PHYSICAL REVIEW B **70**, 081301(R) (2004)

Magnetization of nanoscopic quantum rings and dots

J. I. Climente, J. Planelles,* and J. L. Movilla
Departament de Ciències Experimentals, UJI, Box 224, E-12080 Castelló, Spain
(Received 21 May 2004; published 10 August 2004)

The magnetization of one- and two-electron quantum dots and a series of quantum rings with increasingly larger inner radii is calculated using a three-dimensional model with realistic finite confining potential, including strain and Coulomb effects. A change in topology leads to a sharp response in the calculated magnetization. The magnetization is also extremely sensitive to changes in the length of the inner radius of the ring. These results suggest the use of magnetization as a tool, complementary to far-infrared spectroscopy, for probing the topology of nanocrystals. Our calculations also reveal that atomic Zeeman splitting and, more especially, electron-electron interaction induce significant changes in the magnetic moment of a quantum ring of nanoscopic size.

DOI: 10.1103/PhysRevB.70.081301 PACS number(s): 73.21.−b, 75.75.+a, 71.70.Ej

Magnetization measurements provide direct access to the quantum electronic structure of semiconductor nanocrystals, often outperforming transport or far-infrared absorption experiments.[1,2] For example, in few-electron parabolic quantum dots the generalized Kohn theorem prevents dipole-allowed transitions from revealing many-body effects.[3] In contrast, magnetization studies have been useful to observe some of these effects, such as the spin-singlet-spin-triplet transitions of the ground state.[4] In mesoscopic quantum rings, magnetization has also been used to investigate the electronic properties of these nonsimply connected quantum systems.[5,6]

Recently, self-assembled InAs/GaAs rings, which are in the nano-scale, have been synthesized.[7] These nanocrystals have been imaged by atomic force micrography,[8] but the question of whether they preserve the ring-like topology after being covered with GaAs or not is difficult to assess. Far-infrared experiments of one- and two-electron nanoscopic rings in a magnetic field have been carried out in order to clarify this issue.[9,10] Although the results seem to agree well with theoretical predictions for ring structures,[9–11] the low resolution of the reported absorption spectra makes any complementary confirmation highly desirable. Very recently it has been reported that magnetization can be used as a tool for probing the reduction of symmetry in quantum dots.[12–14] In this work we show that magnetization also reveals the topology of a nanocrystal.

The predicted response of nanoscopic rings to homogeneous magnetic fields seems to be different to that of mesoscopic rings,[15] then the effect of electron-electron interactions may also be different. In the case of mesoscopic few-electron rings where only the lowest Landau level is populated, electron-electron interactions do not play a significant role in magnetization.[6] Since, to our knowledge, the only theoretical study on the magnetization of few-electron nanoscopic rings that has been performed so far only considers independent particles,[16] we include in this note the study of the magnetization of two-electron rings and dots with and without Coulomb interactions in order to assess the role of electron-electron interaction in nanoscopic sized rings.

The model we use is that in Ref. 11. The one-band effective mass Hamiltonian for the electron states, including a magnetic field perpendicular to the ring plane, can be written in atomic units as

$$\mathcal{H}_e = \left(-\frac{1}{2}\nabla\left(\frac{1}{m^*(E_{n,m};\rho,z)}\nabla\right) + \frac{(B\rho)^2}{8m^*(E_{n,m};\rho,z)} + \frac{Bm}{2m^*(E_{n,m};\rho,z)} + \frac{1}{2}\mu_B g(E_{n,m};\rho,z)B\sigma + V_c(\rho,z) + a_c\varepsilon_{hyd}(\rho,z)\right), \quad (1)$$

