(r, \phi) = \frac{1}{2} m^* \alpha_0^2 r^2 \left[ 1 + \sum_{p=1}^{p_{\text{max}}} \alpha_p \cos(2p\phi) \right] + V_0 \exp(-\gamma r^2),$$ (1)
Orbital and spin magnetization of quantum dots and rings.

where the parameters $\alpha_p$ can be used to break the circular symmetry of the parabolic confinement, and $\gamma$ and $V_0$ control a circular hill in the center of the dot in order to change it into a ring. The electron-electron interaction is treated in the Hartree-Fock Approximation (HFA) at a finite temperature $T$. We only consider the $z$-spin component of each electron. The effective single-electron Schrödinger equation is solved iteratively in the mathematical basis of the Fock-Darwin wave functions [7, 6]. In the HFA we have a nonlocal equation of motion and no explicit single-electron Hamiltonian. Thus, the current density does not have the same simple local expression as in the Hartree approximation. Instead, by defining the current density as

$$ j = -e \dot{r} = \frac{ie}{\hbar} [H, r] $$

we construct the matrix element of the contribution of each Hartree-Fock state $| \alpha \rangle$ of the orbital magnetization operator $M_o = r \times j$ and sum up the total magnetization of the system

$$ M_o = \sum_\alpha f_\alpha \langle \alpha | M_o | \alpha \rangle, $$

where $f_\alpha$ is the occupation of the state $| \alpha \rangle$ according to the equilibrium Fermi distribution.

In order to see what can happen in a system with more electrons, and also to verify the main features in our calculation, we compute the magnetization for a tight-binding lattice model with 100 sites with coordinates $(x, y) \equiv (na, ma)$, with $n, m = 1, 2, \ldots, 10$, $a$ being the lattice constant [4]. In this model the Hamiltonian is written as

$$ H = \sum_{n,m} \left[ V_{nm} |n,m\rangle \langle n,m| + t \left( e^{i\pi m\phi} |n,m\rangle \langle n+1,m| + e^{-i\pi m\phi} |n,m\rangle \langle n,m+1| + h.c. \right) \right] 
+ U_c \sum_{n,m \neq n', m'} \frac{\nu_{nm}}{(n-n')^2 + (m-m')^2} |n,m\rangle \langle n',m'|, $$

where $V_{nm}$ is a potential energy on each site, $t$ is the energy of hopping between nearest-neighbor sites, $\phi$ is the magnetic flux through the unit cell in units of magnetic flux quanta, $U_c$ is the Coulomb energy in units of $t$, and $\nu_{nm}$ is the site occupation. The inclusion of the Coulomb energy corresponds here to the Hartree approximation. The tight binding model is indeed more primitive, but with the number of sites chosen here it can reasonably describe a quantum dot of 100 nm width in a magnetic field up to 5 T. More details on the applicability of the tight-binding model can be found in [4] and references therein. The main advantages of this model is that we can easily use it for more electrons than the continuous model with the Darwin-Fock basis. Also, we can easily define potential barriers inside, through the on-site potentials $V_{nm}$, and give various shapes to the dot, or change it into a ring.

3. Results

In accordance with experiments on magnetization of quantum dots [1] we use GaAs parameters, $m^* = 0.067 m_e$, $\kappa = 12.4$, and $g^* = -0.44$. In Fig. 1 we show the magnetization for 230 and 40 electrons in a quantum dot, in the HA. For that many electrons we do not expect important exchange effects. For magnetic fields above 2 T we see de Haas-van Alphen oscillations and for the 40 electrons at $T = 1$ K sharper oscillations are superimposed due to the Aharonov-Bohm effect and finer details in the density of states [2]. Clearly, the
Orbital and spin magnetization of quantum dots and rings.

Figure 1. The orbital magnetization of 230 electrons at $T = 1$ K (a), and 40 electrons at $T = 1$ and 8 K (b) in a quantum dot in the Hartree approximation in units of $\mu_B$. Due to the high number of electrons and large $B$ range for $N = 230$ three different sizes of the basis sets are used in the calculation and indicated with color on the graph. $\hbar \omega_0 = 6$ meV for $N = 230$ and $\hbar \omega_0 = 3.37$ meV for $N = 40$, no spin, and circular symmetry.

