Spatially dependent Kondo effect in Quantum Corrals

Enrico Rossi and Dirk K. Morr

Department of Physics, University of Illinois at Chicago, Chicago IL 60607
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We study the Kondo screening of a single magnetic impurity inside a non-magnetic quantum corral located on the surface of a metallic host system. We show that the spatial structure of the corral’s eigenmodes lead to a spatially dependent Kondo effect whose signatures are spatial variations of the Kondo temperature, $T_K$. Moreover, we predict that the Kondo screening is accompanied by the formation of multiple Kondo resonances with characteristic spatial patterns. Our results open new possibilities to manipulate and explore the Kondo effect by using quantum corrals.

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The Kondo effect exhibited by a magnetic impurity is one of the most fundamental and important phenomena in condensed matter physics [1, 2, 6]. Over the last few years, the emergence of a Kondo effect in confined host geometries with discrete energy levels, such as quantum dots [4], nanotubes [3] and molecules [8] has attracted significant experimental [1, 7] and theoretical [5, 6] interest. Discrete eigenmodes have also been observed in quantum corrals located on metallic surfaces [8]. Recently, Manoharan et al. using scanning tunneling microscopy (STM) showed that the spatial structure of these eigenmodes can be employed to create the quantum image of a Kondo resonance [10]. While a series of theoretical studies successfully explained the formation of this quantum image [11], the question whether the eigenmodes’ spatial structure leads to a spatially dependent Kondo effect for different positions of a magnetic impurity inside the quantum corral, has not yet been addressed.

In this Letter, we answer this question by studying the Kondo screening of a single magnetic impurity inside a non-magnetic quantum corral located on the surface of a metallic host. Combining a large-$N$ expansion [3, 12, 13] with a generalized $T$-matrix approach [14] we show that the spatial structure of the corral’s eigenmodes leads to a spatially dependent Kondo effect whose signatures are spatial variations of the Kondo temperature, $T_K$, and of the critical coupling, $J_{cr}$. Specifically, $T_K$, is the largest and $J_{cr}$ the smallest, at those locations where the density of states (DOS) of the lowest energy eigenmode possesses a maximum. Moreover, we find that the screening of the magnetic impurity leads to the formation of multiple Kondo resonances with characteristic spatial patterns that provide clear experimental signatures of the spatially dependent Kondo effect. Our results demonstrate that quantum corrals provide a new possibility to manipulate and explore the nature of the Kondo effect.

While the large-$N$ approach [3, 12, 13] provides a qualitatively correct description of all salient features of the Kondo effect [2], its interpretation requires some care. In particular, in the large-$N$ approach, the onset of Kondo screening occurs via a sharp transition, such that for a given $J (T)$, a Kondo effect occurs for $T < T_K (J > J_{cr})$. This sharp transition is an artifact of the large-$N$ approach [3, 12, 13], and hence $T_K$ and $J_{cr}$ should rather be interpreted as crossover values. However, this interpretation does not change the main result of our study, viz. $T_K$ and $J_{cr}$ exhibit a pronounced spatial dependence with clear experimental signatures.

We consider a system consisting of a quantum corral with $M$ non-magnetic impurities located on the surface of a metallic host, and a single magnetic impurity inside the corral. This system is described by the Hamiltonian

$$H = -\sum_{i,j,\sigma} t_{ij} \epsilon_{i,\sigma} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_{i,\sigma} \epsilon_{i,\sigma} c_{i,\sigma}^{\dagger} c_{i,\sigma}$$

$$+ J S \cdot \sigma c_{R,\sigma}^{\dagger} c_{R,\sigma},$$

where $\epsilon_{i,\sigma}$ are the fermionic creation and annihilation operators for a (host) conduction electron at site $i$ with spin $\sigma$, and $t_{ij}$ is the hopping element between sites $i$ and $j$. In the following, we consider a two-dimensional (2D) host metal on a square lattice with dispersion $\epsilon_k = k^2/2m - \mu$ where $\mu$ is the chemical potential. We set the lattice constant $a_0$ to unity and use $E_0 \equiv h^2/ma_0^2$ as our unit of energy. The primed sum runs over all positions $r_{i}$ ($i = 1, \ldots, M$) of the $M$ corral impurities with identical non-magnetic scattering potential $U$. The last term in Eq. (1) describes the Kondo interaction between the conduction electrons and the magnetic impurity, located at site $R$ with magnetic moment $S$ and scattering strength $J$. Below, we consider for concreteness a magnetic impurity with spin $S = 1/2$.