where $m=0,\pm1,\pm2,\ldots$ is the quantum number of the projection of the angular momentum onto the magnetic field (B) axis, n is the main quantum number, $V_c(\rho,z)$ is the finite confinement potential corresponding to the geometries shown in the insets of Fig. 1, and $m^*(E_{n,m};\rho,z)$ and $g(E_{n,m};\rho,z)$ stand for the energy- and position-dependent mass and Landé factor, respectively.[16] a_c denotes the hydrostatic deformation potential for the conduction band, and ε_{hyd} is the hydrostatic strain, which we calculate within the framework of the isotropic elastic theory.[17,18] It should be underlined that V_c must be a step-like, finite confinement potential in order to achieve a realistic description of the effect of the inner hole and the magnetic field penetration into the ring region.[15,19] Finally, since exchange and correlation effects are known to have a strong influence on the magnetization of quantum dots with interacting electrons,[1,20] a configuration interaction procedure is used to calculate the two-electron eigenstates and eigenenergies. The two-electron states can be labeled by the z projection of the total angular momentum $M=m_1+m_2$, total spin $S=\sigma_1+\sigma_2$, and main quantum number N.[11] The total magnetization of the nanocrystals at zero temperature is defined by

$$M = -\frac{\partial E_{tot}}{\partial B}, \quad (2)$$

where E_{tot} is the total energy for a given N-electron system.

We investigate self-assembled InAs quantum dots and rings embedded in a GaAs matrix. The dot is lens-shaped and the shape of the rings is a cut torus. The cross sections of

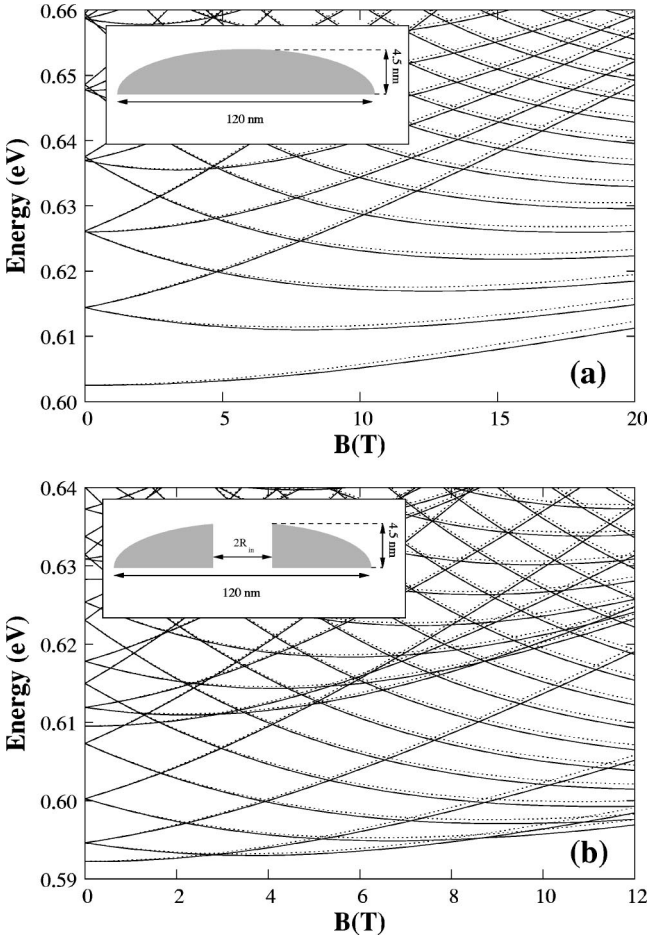

FIG. 1. Energy levels vs magnetic field of one electron in a quantum dot (a) and in a quantum ring with $R_{in}=5$ nm (b). Solid lines denote spin α levels, and dotted lines spin β levels. The insets show the cross section of the investigated dot (upper panel) and ring (lower panel).

the dot and rings can be seen in the insets of Figs. 1(a) and 1(b), respectively. Following recent measurements,[8] we take the height at the inner edge of the cross section of the rings to be 4.5 nm and then we let it decrease as a spherical casket. The outer radius of the rings is fixed at the approximate experimental value of 60 nm and the inner radius (R_{in}) is varied from 0 to 10 nm. The same material parameters as in Ref. 11 are used here. We have assumed the InAs/GaAs band-offset, $V_c(\text{matrix})=0.77$ eV, to be the confinement potential. Such a potential has successfully described the experimental far-infrared resonances of InAs rings.[11] However, its finite magnitude allows some electron density charge to spread over the inner hole of the ring, so that introducing an inner hole does not actually change the topology of the electronic density distribution from a simple to a twofold connected one. Instead, it produces a rather gradual transition. Assuming higher confinement barriers would lead to a further enhanced quantum ring-like electronic structure,[21] but again it is worthwhile noting that our conclusions are obtained for a realistic, finite, value of the confinement potential. Equation (1) is integrated numerically by employing finite differences in a two-dimensional grid (ρ,z). The

