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Quantum entanglement in elliptical quantum corrals

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ABSTRACT

Quantum corrals present interesting properties due to the combination of confinement and, in the case of elliptical corrals, to their focalizing properties. We study the case when two magnetic impurities are added to the non-interacting corral, where they interact via a superexchange AF interaction J with the surface electrons in the ellipse. Previous results showed that, when both impurities are located at the foci of the system, they experience an enhanced magnetic interaction, as compared to the one they would have in an open surface. For small J and even filling, they are locked in a singlet state, which weakens for larger values of this parameter. When J is much larger than the hopping parameter of the electrons in the ellipse, both spins decorrelate while forming a local singlet with the electrons of the ellipse, thus presenting a confined RKKY–Kondo transition.

We interpret this behaviour by means of the von Neumann entropy between the localized impurities and the itinerant electrons of the ellipse: for small J the entropy is nearly zero while for large J it is maximum. In addition, the local density of states provides us with a concrete experimental tool for detecting the Kondo regime.

1. Introduction

Modern laboratory techniques have allowed an important progress in the comprehension of quantum phenomena in solid state structures at the nanoscopic scale. This has been possible thanks to the design, modelling and fabrication of devices for quantum confinement and the control of atoms, photons and electrons. One of its consequences has been to motivate the development of novel applications in nanotechnology, particularly in quantum electronics.

At the same time, an innovative theory such as quantum information has evolved into a new paradigm in computation and communication that has overcome the limits of classical information [1]. While classical bits in binary logic take two possible values, zero and one, quantum computation is based on new quantum units of information or qubits, which represent a superposition of ones and zeros. Its multiple applications (computation, communication, cryptography or quantum teleportation, among others) require a controlled manipulation of light and matter at the quantum level.

In this sense nanostructured materials play an important role [2,3]. Among these we can mention the so-called quantum corrals, where the electrons remain quantically confined by means of a geometrical array of adatoms deposited on the surface of nobel metals, forming a nearly closed structure. These systems have allowed the observation of surprising effects such as quantum mirages [4,5], where the introduction of an impurity on one of the foci of an elliptical structure formed a ghost image in the empty one. These systems are excellent candidates for technological applications in quantum information and spintronics [6–8]. For example, by adding a magnetic atom on one focus the quantum mirage could be used as a geometric protection of magnetic qubits against decoherence. In addition, quantum entanglement can be robust if two magnetic impurities are added at the foci. Also feasible is the implementation of logical gates of one and two qubits. In this case, these corrals could serve as elementary prototypes of quantum computers.

In a recent work we have shown that, when a magnetic impurity is added to a focus, an image is formed at the other focus, which can be observed in the local density of states (DOS) when the Kondo effect is operative [9,10]. This implies that in any system with focalizing properties, two impurities which are located at relatively large distances could strongly interact. We have studied the problem with two impurities [11–13] where we have calculated the time response to localized stimulations and the degree of quantum entanglement for different partitions of the system.

In this work we present results for the quantum entanglement between two localized magnetic impurities which interact antiferromagnetically with the itinerant surface electrons of the

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ellipse. We find that, when this interaction is weak, the spins are strongly entangled in a singlet state while they are disentangled from the elliptical degrees of freedom. For large interactions, instead, the spins decorrelate while increasing their entanglement with the electrons. This state can be characterized by measuring the local density of states at the foci.

2. The model

In Fig. 1 we sketch the model used, which consists of a hard-wall ellipse with non-interacting electrons, which interact via an antiferromagnetic superexchange interaction with two localized spins with $S=1/2$ situated at the foci. We have taken the Fermi energy to coincide with the twenty-third one-body eigenstate for this eccentricity to resemble the experiments. However, other Fermi levels lead to similar results provided the weight of the wave function at the foci is appreciable.

The Hamiltonian of the model reads

$$H = H_{el} + J(\mathbf{S}_1.\boldsymbol{\sigma}_1 + \mathbf{S}_2.\boldsymbol{\sigma}_2), \tag{1}$$

where

$$\mathbf{S}_i \cdot \boldsymbol{\sigma}_i = \mathbf{S}_i^z \cdot \boldsymbol{\sigma}_i^z + \tfrac{1}{2}(\mathbf{S}_i^+ \boldsymbol{\sigma}_i^- + \mathbf{S}_i^- \cdot \boldsymbol{\sigma}_i^+), \tag{2}$$

$\sigma_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}$, $\sigma_i^z = (n_{i\uparrow} - n_{i\downarrow})/2$, with $n_{i\sigma}$ the number operator and $c_{i\sigma}$ the destruction operator of an electron with spin σ in focus i of the ellipse. In the basis of eigenstates $|\alpha\rangle$ of the ellipse, these local operators can be expanded as $c_{i\sigma} = \sum_\alpha \Psi_{\alpha i} c_{\alpha\sigma}$, where $c_{\alpha\sigma}$ and $\Psi_{\alpha i}$ are the destruction operator and amplitude in state $|\alpha\rangle$. H_{el} is the Hamiltonian of the isolated ellipse with infinite walls and hopping matrix element t^*.

