Magnetization of noncircular quantum dots

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Abstract

We calculate the magnetization of quantum dots deviating from circular symmetry for noninteracting electrons or electrons interacting according to the Hartree approximation. For few electrons the magnetization is found to depend on their number, and the shape of the dot. The magnetization is an ideal probe into the many-electron state of a quantum dot.

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I. INTRODUCTION

The internal electron structure of quantum dots has been explored by far-infrared (FIR) absorption, Raman scattering, and tunneling. The FIR absorption can only be used to detect center-of-mass oscillations of the whole electron system if it is parabolically confined in a circular quantum dot that is much smaller than the wavelength of the incoming radiation, i.e., the absorption is according to the extended Kohn theorem. Collective excitations due to relative motion of the electrons are observed in dots where either the circular symmetry is broken, the radial confinement is not parabolic, or Raman scattering is used to inelastically transfer finite momentum with a radiation of shorter wavelength to the electron system. A similar blocking effect has been found in the transport excitation spectroscopy of a quantum dot, where correlation between the multi-electron states suppresses most of the energetically allowed tunneling processes involving excited dot states. Transitions in Raman scattering measurements do follow certain selection rules but there is no general mechanism blocking a wide selection of collective modes comprised of relative motion of the electrons. Together these three methods have proven invaluable for the exploration of excitations in quantum dots and have supplied important indirect information about the ground state of the electron system.

Recently it has been realized that new or improved methods to measure the magnetization of a two-dimensional electrons gas (2DEG) give important information about the structure of the many-electron ground state. We are aware of an effort to extend these measurements to nanostructured 2DEG’s, arrays of quantum wires or dots.

The magnetization has been calculated for large ”semi-classical“ circular quantum dots with noninteracting electrons, or two ”exactly“ interacting electrons in a square quantum dot with hard walls and an impurity in the center to investigate how it changes the effect of the electron-electron interaction on the magnetization.

In this paper we show that magnetization measurements of isolated dots can reveal information about the shape of a dot and the number of electrons in it. In addition, the magnetization is shown to be very sensitive to the electron-electron interaction.

II. MODEL

We consider a very general angular shape of the quantum dot, thus neither the total angular momentum of the system nor the angular momentum of the effective single particle states in a mean field approach is conserved. The Coulomb interaction 'mixes' up all elements of the functional basis used and we limit ourselves to the Hartree approximation (HA) in order to be able to calculate the magnetization for up to five electrons. The confinement potential of the electrons in the quantum dot is expressed as

$$V(r, \phi) = \frac{1}{2} m^* \omega_0^2 r^2 \left[ 1 + \sum_{p=1}^{p_{\text{max}}} \alpha_p \cos(2p\phi) \right],$$

representing an elliptic confinement when $\alpha_1 \neq 0$ and $\alpha_p = 0$ for $p \neq 1$, and a square symmetric confinement when $\alpha_2 \neq 0$ and $\alpha_p = 0$ for $p \neq 2$. We use the Darwin-Fock basis; the eigenfunctions of the circular parabolic confinement potential in which the natural length scale, $a$, is given by
where \( \omega_c = eB/m^*c \) is the cyclotron frequency of an electron with an effective mass \( m^* \) in a perpendicular homogeneous magnetic field \( B \). The states are labelled by the radial quantum number \( n_r \) and the angular quantum number \( M \).

The total magnetization with an orbital contribution \( M_o \) defined in terms of the quantum thermal average of the current density, and the spin contribution \( M_s \) derived from the average value of the spin density is defined as

\[
M_o + M_s = \frac{1}{2} \int_{R^2} d\mathbf{r} (\mathbf{r} \times \langle \mathbf{J}(\mathbf{r}) \rangle) \cdot \hat{n} - g\mu_B \int_{R^2} d\mathbf{r} \langle \sigma_z(\mathbf{r}) \rangle,
\]

where \( \mu_B \) is the Bohr magneton. The equilibrium local current is evaluated as the quantum thermal average of the current operator,

\[
\hat{J} = -\frac{e}{2} \left( \hat{\mathbf{v}} |\mathbf{r}\rangle \langle \mathbf{r}| + |\mathbf{r}\rangle \langle \mathbf{r}| \hat{\mathbf{v}} \right),
\]

with the velocity operator \( \hat{\mathbf{v}} = [\hat{\mathbf{p}} + (e/c) \hat{\mathbf{A}}(\mathbf{r})]/m^* \), \( \hat{\mathbf{A}} \) being the vector potential. For the finite electron system of a quantum dot the total magnetization can equivalently be expressed via the thermodynamic formula

\[
M_o + M_s = -\frac{\partial}{\partial B}(E_{\text{total}} - TS),
\]

where \( S \) and \( E_{\text{total}} \) are the entropy of the system and its total energy, respectively. In GaAs \( M_s \) is a small contribution and within the HA it is a trivial one. Thus, we neglect the spin degree of freedom here, but admittedly the spin can be of paramount importance in connection with exchange effects on the orbital magnetization.