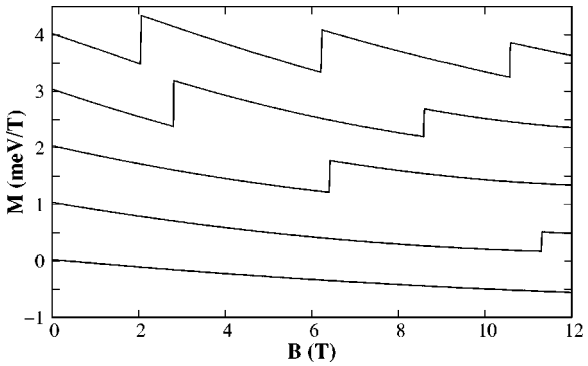

FIG. 2. Magnetization of one-electron nanocrystals with increasing inner radius. From bottom to top the curves correspond to $R_{in}=0$ nm, $R_{in}=1$ nm, $R_{in}=2$ nm, $R_{in}=5$ nm and $R_{in}=10$ nm. The curves are offset by 1.0 meV/T.

configuration interaction calculations include all the single-particle states up to 35 meV away from the ground state for the ring structures and up to 50 meV for the quantum dot. We have checked that the use of larger basis sets does not significantly change the low-lying two-electron states within the range of the magnetic field that is studied.

Figure 1 shows the electronic structure vs a magnetic field for nanocrystals with $R_{in}=0$ (a), and $R_{in}=5$ nm (b). Solid lines are used for spin up and dotted lines for spin down levels. It can be seen that the changes induced by the presence of the inner hole of the ring in the monoelectronic energy structure are dramatic. It significantly reduces the energy spacing between consecutive azimuthal levels ($m=0,\pm1,\pm2,\ldots$) at $B=0$. As a result, changes in the z component of the ground state angular momentum, from $m=0$ to $m=-1$ and from $m=-1$ to $m=-2$, take place at 2.8 and 8.6 T, respectively, while the quantum dot ground state is $m=0$ over the whole range under study, 0–20 T. Indeed, these angular momentum changes in the ground state never occur in the one-electron dot, where the low-lying levels converge to the first Landau level without crossings.[3] Although differences between quantum dot and ring energy structure were expected from the topological change of the potential, their magnitude is worth highlighting. Typical InAs self-assembled rings have an inner radius ranging between 10 and 15 nm.[8,9] Therefore, the evolution of their energy levels with a magnetic field will show a behavior that is clearly different to that of a quantum dot. This can be seen in Fig. 2, where the magnetization curves of a quantum dot and quantum rings with increasingly larger inner radii are depicted. The magnetization curves are offset by 1.0 meV/T for clarity. In the quantum dot limit ($R_{in}=0$), magnetization is smooth over the entire range of studied magnetic fields. However, an inner radius as small as $R_{in}=1$ nm already leads to a discontinuity (or step) at 11.3 T. Such a step is related to the change in ground state angular momentum in the quantum ring, as described above. By increasing the inner radius, the step shifts toward weaker magnetic fields and becomes sharper. This is because the slope of the energy levels in a magnetic field gets steeper as the ring becomes narrower.[16] An inner radius of $R_{in}=5$ nm already yields two steps that can be seen at 2.8 and 8.6 T. These steps correspond to the

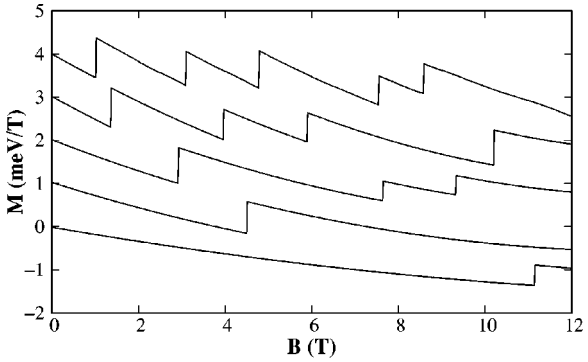

FIG. 3. Magnetization of two-electron nanocrystals with increasing inner radius. From bottom to top the curves correspond to $R_{in}=0$ nm, $R_{in}=1$ nm, $R_{in}=2$ nm, $R_{in}=5$ nm and $R_{in}=10$ nm. The curves are offset by 1.0 meV/T.