The experimental situation is a bit more complicated [1], especially when it comes to comparing the magnetization in the regimes of high and low magnetic field.

For only few electrons in a dot their spin configuration becomes essential and the exchange interaction between them can not be neglected. To better appreciate the effects of the interaction we display in Fig. 2 the magnetization of a quantum dot with 4 electrons as it is changed into a quantum ring by increasing $V_0$, the height of the central hill in the confinement potential (eq. [1]). The energy spectrum for a infinitely narrow ring is periodic in the magnetic flux through it. But in the case of a ring of finite width the energy spectrum for a single electron is a mixture of the ring spectrum and the Fock-Darwin spectrum for a parabolic circular quantum dot, see Fig. 2b. For low magnetic field the spectrum is almost periodic for the lowest energy levels, and at a higher field a Landau band structure emerges as the effective magnetic length becomes comparable to or smaller than the width of the ring. The magnetization in Fig. 2a starts to show oscillations as the system becomes more ring like, but never becomes exactly periodic as is known for a thin ring.

The electron-electron interaction changes the magnetization considerably, especially the exchange interaction. If we first look at the pure dot confinement, $V_0 = 0$ in Fig. 2c, we notice a jump in $M_o$ between 1 and 2 T, but the curve in the Hartree approximation, not shown here, is smooth. In the HA, at finite $T$, when the magnetic field increases the electrons are gradually pushed to occupy states with a higher angular momentum quantum number $M$. In the HFA, at low $T$, the states are either occupied or empty, and the sharp differences in the exchange energy lead to jumps in the magnetization as $B$ increases.

In a quantum ring, i.e. for large values of $V_0$, the electrons are barred from the center region so states with low $M$ are not occupied for low $B$. When the magnetic field is increased more complex reorganization of the occupation of the $M$ states occurs and thus more jumps are seen in the orbital magnetization $M_o$. The effective single-electron Hartree-Fock energy spectrum shown in Fig. 2d reflects this fact. For all but the lowest magnetic field values we have a strong enhancement of the spin splitting, the system is spin polarized, and we have a large gap around the chemical potential $\mu$.

For the lowest two values of the magnetic field we do not get the system spin-polarized and we have not been able to attain the correct ground state as can be confirmed by the fact that we do not get a vanishing orbital magnetization for $B \approx 0$. Here the $\pm M$ states are not
Orbital and spin magnetization of quantum dots and rings.

Figure 2. For the noninteracting system the magnetization in units of $M_0 = \mu_B$ (a), and the energy spectrum (b), and for the interacting system the magnetization (c) and the effective energy spectrum (d). The interaction is treated in the Hartree-Fock approximation, and the system evolves from a dot to a ring with increasing $V_0$. The chemical potential is indicated with a continuous curve in the subfigures for the energy which are for $V_0 = 30$ meV. $\hbar \omega_0 = 3.37$ meV, and $N = 4$. $T = 1$ K.

symmetrically occupied as should be. This is a common problem with the HFA, the system gets trapped in a final state that is not the ground state and we have to start the iterations with many different initial conditions to map out possible final states in the calculation. It should though be mentioned here that all the final states here have the same angular symmetry as the initial state, we shall come back to this point below.

In Fig. 3 we show some results obtained with the tight-binding model for a square quantum dot with $n=2$, 3, and 12 electrons. Since in the tight-binding model the electrons have no spin degree of freedom the magnetization for 2 electrons in Fig. 3a corresponds to the results for 4 electrons in Fig. 2a except for the influence of the exchange. (Direct correspondence can be found to the results of Magnúsdóttir [6]). By putting an energy $V_{nm} = V_0$ to 16 central sites we define a square quantum ring. The values of $V_0$ are shown in Fig. 3 in units of the hopping energy $t$. Fig. 3b, reproduces the oscillations seen in Fig. 2a for the noninteracting electrons in a ring, despite, the differences in the geometrical shape, but, as expected, it does not show the sharp jumps created by the exchange interaction seen in Fig. 2c. In the case of 12 electrons in a square dot ($V_0 = 0$) the magnetization displayed in Fig. 3c shows the first signs of de Haas-van Alphen oscillations caused by the density of states at the Fermi level. Interestingly, the oscillations are subdued in the corresponding ring except in the regime corresponding to the last oscillation in $M_0$ for the dot, when the chemical potential
is in the lowest band in the energy spectrum seen in Fig. 3d.

