Spin transitions in semiconductor quantum rings

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Abstract. We adopt the path integral Monte Carlo method to accurately resolve the total spin of the ground state of electrons confined in a quantum ring with different geometries. Using this method, an evaluation of the ground state of three electrons in a ring shows a spin transition to the fully polarized state by increasing the radius and thereby enhancing the Coulomb interaction. The total spin of the ground state is determined by the mutual interplay of confinement and electron-electron interaction. An analysis of the four-electron ring demonstrates that in this case no spin transitions take place. Furthermore, the effect of geometric distortion of the ring on its ground state has been investigated. Elliptically deforming the ring breaks the symmetry of the system and leads to the removal of orbital degeneracy. For strong distortion the splitting between hybridized states is sufficient to overcome the exchange-energy saving associated with a higher spin state. We have found that this effect removes the polarization of three electrons. Even in a four-electron ring the ground state is forced by the distortion to be unpolarized and thus suppressing the Hund’s rule ground state.

1. Introduction

The interest in spin effects in semiconductor nanostructures has grown during the last decades due to their possible application as spintronic devices. Most prominent representatives are quantum dots which can be manufactured to contain a defined small number of electrons. Particularly methods for manipulating and preparing the spins in nano devices are required to build spintronic devices. Among other applications, the use of quantum dots as spin filters, memory devices and qubits in quantum computers are proposed [1, 2].

Ring shaped quantum dots, referred to as quantum rings, are a promising class of nanostructures because the electrons are additionally confined on a circular orbit which will be shown to enhance spin effects. Different radii and ring widths can be experimentally realized depending on the process of manufacture [3, 4]. The ground-state transition solely induced by changing the geometry of the ring is a salient question. Recent theoretical investigations indicated that changes in ring size are accompanied by an alteration of the total spin of the ground state [5, 6]. We have performed a comprehensive numerical study of the dependence of the ground-state spin on two ring parameters which are diameter and elliptical distortion. The results showed in particular that the system can be driven to ferromagnetism by increasing the diameter.
2. Model and method

The Hamiltonian of $N$ interacting electrons in a quantum ring is written as

$$\mathcal{H} = \sum_i^{N} \mathcal{H}_i^{(1)} + \sum_{i<j}^{N} \frac{e^2}{\kappa |\mathbf{r}_i - \mathbf{r}_j|},$$  

(1)

where $\kappa$ denotes the dielectric constant of the bulk and the ring is assumed to be perfectly flat, i.e. the electron motion is strictly two-dimensional. The one-particle Hamiltonian $\mathcal{H}_i^{(1)}$ describes an electron confined in radial direction by a displaced harmonic confinement

$$\mathcal{H}_i^{(1)} = \frac{\mathbf{p}_i^2}{2m^*} + \frac{1}{2} m^* \omega_0^2 (r_i - r_0)^2,$$

(2)

where $r_0$ is the radius of the ring, $r_i$ the radial coordinate of the electron and $m^*$ its effective mass. The electrons move freely in angular direction and are bounded in radial direction. We may relate the confinement frequency $\omega_0$ to the width of the ring defined as $W = 2r_0$, where $l_0 = \sqrt{\hbar/m^*\omega_0}$ is the characteristic length of the displaced harmonic oscillator. In the following, lengths and energies are given in effective Bohr radii $a_0^* = \frac{\hbar^2}{m^*e^2}$ and effective Hartree $E_{H}^* = \frac{\hbar^2}{m^*a_0^{*2}} = \frac{e^2}{m_a}$, respectively. For example, taking GaAs rings the units of length and energy are $a_0^* = 9.8$nm and $E_{H}^* = 12$meV. The ring radius $r_0$ of experimentally realized quantum rings is of the order of 10 to 100 nm while the confinement $\hbar \omega_0$ varies between 1 up to a few meV [3, 4].