level crossings in the ground state shown in Fig. 1(b). An inner radius of $R_{in}=10$ nm yields three steps at about 2, 6.2, and 10.6 T. It should be noted that the magnetization curves are not periodic. This is due to the penetration of the magnetic field into the ring region.[5,15] Finally, by increasing the magnetic field the additionally arising steps gradually become flatter due to the smaller changes in slope at the crossing points (see Fig. 1(b)). It can be concluded from Fig. 2 that the magnetization of a one-electron quantum dot is markedly different to that of any quantum ring. These differences can be traced at relatively low magnetic fields, even for inner holes as small as $R_{in}=1$ nm.

In quantum dots, electron-electron interaction pushes the magnetization steps toward lower values of the magnetic field.[20] Hence, we calculate the magnetization of a two-electron dot and rings with various inner radii to investigate whether it is possible to distinguish them by means of fields that are even weaker than in the one-electron case. The corresponding results are plotted in Fig. 3, the curves being offset by 1.0 meV/T. A major difference with respect to one-electron magnetization can be found in the magnetization curve of the quantum dot: whereas in Fig. 2 no step was present in the $R_{in}=0$ curve, in Fig. 3 a step shows up at 11.15 T. The origin of this new step is the spin-singlet-spin-triplet transition that the exchange energy induces in the ground state of two-electron dots.[22] Such spin oscillations are also present in the ground state of two-electron quantum rings,[11] and thus a step can be also seen in the $R_{in}=1$ nm curve, but at a magnetic field that is much lower than that of the dot. Further steps appear when the size of the inner hole increases. In general, the steps of the two-electron quantum ring magnetization show up at weaker fields than in the one-electron case. This is mostly due to the exchange interaction. Our results highlight the fact that low-field magnetization measurements unambiguously reveal the topology of covered InAs/GaAs nanocrystals with one or two electrons. It should be stressed that ring morphology is evidenced by the presence and the position of the magnetization steps. This probe can be complemented with estimates of the circular symmetry also performed using magnetization data, since asymmetry leads to variations in the size of the steps, rather than in their positions.[12,13]

In order to study the influence of Coulomb interaction on the magnetization of nanoscopic rings, in Fig. 4 we illustrate the magnetization curves of a one- and two-electron quantum ring with $R_{in}=5$ nm, and those of the one- and two-electron quantum dots, which are shown for comparison. Figures 4(a) and 4(b) show the magnetization of the one-electron dot and

