Quantum Corrals, Eigenmodes and Quantum Mirages in s-wave Superconductors

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We study the electronic structure of magnetic and non-magnetic quantum corrals embedded in s-wave superconductors. We demonstrate that a quantum mirage of an impurity bound state peak can be projected from the occupied into the empty focus of a non-magnetic quantum corral via the excitation of the corral's eigenmodes. We observe an enhanced coupling between magnetic impurities inside the corral, which can be varied through oscillations in the corral's impurity potential. Finally, we discuss the form of eigenmodes in magnetic quantum corrals.

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The interaction of nanoscale impurity structures with fermionic quantum many-body systems has led to the observation of a large number of novel physical phenomena over the last few years. In superconducting (SC) systems, quantum interference of electronic waves that are scattered by a small number of impurities can lead to the splitting of impurity states, as observed in the one-dimensional chains of the high-temperature superconductor YBa$_2$Cu$_3$O$_{6+x}$ [1-4], and discussed theoretically for these chains as well as two-dimensional (2D) $d_{x^2-y^2}$-wave [5] and s-wave superconductors (SSC) [6,7].

In more complex impurity structures, such as quantum corrals, the existence of discrete eigenmodes can be employed for the creation of quantum mirages. This effect was beautifully demonstrated by Manoharan et al. [1] who used the Kondo-resonance of a magnetic impurity located in the focus of an elliptical quantum corral as the “electronic candle” whose quantum image was projected into the empty focus. A nice theoretical explanation of this phenomenon was subsequently provided in a series of articles [8].

Of particular interest is the possibility that nanoscale impurity structures can provide insight into the nature of complex electronic systems. In general, one expects that strong electronic correlations or changes in the electronic structure due to broken symmetries affect the spatial patterns of eigenmodes in quantum corrals and provide novel “electronic candles” whose spectroscopic signatures can be projected. As a first step in the investigation of this idea, we study in this Letter quantum corrals that are embedded in an s-wave superconductor with non-trivial correlations arising from particle-hole mixing. We consider a variety of quantum corrals consisting of non-magnetic or magnetic impurities with constant or oscillating scattering potentials. Magnetic impurities that are placed inside the corral induce bound states whose spectroscopic signatures are observed in the density-of-states (DOS). We utilize these peaks as the “electronic candle” to investigate the corral’s electronic properties. We demonstrate that by placing a magnetic impurity in one of the corral’s foci, a quantum image of its bound state peaks is projected into the empty focus via the excitation of the corral’s eigenmodes. These eigenmodes also lead to an enhanced coupling between magnetic impurities inside the corral.

We illustrate how the spatial pattern of eigenmodes can be changed through oscillations in the corral’s impurity potential or the relative alignment of impurity spins in magnetic corrals. These results provide a new tool for manipulating the interaction between magnetic impurities, a topic of great current interest in the field of spin electronics and quantum information technology.

To study the electronic structure of quantum corrals we employ a $T$-matrix formalism [6,9,10,11,12] which was generalized to describe electronic scattering off a large number of impurities. In a fully gapped SSC, magnetic impurities with spin $S$ can be treated as classical variables [11] since no Kondo-effect exists for sufficiently small coupling between the impurity and delocalized electrons [13]. In the Nambu formalism, the electronic Greens function in the presence of $N$ impurities located at $r_i$ is

$$\hat{G}(r, r', \omega_n) = \hat{G}_0(r, r', \omega_n)$$

$$+ \sum_{i,j=1}^N \hat{G}_0(r_i, r_j, \omega_n) \hat{T}(r_i, r_j, \omega_n) \hat{G}_0(r_j, r', \omega_n),$$

(1)

where one has for the $\hat{T}$-matrix

$$\hat{T}(r_i, r_j, \omega_n) = \hat{V}_i \delta_{i,j} + \hat{V}_i \sum_{l=1}^N \hat{G}_0(r_i, r_l, \omega_n) \hat{T}(r_l, r_j, \omega_n),$$

(2)

and

$$\hat{G}_0^{-1}(k, i\omega_n) = [i\omega_n \tau_0 - c_k \tau_3] \sigma_0 + \Delta_0 \tau_2 \sigma_2;$$

$$\hat{V}_i = \frac{1}{2} (U_i \sigma_0 + J_i S \sigma_3) \tau_3.$$  

(3)

$\hat{G}_0(k, i\omega_n)$ is the electronic Greens function of the unperturbed (clean) system in momentum space, $\sigma$, $\tau$ are the Pauli-matrices in spin and Nambu-space, respectively, and $\Delta_0$ is the SC gap. We assume that the corral is located at the surface of an SSC, and thus consider for simplicity a 2D electronic system. Its normal state dispersion