The purpose of our calculations is to determine the ground state of the Hamiltonian (1) during the crossover between different ring geometries. We utilize the path integral Monte Carlo method which yields numerically exact results. The partition function for $N$ electrons at an inverse temperature $\beta = 1/k_B T$ with $k_B$ the Boltzmann constant reads [7, 8]

$$Z = \frac{1}{N!} \sum_{\mathcal{P}} (-1)^p n(\mathcal{P}) \int d\mathbf{R} \langle \mathbf{R} | e^{-\beta \mathcal{H}} | \mathcal{P} \mathbf{R} \rangle,$$

(3)

with

$$n(\mathcal{P}) = \sum_{\sigma_1,...,\sigma_N = \pm \frac{1}{2}} \delta_{\sigma_1,\mathcal{P}(\sigma_1)} \cdots \delta_{\sigma_N,\mathcal{P}(\sigma_N)}.$$

(4)

A set of coordinates $\mathbf{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is introduced with $\mathbf{r}_i$ being the position of the $i$-th particle with spin projection $\sigma_i$. $\mathcal{P}$ denotes a permutation (with parity $p$) of the particle labels. In order to numerically evaluate the partition function, the diagonal elements of the density matrix $e^{-\beta \mathcal{H}}$ are expanded in a path integral

$$\langle \mathbf{R} | e^{-\beta \mathcal{H}} | \mathcal{P} \mathbf{R} \rangle = \int d\mathbf{R}_1 \int d\mathbf{R}_2 \ldots \int d\mathbf{R}_{M-1} \times \langle \mathbf{R} | e^{-\beta \mathcal{H}} | \mathbf{R}_1 \rangle \ldots \langle \mathbf{R}_{M-1} | e^{-\beta \mathcal{H}} | \mathcal{P} \mathbf{R} \rangle,$$

(5)

where $M$ is referred to as the number of time slices. Using (5), the partition function can be evaluated by statistically sampling the discrete path $\{\mathbf{R}, \mathbf{R}_1, \ldots, \mathbf{R}_{M-1}, \mathcal{P} \mathbf{R}\}$ [8]. Thermodynamic observables are computed using the partition function, specifically the free energy

$$E = -\frac{\partial \ln Z}{\partial \beta}.$$  

(6)

In the following, the temperature is set to $k_B T = 0.1 \hbar \omega_0$ which is low enough to ensure that the partition function receives contributions mainly from the lowest energy state but remains still computationally feasible. The objective is to discriminate the lowest energy states by their
total spin which is preserved in the system. This can be achieved by diagonalizing the density matrix in the space of $S^2$ states by employing group theory which yields new coefficients $n(P)$ in equation 4 [9]. In the case of two electrons, for instance, the density matrix can be decomposed in two sectors corresponding to $S = 0$ and $S = 1$. By taking the partial trace relative to a basis with fixed total spin $S$, energies $E_S$ can be obtained. The total spin of the ground state can be accurately specified monitoring the sign of the energy difference $\Delta_{S,S'} = E_{S'} - E_S$. The ground state exhibits a transition of its total spin from $S$ to $S'$ if the sign of $\Delta_{S,S'}$ becomes negative.

3. Results

3.1. Circular quantum ring

The dominant interaction in a quantum ring strongly depends on the radius. The kinetic energy of a narrow circular ring scales roughly with the inverse square of the radius, whereas the interaction energy drops inversely with increasing ring radius. The continuous crossover from a weakly to a strongly interacting system is explored by calculating the energy differences $\Delta_{S,S'}$ as can be seen in figure 1 (a). The confinement energy $\hbar \omega_0 = 2.0E^*_H$ is kept fixed while tuning the ring radius. A spin transition of the ground state is seen in the case of three electrons populating the ring while for four electrons no transition occurs. Regarding small radii, the ground state is $S = \frac{1}{2}$ which can be understood considering the energy levels of the system. Supposing that the radial motion of the electrons is much slower than the circular motion ($\omega_0 r^2_0 > 1$), the energy levels are given by a rigid rotator with a two-fold degeneracy (left/right motion) and a non-degenerate ground state. The weakly interacting electrons occupy the lowest single-particle levels giving rise to the $S = \frac{1}{2}$ ground state. Increasing the ring radius leads to a spin transition to $S = \frac{3}{2}$. The gap between the single-particle energy states is reduced leading to a fully polarized system which minimizes the exchange energy. Finally, the energy difference between all spin-states vanishes for large radii while approaching a classical limit. Such spin transition, however, is absent in a four-electron system (cp. figure 1 (a)). The ground state is given by Hund’s rule with a total spin of $S = 1$ over the whole range of possible radii. The lowest single-particle levels are occupied by the electrons. In the degenerate level, however, the electrons maximize their spin reducing the exchange energy. Single-particle states with higher angular momentum are not occupied because their energy is too large. In the limit of large radii, again, all spin states coincide energetically, but without an alteration of the ground-state spin.