In the large-$N$ approach [3, 12, 13], the spin $S$ of the magnetic impurity is expressed in terms of fermionic operators, $f_{m}^{\dagger}, f_{m}$, that obey the constraint $\sum_{m=1..N} f_{m}^{\dagger} f_{m} = 1$ with $N = 2$ being the number of fermionic flavors for a magnetic impurity with spin $S = 1/2$. Within a path integral approach, the constraint is enforced by means of a Lagrange multiplier $\epsilon_f$ and the exchange interaction in Eq. (1) is decoupled via a Hubbard-Stratonovich field, $s$. $\epsilon_f$ is interpreted as the energy of the $f$ electrons, and $s^2$ represents their hybridization with the conduction electrons. By minimizing...
the effective action on the saddle point level, one obtains the self-consistent equations \[ \tag{2a} \]

\[
T \sum_n \frac{1}{i\omega_n - \epsilon_f - s^2 G_c(R, R, i\omega_n)} = \frac{1}{N} \quad \tag{2b}
\]

\[ G_c, \text{ the conduction electrons' Green's function in the presence of the corral only, is given by} \]

\[
G_c(r, r', i\omega_n) = G_0(r - r', i\omega_n) + \sum_{j,l} G_0(r - r_j, i\omega_n) \times T_{jl}(i\omega_n) G_0(r_l - r', i\omega_n) \quad \tag{3}
\]

where \( G_0 = 1/(i\omega_n - \epsilon_f) \) is the Green's function of the unperturbed host system in momentum space. The \( T \)-matrix is obtained from the Bethe-Salpeter equation

\[ T_{ij}(i\omega_n) = U \delta_{ij} + U \sum_l G_0(r_l - r_i, i\omega_n) T_{il}(i\omega_n). \quad \tag{4} \]

In the presence of the magnetic impurity, the total Green's function of the conduction electrons is given by

\[
G_{c, \text{tot}}(r, r', i\omega_n) = G_c(r, r', i\omega_n) + s^2 G_c(r, R, i\omega_n) F(i\omega_n) G_c(R, r', i\omega_n), \quad \tag{5}
\]

where \( F = [(i\omega_n - \epsilon_f - s^2 G_c(R, R, i\omega_n))^{-1} \) is the Green's function of the \( f \) electrons. In the presence (absence) of the magnetic impurity, the host system's DOS, \( N_{c, \text{tot}}(\epsilon_f) \), is obtained from Eq.3 (Eq.4) via \( N_{c, \text{tot}}(\epsilon_f)(r, \omega) = -2 \text{Im}[G_{c, \text{tot}}(r, r, \omega + i\delta)]/\pi \) with \( \delta = 0.0025 E_0 \).

In what follows, we consider a circular quantum corral of radius \( r = 10a_0 \) consisting of \( M = 81 \) non-magnetic impurities with \( U = 2.5 E_0 \) [see Fig. 1(b)]. In the absence of the magnetic impurity, the DOS, \( N_c \), exhibits well separated eigenmodes [Fig. 1(a)] that possess distinct spatial patterns, as shown in Figs. 1(b) and (c) for the eigenmodes denoted by (1) and (2) in Fig. 1(a). We expect that the spatial structure of the Kondo effect is determined by that of the lowest energy eigenmode as long as the Kondo temperature, \( T_K \), is smaller than the energy splitting between modes. To test this conjecture, we set \( \mu = 0.077 E_0 \), such that the mode shown in Fig. 1(b) is located at the Fermi energy.

In Fig. 1 we present \( J_{cr} \) as a function of temperature for two positions \( R_{1,2} \) of the magnetic impurity, corresponding to the minimum \( |R_1| = (0, 0) \) and maximum \( |R_2| = (5, 0) \) in the DOS of the zero-energy mode. In the limit \( T \rightarrow 0 \), the behavior of \( J_{cr} \) at \( R_{1,2} \) is qualitatively different: while \( J_{cr} \sim T \) at \( R_2, J_{cr} \) saturates to a finite value at \( R_1 \). This result can be understood by considering a model in which the fermionic excitation spectrum inside the corral consists of discrete eigenmodes, described by the Green’s function \( G_c(r, i\omega_n) = \sum_l \phi_l(r)/(i\omega_n - \Omega_l) \), where \( \Omega_l \) and \( \phi_l(r) \) are the energy and the spectral weight of the \( l \)th mode at position \( r \), respectively. With this form of \( G_c, \) Eq.2b yields

\[
\frac{1}{J_{cr}} = -\sum_l \frac{\phi_l(R)}{\Omega_l} \left[ n_F \left( \frac{\Omega_l}{T} \right) - \frac{1}{2} \right]. \quad \tag{6}
\]
Taking one mode to be located at zero energy, $\Omega_0 = 0$, while for all other modes $|\Omega| \gg T$, one finds in the low-temperature limit $\varphi_p(R)/4T \approx \sum_{\ell \neq p} \varphi_\ell(R)/2|\Omega|$, that $J_{cr} \approx 4T/\varphi_p(R)$. This low-temperature behavior is observed at $R_2$ since $\varphi_p(R_2) \neq 0$ for the zero-energy mode shown in Fig. 1(b). In contrast, one has $\varphi_p(R_1) = 0$, implying that for $T \to 0$, $J_{cr}(R_1)$ saturates to a non-zero value given by $J_{cr} \approx 1/\sum_{\ell \neq p} \varphi_\ell(R_1)/2|\Omega|$. In Fig. 2 we also plot the temperature dependence of $J_{cr}$ for a system without quantum corral, $J_{cr}^0$, which is qualitatively similar to that of $J_{cr}(R_2)$ due to the non-zero DOS of the unperturbed, metallic host at $\omega = 0$. Since $J_{cr}^0$ lies between $J_{cr}(R_1)$ and $J_{cr}(R_2)$, a quantum corral can either facilitate (at $R_2$) or suppress (at $R_1$) the screening of a magnetic impurity. Finally, the difference in $J_{cr}$ between $R_1$ and $R_2$ is quite substantial already for rather weak scattering potential $U$, as follows from Fig. 2 where the filled [open] square and circle represent $J_{cr}$ at $R_1$ [$R_2$] for a corral with $U = 0.2E_0$ and 0.5$E_0$, respectively. This demonstrates the robustness of the spatially dependent Kondo effect even for small $U$.