In this basis the spin operators are expressed as

$$\sigma_i^z = \frac{1}{2}\sum_{\alpha_1\alpha_2} \Psi_{\alpha_1 i}^* \Psi_{\alpha_2 i}(c_{\alpha_1\uparrow}^\dagger c_{\alpha_2\uparrow} - c_{\alpha_1\downarrow}^\dagger c_{\alpha_2\downarrow}),$$
$$\sigma_i^+ = \sum_{\alpha_1\alpha_2} \Psi_{\alpha_1 i}^* \Psi_{\alpha_2 i} c_{\alpha_1\uparrow}^\dagger c_{\alpha_2\downarrow}. \tag{3}$$

In order to perform the many-body calculations, we have solved this Hamiltonian numerically with exact diagonalization for a small number of levels L and using the Lanczos technique for larger systems and different fillings corresponding to an even (closed shell) or odd (open shell) number of particles, N.

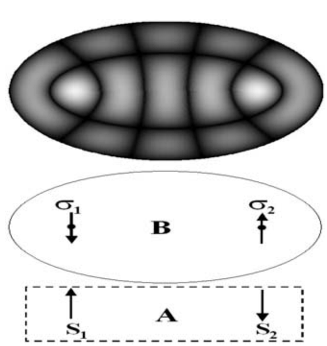

Fig. 1. (a) System under consideration: squared modulus of the eigenstate at the Fermi energy for the non-interacting ellipse with eccentricity $\varepsilon = 0.6$. White and black represent high and low electron densities, respectively. (b) Graphical representation: S_1 and S_2 are the impurity spins at the foci of the ellipse which interact with the localized spins σ_i via a superexchange interaction J. The lines indicate the partition considered for the calculation of the von Neumann entropy between subsystems A and B.

3. Quantum entanglement

A very important quantity in quantum information is the von Neumann or quantum entropy [1]. Given a quantum system A in a mixed state described by a density operator ρ_A, the quantum entropy is defined as

$$S = -\mathrm{Tr}(\rho_A \log_2 \rho_A). \tag{4}$$

This entropy is a measure of uncertainty in the mixed state. If we consider a system in a pure state $|\psi\rangle$ and divide it into two parts, A and B, the entanglement between A and B is defined as the entropy of either part as $E = -\mathrm{Tr}(\rho_A \log_2 \rho_A) = -\mathrm{Tr}(\rho_B \log_2 \rho_B)$ where the density matrices are defined as $\rho_{i'i}^A = \sum_j \psi_{ij}^* \psi_{i'j}$, and ψ_{ij} is the projection of the pure state $|\psi\rangle$ onto states i and j corresponding to parts A and B of the system, respectively, and similarly for $\rho_{j'j}^B$. When the density matrices are diagonalized obtaining the eigenvalues ω_i^A, the entropy has a simpler form

$$S = -\sum_i \omega_i^A \log_2 \omega_i^A = -\sum_i \omega_i^B \log_2 \omega_i^B. \tag{5}$$

The quantum entropy is positive and lower than the smallest of the dimensions of A and B. If $|\psi\rangle$ is formed as a direct product of states in A and B ($\omega_1^A = \omega_1^B = 1$) then $S = 0$ and there is no entanglement. On the contrary, when all states in A combine with all states in B (completely mixed density operator, $\omega_i = 1/d$, where d is the smallest dimension of the Hilbert spaces of A and B), then $S_{max} = \log_2(d)$.

We will study a particular partition which consists of considering the localized spins separated from the ellipse (Fig. 1b). This helps us understand the entanglement of the spins and the rest of the ellipse while varying the magnetic interaction.

For this partition we find that the entropy increases with J and has a slightly different behaviour for even and odd particles in the ellipse (Fig. 2). For the even case and small interaction, the entropy is negligible because the spins are locked into a singlet state [11] and the ground state consists of a direct product between this singlet and the ground state of the non-interacting ellipse. This state can be thought of as due to an effective RKKY interaction via the itinerant electrons, which is enhanced due to confinement. When J increases, again more states get involved, the localized spins are no longer in a singlet and the entropy or entanglement increases. In the largest entangled case we have in A a product of all four spin states ($|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$), which

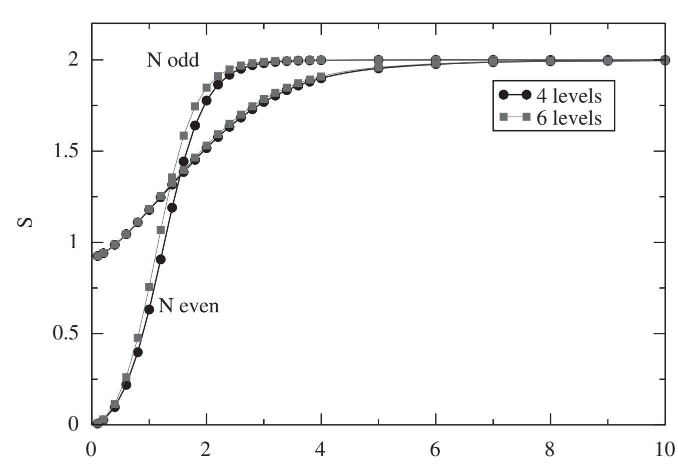

Fig. 2. Quantum entropy as a function of the magnetic interaction for even and odd fillings. The increase in the entanglement between the localized spins and the ellipse with J is clearly observable.