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is given by \( \epsilon_k = k^2/2m - \mu \) (\( \hbar = 1 \)), where \( \mu = k_F^2/2m \) is the chemical potential and \( k_F = \pi/2 \) is the Fermi wavevector (lattice constant \( a_0 = 1 \)). We set \( 1/(m\Delta_0) = 30 \), yielding a SC coherence length of \( \xi_c = k_F/(m\Delta_0) = 15\pi \). Moreover, \( \hat{V} \) is the scattering matrix at \( r_i \), with \( U_i \) and \( J_i \) being the potential and magnetic scattering strengths of the impurity. Unless otherwise noted, we take for definiteness \( U_i/2\Delta_0 = 30 \) (\( J_i = 0 \)) for non-magnetic impurities, and \( J_i S/2\Delta_0 = 30 \) (\( U_i = 0 \)) for magnetic impurities. These values are taken to demonstrate the qualitative features of our results which are robust against changes in the scattering strengths or in the form of the fermionic dispersion. The DOS, \( N(r, \omega) \), is obtained from a numerical computation of Eqs. (1) and (2) with \( N(r, \omega) = A_{11} + A_{22}, A_{ii}(r, \omega) = -\text{Im} \, G_{ii}(r, \omega + i\delta)/\pi \), and \( \delta = 0.02\Delta_0 \).

We first study an elliptical corral with semi-axes \( a = 20, b = 15 \), and eccentricity \( e = \sqrt{7}/4 \), that consists of 100 non-magnetic impurities. Defining the center of the corral as \((0, 0)\), we place a magnetic impurity in the corral’s focus at \( f_+ = (13, 0) \), while leaving the other focus at \( f_- = (-13, 0) \) empty. In Fig. 1a, we present the DOS in the focii at \( f_+ \). As expected, the magnetic impurity induces a bound state resulting in a particle- and hole-like peak in the DOS at frequencies \( \Omega_b^{(1,2)}/\Delta_0 = \mp 0.4 \), respectively. A quantum mirage of these peaks emerges in the empty focus at \( f_- \). The formation of this quantum image through excitations of the corral’s eigenmodes becomes evident when we consider the spatial DOS pattern at \( \Omega_b^{(2)} \) as shown in Fig. 1b. All plots of the spatial DOS shown in the following possess the same intensity scale to facilitate a direct comparison, with light (dark) color indicating a large (small) DOS. In addition to the quantum mirage, we observe DOS oscillations, representing the excited eigenmodes of the corral. By increasing the corral’s impurity potential \[15\], the eigenmodes as well as the impurity bound state become more confined inside the corral. The presence of two bound state peaks at \( \Omega_b^{(1,2)} \) that arise from particle-hole mixing in the SC state allows us to study eigenmodes at different excitation energies. Note, e.g., that the spectral weight in the DOS at \( \Omega_b^{(1)} \) (Fig. 1c) is much more concentrated around \( f_+ \) than at \( \Omega_b^{(2)} \) (Fig. 1d) concomitant with a weaker excited eigenmode and quantum mirage. It was noted earlier \[2\], that eigenmodes can be only excited if the excitation (via the impurity bound state) takes place at a position where the spectral weight of the eigenmode is large, and if the excitation energy, i.e., \( \Omega_b^{(1,2)} \), is close to the eigenmode’s energy. For \( U_i = \infty \), no eigenmodes exist inside the SC gap, and the eigenmodes closest to the Fermi energy and large spectral weight close to the focii are located at \( \Omega_{m^{(\pm)}}^{(1)}/\Delta_0 = \pm 1.1 \). Since the mode’s amplitude at \( \Omega_m^{(\pm)} \) is considerably larger than that at \( \Omega_{m^{(-)}}^{(1)} \), the DOS oscillations and thus the quantum mirage at \( \Omega_b^{(1)} \) are weaker, leading to a concentration of spectral weight around \( f_+ \). This demonstrates that the eigenmodes act as “waveguides” for the projection of the bound state peaks into a quantum image \[15\].

The effect of a corral on the DOS strongly depends on the ratio of the decay length, \( \xi_d = \xi_c/\sqrt{1 - (\Omega_b/\Delta_0)^2} \), and the corral’s semi-axes. In the above case, \( \Omega_b^{(1,2)}/\Delta_0 = \pm 0.4 \), \( \xi_d = 16.4\pi \gg a, b \) and the spatial DOS pattern at \( \Omega_b^{(2)} \) is significantly different for a magnetic impurity at \( f_+ \) with (Fig. 1c) and without a corral (Fig. 1d). Note that the presence of a corral also shifts \( \Omega_b^{(1,2)} \) from \( \Omega_b^{(1,2)}/\Delta_0 = \pm 0.575 \) (no corral) to \( \Omega_b^{(1,2)}/\Delta_0 = \pm 0.4 \). In contrast, if \( \xi_d \ll a, b \) the bound state wave-function at
the position of the corral wall is exponentially suppressed, no eigenmodes can be excited, and the spatial DOS pattern of a single magnetic impurity remains unchanged in the presence of a quantum corral [15]. Note, however, that $\xi_d$ can become arbitrarily large by increasing $J_S$ such that $|\Omega_b^{(1,2)}|/\Delta_0 \to 1$.