In Fig. 2(a) we present $J_{cr}$ along $R = (x, 0)$ inside the corral for $T = 0.005E_0$. A comparison with the DOS of the zero-energy mode in Fig. 3(b) along the same path shows that $J_{cr}(R)$ exhibits as expected a minimum at $R = (5, 0)$ where the DOS possesses a maximum. Complementary to this result, we plot in Fig. 3(c) the spatial dependence of $T_K$, which exhibits the same spatial dependence as (a) the DOS in Fig. 3(b), and (b) the hybridization, $s^2$ for $T \to 0$ (not shown). Hence, a magnetic impurity with a given $J$ exhibits characteristic signatures of Kondo screening (see below), only for those locations inside the corral, for which $T < T_K(R)$. This result remains qualitatively unaffected by the interpretation of $T_K$ as a crossover. A comparison of $T_K(R)$ with the spatially uniform $T_K$ in the absence of a corral [dotted line in Fig. 3(c)] for $J = 1.3E_0$ shows that $T_K(R)$ is increased inside the corral for $3 \leq x \leq 7$, and suppressed otherwise. This opens the possibility to custom-design $T_K$ for a magnetic impurity inside a quantum corral.

In Figs. 4(a) and (b), we present $N_c^{tot}$ and the $f$ electrons’ DOS, $N_f = -NIm[F(R, \omega)]/\pi$, respectively, as a function of energy at $T = 0.005E_0$ for an impurity with $J = 1.45E_0$ and $R = (5, 0)$, yielding $T_K = 0.0145E_0$. We find that Kondo screening is accompanied by multiple Kondo resonances, a phenomenon characteristic of the discrete excitation spectrum in a host system. A comparison of Figs. 4(a) and (b) shows that away from the Fermi energy, each corral eigenmode induces a single Kondo resonance, leading to a small shift of the eigenmode energy from its unperturbed value. In contrast, level repulsion between the unperturbed $f$-level and the corral’s zero-energy eigenmode leads to two Kondo resonances almost symmetrically located around $\omega = 0$. This splitting of the corral’s eigenmode into two Kondo resonances is one of the most prominent signatures of Kondo screening in the DOS. Note that due to the frequency dependence of $N_c$, the width of the low-energy Kondo resonances is not set by $T_K$.

The spatial form of $N_c^{tot}$ at several frequencies is shown in Fig. 5. A comparison of Figs. 5(b) and 5(a) shows that Kondo screening of the impurity strongly suppresses the DOS of the zero-energy eigenmode at the impurity position, $R$, and its mirror site $-R$. The same result holds for eigenmodes away from zero energy [see, e.g. Figs. 5(c) and 5(b)]. In contrast, the DOS of the Kondo resonance at $\omega = -0.019E_0$ possesses a peak around $R$, with a weaker image at the mirror site, $-R$, while the resonance at $\omega = 0.018E_0$ only exhibits a peak in the DOS at the mirror site, but not at $R$. We find that similarly strong signatures of Kondo screening in the DOS exist for all locations of the magnetic impurity with $T < T_K(R)$.

Finally, results similar to the ones discussed above are
FIG. 4: (Color online) (a) $N_{t o t}^c$ and (b) $N_f$ as a function of frequency for $R = (5, 0), J = 1.45E_0, T = 0.005E_0, \epsilon_f = 0.02E_0$ and $s^2 = 0.03E_0^2$.

FIG. 5: (Color online) Spatial form of $N_{t o t}^c$ at (a) $\omega = 0$ and at three of the Kondo resonances shown in Fig. 4: (b) $\omega = 0.0625E_0$, (c) $\omega = -0.019E_0$, (d) $\omega = 0.018E_0$.

also found in other corral geometries and for different spatial structures of the low-energy eigenmodes. Moreover, we expect that the spatially dependent Kondo effect is robust against the inclusion of an electron-electron interaction in the host system as long as the relevant eigenmodes are located near the Fermi energy.

In summary, we studied the Kondo screening of a magnetic impurity inside a non-magnetic quantum corral. We showed that the spatial structure of the corral’s low-energy eigenmode leads to spatial variations in the Kondo temperature and the critical coupling. The spectroscopic signature of the Kondo effect are multiple Kondo resonances in the DOS with distinct spatial patterns. Our results show that quantum corrals provide a new possibility to explore and manipulate the Kondo effect.

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