In order to check the numerical results we have verified that both definitions \( (3) \) and \( (5) \) give identical results within our numerical accuracy for \( T = 1 \) K, even when the entropy term of \( (5) \) is neglected.

### III. RESULTS

In the numerical calculations we use GaAs parameters, \( m^* = 0.067m_0 \), and \( \kappa = 12.4 \). Furthermore, we select the confinement frequency \( \hbar \omega_0 = 3.37 \) meV in order to study quantum dots with few electrons in the regime where the energy scale of the Coulomb interaction is of same order of magnitude or larger than the quantization energy due to the geometry and the magnetic field.

To make clear the information about the structure of the ground state discernible in the curves of the magnetization versus the magnetic field \( B \) we start by investigating a dot with noninteracting electrons. The magnetization of 2-5 electrons in an elliptic quantum dot is shown in Fig. [1] for different degree of deviation from a circular shape. For comparison the total energy \( E_{\text{total}} \) for the same number of electrons, and the single-electron spectrum for a dot with an elliptical shape is presented in Fig. [2]. Sharp jumps in the magnetization can be
correlated with "discontinuities" in the derivative of $E_{\text{total}}(B)$ reflecting crossing of single-electron states. A jump represents a change in the electron structure of the dot. In a circular dot, or a nearly circular dot, each single-electron state can be assigned a definite quantum number $M$ for the angular momentum. As the magnetic field is increased the occupation of a state with a higher angular momentum is energetically favorable. The mean value of the radial electron density moves away from the center, the moment of inertia increases, and in order to conserve the total energy the equilibrium current is reduced leading to weaker magnetization. In addition to this over-simplified semiclassical picture the persistent equilibrium current, even in a circular dot, has a nontrivial structure as a function of the radial coordinate $r$ that can lead to the sign change of the magnetization.

For which range of $B$ the effects of the geometry are strongest can be understood in the following way: For low magnetic field $B \sim 0$ the increased elliptic shape results in a change of the curvature of some of the single-electron energy levels, i.e. those that are degenerate for circular dots. If we look at the magnetization for $N_s = 2$ it only differs at low $B$ for different $\alpha_1$ reflecting the fact that the lowest occupied single-electron state has almost unchanged curvature for low $B$, but the second state is affected. In the case of three electrons the change in the curvature of the second and the third state for low $B$ cancels leaving the magnetization unaffected by the change in the shape for low magnetic field. Instead, the magnetization changes with $\alpha_1$ around $B \sim 1$ T where the third and the fourth single electron state cross. The crossing point varies with $\alpha_1$ shifting the location of the jump in the magnetization. In this same sense all the variation in the magnetization can be referred back to the single electron energy spectrum, and thus the total energy.

So, what changes do we observe when we change the degree of a square deviation of a quantum dot instead of the elliptical shape? The corresponding graphs for the magnetization and the energy can be seen in Fig. 3 and 4, respectively in case of square deviated dots. The square deviation does not lift the degeneracy of the second and the third single-energy levels at $B = 0$ and it does not move strongly the crossing point between the third and the fourth energy level. The magnetization for $N_s = 2$ and 3 is thus not strongly affected by increased square shape of a quantum dot. On the other hand, the magnetization is strongly affected by the change in the shape of dots with four or five electrons. The large change in the anticrossing seen in the single-energy spectrum (at $B \approx 2.3$ T) with increasing $\alpha_2$ is clear in the magnetization.

The main difference in the magnetization of a quantum dot with an elliptical or square shape comes from the fact that the elliptical deviation has nonzero matrix elements between single electron states with a dominant contribution of basis states of a circular dot satisfying $|\Delta M| = 2$, whereas the square shape can only connect states with the dominant contribution satisfying $|\Delta M| = 4$. For weak deviation the square shaped dot thus needs the occupation of more states than the elliptical one to show effects in the magnetization different from the magnetization of a circular quantum dot.

Within the Hartree approximation the essential structure of the effective single electron spectrum remains, i.e. the anticrossing typical for the square shape and the lifting of the degeneracy of the second and third energy level typical for the elliptic shape. The finer details of the spectrum depend on the number of electrons in the dot as is expected in an effective potential. The electron-electron interaction in a circular dot can not change the angular symmetry of the dot, but as soon as this symmetry is broken by the confinement potential the
interaction further modifies the angular shape of the dot. In Fig. 5 and 6 the magnetization for three and four interacting electrons is compared to the magnetization of noninteracting electrons. The Coulomb repulsion between the electrons causes changes in the electron structure to occur for lower magnetic field $B$. It is energetically favorable for electrons to occupy states associated with higher angular momentum earlier when $B$ is increased in order to reduce the overlap of their wavefunctions. The jumps in the magnetization are thus shifted toward lower $B$.

In the noninteracting case the magnetization of three electrons in a square shaped dot did not vary much with increased deviation from a circular shape, see Fig. 3. Quite the opposite happens for three interacting electrons in the same system, the reason being that the interaction enhances the deviation and thus the size of the anticrossing energy gap in the effective single electron spectrum. This behavior is only observed in dots with few electrons, in larger dots the interaction generally smoothens the angular shape of the dots.