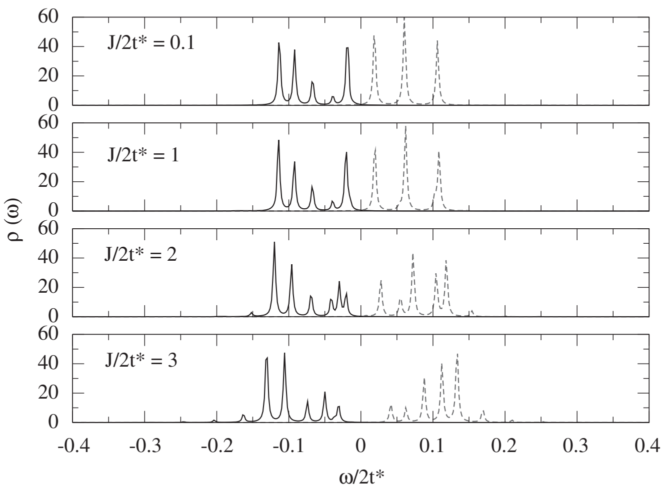

Fig. 3. Local density of states at one focus of the ellipse for occupied (full lines) and unoccupied (broken lines) levels. Here we have considered $L = 8$ energy levels, $N = 10$ electrons in the ellipse and different values of the interaction J.

appear with equal probability. The spins are completely decoupled and form local Kondo singlets with the electrons.

For the odd case and small J, the spins are in a mixture of mainly two triplet states because we are considering the $S_z = 1/2$ subspace. Again, for large J, the results match the even case and have maximum entropy ($S = \log_2 4 = 2$).

4. Local density of states

As a means to detect whether the system is in the local Kondo regime we can resort to the observation of the local densities of states defined as

$$\rho(\omega) = -\frac{1}{\pi}\lim_{\eta\to 0^+} \mathrm{Im}\, G(\omega + i\eta + E_0),$$
$$\rho^*(\omega) = -\frac{1}{\pi}\lim_{\eta\to 0^+} \mathrm{Im}\, G^*(-\omega + i\eta + E_0), \quad (6)$$

where

$$G(z) = \langle\psi_0|c^\dagger_{i\uparrow}(z-H)^{-1}c_{i\uparrow}|\psi_0\rangle,$$
$$G(z)^* = \langle\psi_0|c_{i\uparrow}(z-H)^{-1}c^\dagger_{i\uparrow}|\psi_0\rangle, \quad (7)$$

ω is the energy, $i = 1, 2$ are the foci of the ellipse, E_0 is the ground state energy. The quantities defined above correspond to the photoemission and inverse photoemission spectra, respectively.

We present our results in Fig. 3. Here we can distinguish two different regimes. For small J, the spectra consist mainly of the discrete levels of the isolated ellipse. However, when the antiferromagnetic superexchange interaction J increases ($J/2t^* > 1$), a pseudogap or a reduction of the local DOS starts developing, showing the transition to a different state. This reduction is a consequence of the Fano interference between the states of the ellipse and the localized spin when the many-body Kondo singlet is formed [14], thus signalling the mutual decoupling of the two impurities and the onset of the local Kondo state.

5. Conclusions

We have studied an elliptical confined system with focalizing properties in the presence of two localized impurities which interact antiferromagnetically (via J) with the itinerant electrons of the corral. We found a different behaviour for even and odd fillings in the ellipse which shows up in the character of the ground state and the excitations. For the even-particle case and small interaction J, both localized spins are entangled in a (quasi)-singlet state. When increasing the antiferromagnetic interaction J, an interesting feature arises which resembles the RKKY–Kondo-like transition occurring in the two-impurity system: while the localized spins form a singlet state between them for small interactions, this coupling decreases for larger J giving rise to an on-site singlet correlation between the spin and the itinerant electron. For odd number of electrons the effective interaction is ferromagnetic in the ground state. The character of this interaction can be controlled by changing the chemical potential of the system.

In this work we have also analysed the entanglement and von Neumann entropy for a particular partition of the system in the ground state, which offers us an alternative perspective on the problem. When the impurities are locked in a singlet state their entanglement with the ellipse is negligible, while it grows to its maximum value when they decouple from each other and form a local Kondo state with the electrons.

For small to moderate values of J ($J/2t^* \lesssim 1$) we expect the main results synthesized above to hold in the case of more realistic models of quantum ellipses which include tunnelling of the electrons in open corrals and inelastic processes with bulk electrons. In this parameter range the broadening of the relevant energy levels is smaller than their separation [10,5]. When larger interactions are included, higher levels which are more hybridized take part, and models including these processes should be considered.

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