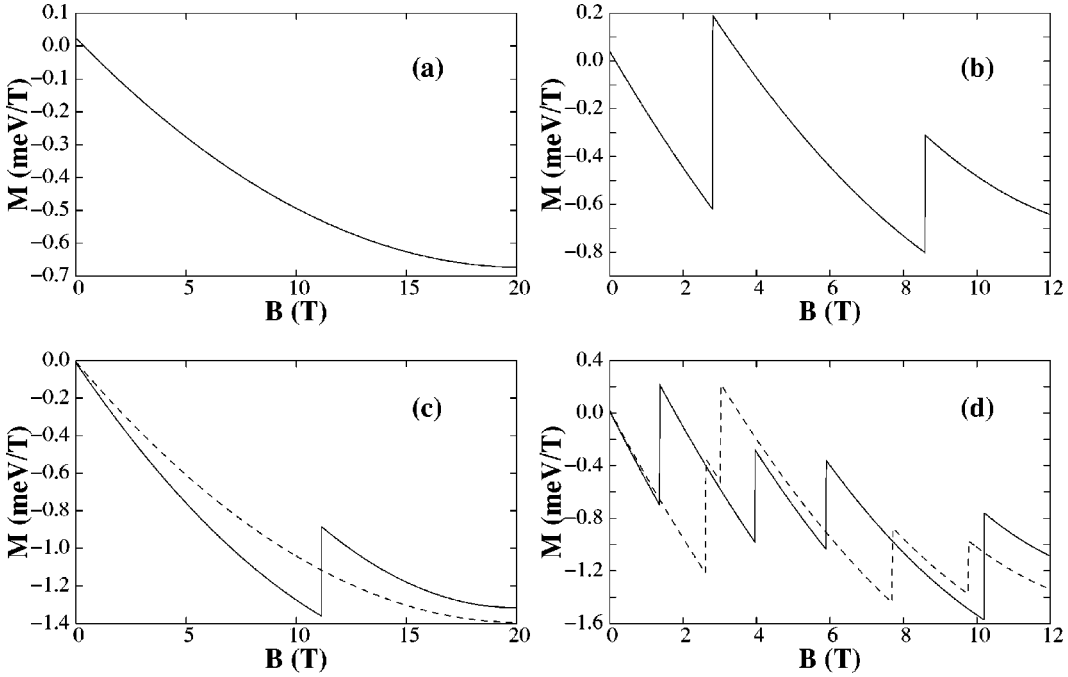

FIG. 4. Magnetization of a one-electron quantum dot (a), a one-electron quantum ring with $R_{in}=5$ nm (b), a two-electron quantum dot (c) and a two-electron quantum ring with $R_{in}=5$ nm (d). In (c) and (d), solid lines represent interacting electrons and dashed lines non-interacting electrons.

ring, and Figs. 4(c) and 4(d) and show the magnetization of the two-electron dot and ring, respectively. In Figs 4(c) and 4(d), solid lines are used for interacting electrons and dashed lines for non-interacting electrons. The two-electron magnetization without Coulomb interaction can be constructed from the single-particle levels of Fig. 1 assuming single occupancy of the two lowest one-electron spin-orbitals (which are not degenerated exactly due to Zeeman splitting) at each value of the magnetic field. Therefore, for the quantum dot the magnetization of non-interacting electrons is the same as that of the one-electron case but about twice as big in magnitude. Only when Coulomb interaction is included a step can be found in the magnetization curve. This originates from the possibility of spin oscillations, which is in turn induced by the electron-electron interaction. Moreover, it can be seen that the electron-electron interaction increases the magnitude of magnetization in the field region $B<11$ T. The underlying reason is that the repulsive Coulomb interaction makes the ground state of interacting electrons be more extended than that of non-interacting ones.[20] For the quantum ring, the two-electron magnetization is clearly different than that of the one-electron case even in the absence of Coulomb interaction. This can be explained in terms of the contribution of the atomic Zeeman term to the one-electron energy structure. In the absence of an atomic Zeeman term, $\sigma=\alpha$ and $\sigma=\beta$ states in Fig. 1(b) would be degenerate and the magnetization of the non-interacting electrons should be similar to that of the one-electron case but with sharper steps. However, the atomic Zeeman term lifts the degeneracy of $\sigma=\alpha$ and $\sigma=\beta$ states at $B\neq 0$. This originates short magnetic field domains where the two-electron ground state is a triplet (around 2 and 8 T in Fig.1(b)), and such triplet ground states give rise to the additional magnetization steps which do not appear in the one-electron case. Moreover, the triplet states domains' grow wider as the magnetic field increases because of its larger Zeeman contribution to the energy. On the other hand, when the Coulomb interaction is considered very important changes take place in the quantum ring magnetization: the position of the steps is very different than that of the non-interacting picture due to variations in the electron interlevel spacing and to exchange interactions, which in turn favor the triplet ground state configuration. The exchange interaction also accounts for the sharper steps coming from the triplet ground state. It is therefore concluded that both atomic Zeeman splitting, which is often neglected in InAs rings calculations (on the grounds that it makes a relatively small contribution to the energy),[9,23] and the Coulomb interaction are essential for a realistic description of the magnetic properties of nanoscopic rings. The role of electron-electron interaction in few-electron nanoscopic rings is thus remarkably different to that predicted for mesoscopic rings using a two-dimensional model with parabolic-like confinement.[6]

In summary, we have studied the magnetization of one- and two-electron nanoscopic dots and rings with different inner radii. Magnetization is very sensitive to the presence and size of an inner hole. Thus, it can be used to probe the topology of a nanocrystal using relatively weak magnetic fields. We have also found that atomic Zeeman splitting and electron-electron interaction cannot be neglected in calculations of magnetic properties of few-electron nanoscopic rings.