**IV. SUMMARY**

The calculation of the magnetization for few electrons in a quantum dot shows that it depends on the shape of the dot and the exact number of electrons present. This is in contrast to the results for large dots with many electrons where the magnetization assumes properties reminiscent of a homogeneous 2DEG.\textsuperscript{4} It is certainly harder to justify the use of the Hartree approximation here than in the case of a calculation of the far-infrared absorption where to a large degree, classical modes - center-of-mass modes - dominate the excitation spectrum. We are fully aware that exchange and correlation effects will be important in the present system,\textsuperscript{21,23} but they will not qualitatively change our results that magnetization measurements are ideal to investigate the many-electron structure of quantum dots.

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REFERENCES

1 T. Demel, D. Heitman, P. Grambow, and K. Ploog, Phys. Rev. Lett. 64, 788 (1990).
2 C. Schüller et al., Phys. Rev. 54, R (1996).
3 P. L. McEuen et al., Phys. Rev. Lett. 66, 1926 (1991).
4 R. C. Ashoori et al., Phys. Rev. Lett. 68, 3088 (1992).
5 R. H. Blick et al., Phys. Rev. B 53, 7899 (1996).
6 P. A. Maksym and T. Chakraborty, Phys. Rev. Lett 65, 108 (1990).
7 D. A. Broido, K. Kempa, and P. Bakshi, Phys. Rev. B 42, 11400 (1990).
8 F. M. Peeters, Phys. Rev. B 42, 1486 (1990).
9 A. V. Chaplik and S. A. Gorov, JETP Letters 52, 31 (1990).
10 V. Gudmundsson et al., Phys. Rev. B 51, 17744 (1995).
11 D. Pfannkuche and S. E. Ulloa, Physical Review Letters 74, 1194 (1995).
12 D. Grundler, I. Meinel, F. S. Bargsteadt, and D. Heitmann, Physica B 249-251, 693 (1998).
13 I. Meinel et al., 24th ICPS Jerusalem, Israel, Editor D. Gershoni, World Scientific (1999).
14 I. Meinel, T. Hengstmann, D. Grundler, and D. Heitmann, Physical Review Letters 82, 819 (1999).
15 S. A. J. Wiegers et al., Physical Review Letters 79, 3238 (1997).
16 M. M. Fogler, E. L. Levin, and B. I. Shklovskii, Phys. Rev. B 49, 13767 (1994).
17 W.-C. Tan and J. C. Inkson, Phys. Rev. B 60, 5626 (1999).
18 W. Sheng and H. Xu, Physica B 256-258, 152 (1998).
19 V. Gudmundsson and R. Gerhardts, Phys. Rev. B 43, 12098 (1991).
20 V. Gudmundsson, S. I. Erlingsson, and A. Manolescu, Phys. Rev. B submitted (1999).
21 D. Pfannkuche, V. Gudmundsson, and P. Maksym, Phys. Rev. B 47, 2244 (1993).
22 C. S. Lent, Phys. Rev. B 43, 4179 (1991).
23 D. Pfannkuche, V. Gudmundsson, P. Hawrylak, and R. Gerhardts, Solid-State Electronics 37, 1221 (1994).
FIG. 1. The effects of increased elliptical deviation on the magnetization of 2-5 noninteracting electrons in a quantum dot. $M_0 = \mu_B = e\hbar/(2m^*c)$, $T = 1$ K, $\hbar\omega_0 = 3.37$ meV.
FIG. 2. The total energy (left), and the single-electron energy spectrum (right) for noninteracting electrons in an elliptic dot with $\alpha_1 = 0.2$. 

FIG. 3. The effects of increased square deviation on the magnetization of 2-5 noninteracting electrons in a quantum dot. $M_0 = \mu_B = e\hbar/(2m^*c)$, $T = 1$ K, $\hbar\omega_0 = 3.37$ meV.
FIG. 4. The total energy (left), and the single-electron energy spectrum (right) for noninteracting electrons in a square dot with $\alpha_1 = 0.4$. 
FIG. 5. The magnetization of a three electron quantum dot in the case of elliptic confinement (left), with $\alpha_1 = 0.2$ and 0.4, and square symmetric confinement (right), with $\alpha_2 = 0.2$, and 0.4 for both interacting (closed symbols), and non-interacting electrons (open symbols). $M_0 = \mu_B = e\hbar/(2m^*c)$, $T = 1$ K, $\hbar\omega_0 = 3.37$ meV.

FIG. 6. The magnetization of a four electron quantum dot in the case of elliptic confinement (left), with $\alpha_1 = 0.2$, and square symmetric confinement (right), with $\alpha_2 = 0.2$, for both interacting and non-interacting electrons. $M_0 = \mu_B = e\hbar/(2m^*c)$, $T = 1$ K, $\hbar\omega_0 = 3.37$ meV.