We next study the evolution of the DOS pattern when the magnetic impurity is moved off the focus for a corral with 88 impurities, $a = 20$, $b = 10$, eccentricity $e = \sqrt{3}/2$ and $f_{\pm} = (\pm 17, 0)$. In Fig. 2a we present the DOS at $\Omega_b^{(2)} = 0.475$ for a magnetic impurity located at $f_+$. The DOS exhibits a similar pattern, including a quantum mirage at $f_-$, as in Fig. 1b, albeit with only one instead of three “side wings” in the excited eigenmode. When we move the impurity off the focus to $(13, 0)$ (Fig. 2b), the bound state energy increases to $\Omega_b^{(1,2)}/\Delta_0 = \mp 0.5$, and only a much weaker quantum mirage emerges at $f_-$. The DOS pattern changes significantly when the magnetic impurity is located at the center of the corral at $(0, 0)$ (Fig. 2c) with $\Omega_b^{(1,2)}/\Delta_0 = \mp 0.725$. Thus, changing the location of the excitation, i.e., the magnetic impurity, leads to different excited eigenmodes and a simultaneous shift in $\Omega_b^{(1,2)}$. In Fig. 2d we plot the DOS in the presence of an oscillating impurity potential along the corral’s wall with $U(\phi) = U_0 \cos \phi$, $U_0/2\Delta_0 = 30$, and $\phi$ being the angle between the x-axis and the line connecting the center of the ellipse with the impurity. This oscillating potential, which might arise, e.g., from charge oscillations in the corral’s wall, weakens the eigenmodes, particularly along the vertical axis of the corral where $U(\phi)$ is small, and almost completely destroys the quantum mirage of the bound state peak.

It was argued in Ref. [7, 8] that quantum interference effects between two magnetic impurities leads to the formation of bonding and antibonding bound states and thus to a frequency splitting of the bound state peaks. We find that this splitting can be enhanced if the magnetic impurities are placed in the foci of a corral. We consider the same corral as in Fig. 1 and assume for definiteness that the spins of the impurities are parallel, however, qualitatively similar results are obtained for arbitrary angle between the impurity spins. As shown in Fig. 3, in the absence of a quantum corral, the energy splitting of the bound state peaks is small, $\delta \Omega_b/\Delta_0 = 0.1$, due to the large distance between the impurities. However, in the presence of the corral the splitting increases...
Finally, we present in Fig. 4 the DOS inside a quantum corral. Spatial DOS pattern for (b) $\Omega_b^{(1)}/\Delta_0 = -0.1$ and (c) $\Omega_b^{(2)}/\Delta_0 = 0.575$ (see (a)).

to $\delta \Omega_b^0/\Delta_0 = 0.65$, implying that the coupling between the two magnetic impurities is enhanced (in the normal state, this effect was discussed in Ref. [12]). Note that for an oscillating impurity potential, as that discussed in Fig. 2d, the splitting decreases to $\delta \Omega_b^0/\Delta_0 = 0.175$.

Finally, we present in Fig. 4 the DOS inside a quantum corral ($a = 20, b = 10$) consisting of 88 magnetic impurities. The corral’s impurity spins are antiferromagnetically aligned and an additional magnetic impurity is located at $f_+ = (17, 0)$. Since the bound states associated with the magnetic impurities are coupled, the DOS exhibits a large number of peaks (Fig. 4a), and we do not observe a well defined quantum image in the empty focus. The DOS pattern changes qualitatively between different bound state energies, as shown in Fig. 4b and c where we present the DOS at $\Omega_b^{(1)}/\Delta_0 = -0.1$ and $\Omega_b^{(2)}/\Delta_0 = 0.575$ (see Fig. 4a). For $\Omega_b^{(1)}$ the spectral weight of the excited eigenmode is predominantly centered around the empty focus, while for $\Omega_b^{(2)}$ most of the spectral weight is located in the vicinity of the occupied focus. Thus, in contrast to non-magnetic corrals, the eigenmodes in a magnetic corral can be concentrated near the occupied or empty focus. For ferromagnetic alignment of the corral spins (not shown) there also exists a large number of bound state peaks in the DOS [13]. However, the spatial distribution of spectral weight associated with these peaks is much more homogeneous, likely due to the stronger scattering for ferromagnetically aligned spins [14] and the resulting larger number of excited eigenmodes.

Finally, we comment on the relevance of pair-breaking effects near magnetic impurities. Since the suppression of the SC gap close to a single magnetic impurities does not alter the DOS’s qualitative features [12], our results presented in Figs. 14 are likely robust against pair-breaking effects. In magnetic corrals, on the other hand, the suppression of the SC gap is potentially relevant and its magnitude could depend on the ferro- or antiferromagnetic alignment of the corral’s spins. Work is currently under way to study the significance of pair-breaking effects and gap suppression in both cases [15].

In summary, we demonstrate that a quantum mirage of an impurity bound state peak can be projected from the occupied into the empty focus of a non-magnetic quantum corral via the excitation of the corral’s eigenmodes. We observe an enhanced coupling between magnetic impurities inside the corral, which can be varied through oscillations in the corral’s impurity potential. This provides a novel tool to manipulate the interaction between magnetic impurities, a topic of great relevance in spin electronics and quantum information technology [10].

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