In GaAs the spin magnetization is generally much smaller than the orbital one due to the small $g$ factor and the small effective mass, but in contrast to the orbital magnetization the fine structure of the spin magnetization can be quite sensitive to the geometrical shape of the system. In Fig. 4 we show the electron density for 4 and 5 spin polarized electrons, for a dot with slight square deviation in the confinement potential, calculated again using the continuous model. These are the ground states and we can correlate the number of peaks with the number of electrons, though that is generally not unique. In the case of 4 spin polarized electrons in a slightly elliptic confinement we have a “homogeneous” spin density seen in Fig. 5. In the same dot we also find an excited state with no total spin polarization but a nice internal spin-density wave shown in Fig. 5. It should be added here that we have repeated the calculations for different shapes, number of electrons and initial parameters. Each time we start with a circular symmetric system we get an end state of the same geometric symmetry. We assume this stability can be explained by the use of polar coordinates and circular basis functions. As soon as the initial state is slightly perturbed away from the circular symmetry the interaction can cause large changes in the symmetry of the end state.
Orbital and spin magnetization of quantum dots and rings.

Figure 4. The electron density for a quantum dot with 4 or 5 spin polarized electrons and a slight square deviation, $\alpha_1 = 0$, $\alpha_2 = 0.1$. $T = 1$ K, $\omega_0 = 3.37$ meV, $g^* = -0.44$.

Figure 5. The spin-density for an excited state and the ground state of a quantum dot with a slight elliptical deviation, $\alpha_1 = 0.1$, $\alpha_2 = 0$. $T = 1$ K, $\omega_0 = 3.37$ meV, $g^* = -0.44$.

4. Conclusions

The magnetization is sensitive to the shape of the dot, to the electron-electron interaction, and to the number of electrons. The deviation from the circular symmetry involves more $M$ states which for few electrons gives the potentiality for more reconfigurations thus producing more oscillations in the magnetization as a function of $B$. The effect is stronger in a ring. The Hartree interaction tends to expand the density and to change the shape, by rounding the corners when the deviation from circular symmetry is slight, or by stretching it in dots with large deviation in order to lower the electrostatic energy. For few electrons the exchange interaction produces abrupt jumps of the magnetization as the exchange energy is very dependent on the exact occupation of the single-electron states.
The oscillations of the magnetization, at low \( T \), are determined by discontinuities of the occupation of the single-particle states, i.e. by the jumps of \( E_F \) or \( \mu \). Such oscillations become the Shubnikov-de Haas oscillations at strong magnetic field. In addition, smaller oscillations occur due to the changes below \( E_F \), in the occupied states. These oscillations can be understood in several ways: the magnetization of an individual state follows the slope of the energy vs. \( B \), which is related to the chirality \( [4] \); changes of the average angular-momentum quantum number \( M \) with \( B \); the shape of the orbits, related to changes in the wave functions with the magnetic field \( B \).

We are aware of the fact that correlation effects may have their influence on the magnetization of dots, as they have for the two-dimensional electron system \( [8] \), both affecting the finer details and the exact location of reconfigurations in the ground state, but as experimental methods have to be refined quite a bit to observe finer details in dots with few electrons we have limited our handling of the electron-electron interaction here to the direct and exchange effects.

Acknowledgments

We acknowledge instructive discussions with A. Aldea and M. Schwarz. The research was partly funded by the Icelandic Natural Science Foundation, and the University of Iceland Research Fund.

References

[1] M. P. Schwarz et al., J. Appl. Phys. 91, 6875 (2002).
[2] E. N. Bogachek, A. G. Scherbakov, and U. Landman, Phys. Rev. B 63, 115323 (2001).
[3] W.-C. Tan and J. C. Inkson, Phys. Rev. B 60, 5626 (1999).
[4] A. Aldea et al., Phys. Rev. B, submitted, preprint cond-mat/0207307 (2002).
[5] W. Sheng and H. Xu, Physica B 256-258, 152 (1998).
[6] I. Magnúsdóttir and V. Gudmundsson, Phys. Rev. B 61, 10229 (2000).
[7] V. Fock, Z. Phys. 47, 446 (1928).
[8] I. Meinel et al., Phys. Rev. B 64, 121306(R) (2001).