![Figure 1](image-url)

**Figure 1.** The energy difference $\Delta_{S,S'} = E_{S'} - E_S$ in a three and four electron ring depending on (a) the ring radius $r_0$ and (b) the elliptical deformation $\delta$. In the former case, only the three electron system exhibits a spin transition $S = \frac{1}{2} \rightarrow S = \frac{3}{2}$ while the four electron ring retains the $S = 1$ ground state. In the latter case, the quantum ring can be completely depolarized for large radii ($r_0 = 2.0$).
3.2. Distorted quantum ring

In this subsection we investigate quantum rings with elliptical shape which form due to crystal strain. In our model, the coordinates are subject to the transformation

\[ x^2 \rightarrow \frac{x^2}{\delta} \quad \text{and} \quad y^2 \rightarrow \delta \cdot y^2, \]

i.e. one semi-axis is stretched whereas the other semi-axis is shortened. Two situations can be observed in the three electron system (cp. figure 1 (b)). In the first case, the ring radius is chosen to be \( r_0 = 1.35a^* \) so that the ground-state spin is \( S = \frac{1}{2} \). The distortion of the ring even increases the energy splitting between the \( S = \frac{1}{2} \) ground state and the excited \( S = \frac{3}{2} \) state. Deformation of the ring reduces the symmetry of the system and thus removes the rotational degeneracy of the single-particle energies. As a consequence, the \( S = \frac{1}{2} \) state mainly occupies the two lowest single-particle states and reduces its energy. In contrast, in the \( S = \frac{3}{2} \) configuration a third single-particle energy level is populated. The three electrons, however, can be initially prepared in a spin-polarized state choosing a radius of \( r = 2.0a^* \). As in the previous case, the system can be forced to an unpolarized ground state as the ring gets distorted.

Regarding four electrons (figure 1 (b)), only the energy difference between \( S = 1 \) and \( S = 0 \) is given since the \( S = 2 \) energy increases monotonically during the distortion process. However, a spin transition of the ground state is taking place as the distortion proceeds. The Hund’s rule ground state of the circular ring is replaced by an \( S = 0 \) ground state. In this state the lowest two single-particle energies are occupied. The energy lowering of single-particle states is sufficient to overcome the exchange-energy savings associated with the Hund’s rule \( S = 1 \) state [10]. In both discussed cases (ring with three and four electrons) the deformation leads to a depolarized ground state. The described effects are related to the competing energy scales of the confinement and the Coulomb interaction. With an elliptical deformation an additional parameter emerges which tunes the gap between previously degenerate single-particle energy levels. Two regimes can be distinguished. In the first case, the system tries to reduce the Coulomb energy leading to a polarized spin configuration associated with exchange-energy saving. In the second case, the ground state of the system is determined by the large spacing between the single-particle energy levels. The system tends to occupy the lowest energy levels and thus minimizes the total spin. In this way the system can be tuned between a polarized and unpolarized ground state.

4. Discussion

In a quantum ring the spin of the ground state strongly depends on ring geometry. The quantum ring can be prepared in a polarized as well as a depolarized ground state for certain electron numbers. The findings are not only important for equilibrium properties but also for transport through rings. Especially, the occurring polarization of the ring can lead to negative differential conductances and even to the phenomenon of spin blockade in transport measurements [11].

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