Financial support from a MEC-FPU grant and UJI-Bancaixa project P1-B2002-01 are gratefully acknowledged.

*Electronic address: planelle@exp.uji.es

[1] V. Gudmundsson, S. I. Erlingsson, and A. Manolescu, Phys. Rev. B **61**, 4835 (2000).
[2] T. H. Oosterkamp, S. F. Godijn, M. J. Uilenreef, Y. V. Nazarov, N. C. van der Vaart, and L. P. Kouwenhoven, Phys. Rev. Lett. **80**, 4951 (1998); M. P. Schwarz, D. Grundler, M. Wilde, Ch. Heyn, and D. Heitmann, J. Appl. Phys. **91**, 6875 (2002).
[3] T. Chakraborty, *Quantum Dots* (Elsevier Science, Amsterdam, 1999).
[4] P. A. Maksym and T. Chakraborty, Phys. Rev. B **45**, 1947 (1992).
[5] W.-C. Tan and J. C. Inkson, Phys. Rev. B **60**, 5626 (1999).
[6] T. Chakraborty and P. Pietiläinen, Phys. Rev. B **50**, 8460 (1994).
[7] J. M. Garcia, G. Medeiros-Ribeiro, K. Schmidt, T. Ngo, J. L. Feng, A. Lorke, J. Kotthaus, and P. M. Petroff, Appl. Phys. Lett. **71**, 2014 (1997).
[8] J. A. Barker, R. J. Warburton, and E. P. O'Reilly, Phys. Rev. B **69**, 035327 (2004).
[9] A. Lorke, R. J. Luyken, A. O. Govorov, J. P. Kotthaus, J. M. Garcia, and P. M. Petroff, Phys. Rev. Lett. **84**, 2223 (2000).
[10] A. Emperador, M. Pi, M. Barranco, and A. Lorke, Phys. Rev. B **62**, 4573 (2000).
[11] J. I. Climente, J. Planelles, F. Rajadell (unpublished).
[12] P. S. Drouvelis, P. Schmelcher, and F. K. Diakonos, Phys. Rev. B **69**, 155312 (2004).
[13] P. S. Drouvelis, P. Schmelcher, and F. K. Diakonos, J. Phys.: Condens. Matter **16**, 3633 (2004).
[14] I. Magnúsdóttir and V. Gudmundsson, Phys. Rev. B **61**, 10229 (2000).
[15] O. Voskoboynikov and C. P. Lee, Physica E (Amsterdam) **20**, 278 (2004).
[16] O. Voskoboynikov, Y. Li, H. M. Lu, C. F. Shih, and C. P. Lee, Phys. Rev. B **66**, 155306 (2002).
[17] J. R. Downes, D. A. Faux, and E. P. O'Reilly, J. Appl. Phys. **81**, 6700 (1997).
[18] J. H. Davies, J. Appl. Phys. **84**, 1358 (1998).
[19] S. S. Li and J. B. Xia, J. Appl. Phys. **89**, 3434 (2001).
[20] W. Sheng and H. Xu, Physica B **256–258**, 152 (1998).
[21] A. Puente and Ll. Serra, Phys. Rev. B **63**, 125334 (2001).
[22] M. Wagner, U. Merkt, and A. V. Chaplik, Phys. Rev. B **45**, 1951 (1992).
[23] H. Hu, J. L. Zhu, and J. J. Xiong, Phys. Rev. B **62**, 16777 (2000); J. B. Xia and S. S. Li, *ibid.* **66**, 035311 (2002); J. Planelles, W. Jaskolski, and J. I. Aliaga, *ibid.* **65**, 033306 (2002); J. I. Climente, J. Planelles, and W. Jaskolski, *ibid.* **68**, 075307 (2003).