Spatially Dependent Kondo Effect in Quantum Corrals

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We study the Kondo screening of a single magnetic impurity inside a nonmagnetic quantum corral located on the surface of a metallic host system. 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. 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 [1–3]. Over the past few years, the emergence of a Kondo effect in confined host geometries with discrete energy levels, such as quantum dots [4], nanotubes [5], and molecules [6], has attracted significant experimental [4–6] and theoretical [7–9] interest. Discrete eigenmodes have also been observed in quantum corrals located on metallic surfaces [10]. Recently, Manoharan *et al.* using scanning tunneling microscopy showed that the spatial structure of these eigenmodes can be employed to create the quantum image of a Kondo resonance [11]. This imaging effect was successfully explained in a series of theoretical studies [12]. However, none of these studies addressed the question of whether the eigenmodes' spatial structure leads to a spatially dependent Kondo effect in which, for example, the Kondo temperature varies with the position of a magnetic impurity inside the quantum corral.

In this Letter, we answer this question by studying the Kondo screening of a single magnetic impurity inside a nonmagnetic quantum corral located on the surface of a two-dimensional metallic host system. Combining a large-N expansion [3,13,14] with a generalized $\hat{T}$-matrix approach [15], 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 $J_{\rm cr}$. Specifically, T_K is the largest and $J_{\rm cr}$ the smallest at those locations where the local density of states (LDOS) of the lowest energy eigenmode possesses a maximum. Moreover, the screening of the magnetic impurity leads to the formation of multiple Kondo resonances with characteristic spatial patterns that provide experimental signatures of the spatially dependent Kondo effect. Our results demonstrate that quantum corrals provide new possibilities to manipulate and explore the Kondo effect.

While the large-N approach [3,13,14] provides a qualitatively correct description of all salient features of the Kondo effect, it is a well-known artifact of this approach [2] that the onset of Kondo screening occurs via a sharp transition, such that for a given J (T), a Kondo effect occurs for $T < T_K$ ($J > J_{\rm cr}$). Hence, T_K and $J_{\rm cr}$ should be interpreted as crossover values. This, however, does not affect the main result of our study, viz., T_K and $J_{\rm cr}$ exhibit a pronounced spatial dependence inside a corral.

We consider a system consisting of a quantum corral with M nonmagnetic impurities located on the surface of a metallic 2D host and a single magnetic impurity inside the corral. This system is described by the Hamiltonian

$$H = -\sum_{\mathbf{i},\mathbf{j},\sigma} t_{\mathbf{ij}} c^\dagger_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + U{\sum_{i,\sigma}}' c^\dagger_{\mathbf{r}_i,\sigma} c_{\mathbf{r}_i,\sigma} + J\mathbf{S}\cdot c^\dagger_{\mathbf{R}\sigma}\tau_{\sigma\sigma'} c_{\mathbf{R}\sigma'}, \tag{1}$$

where $c^\dagger_{\mathbf{i},\sigma} c_{\mathbf{i},\sigma}$ are the fermionic creation and annihilation operators for a conduction electron at site $\mathbf{i}$ with spin σ, and $t_{\mathbf{ij}}$ is the hopping element between sites $\mathbf{i}$ and $\mathbf{j}$. We consider a 2D host metal on a square lattice with lattice constant $a_0 \equiv 1$ and dispersion $\epsilon_{\mathbf{k}} = k^2/2m - \mu$, where μ is the chemical potential. We use $E_0 \equiv \hbar^2/ma_0^2$ as our unit of energy. The primed sum runs over all positions $\mathbf{r}_i$ of the M corral impurities with identical nonmagnetic scattering potential U. The last term in Eq. (1) describes the Kondo interaction between the conduction electrons and the magnetic impurity, located at site $\mathbf{R}$ with spin $S = 1/2$ and scattering strength J.

In the large-N approach [3,13,14], the spin $\mathbf{S}$ of the magnetic impurity is expressed in terms of fermionic operators $f^\dagger_m$, f_m that obey the constraint $\sum_{m=1\ldots N} f^\dagger_m f_m = 1$, with $N = 2$ for a magnetic impurity with $S = 1/2$. Within a path integral approach, the constraint is enforced by means of a Lagrange multiplier ϵ_f, and the exchange interaction in Eq. (1) is decoupled via a Hubbard-Stratonovich field s. ϵ_f is interpreted as the energy of the f electrons, and s represents their hybridization with the conduction electrons. By minimizing the effective action on the saddle point level, one obtains the self-consistent equations [16]

$$T\sum_n \frac{1}{i\omega_n - \epsilon_f - s^2 G_c(\mathbf{R}, \mathbf{R}, i\omega_n)} + \frac{1}{2} = \frac{1}{N}, \quad (2a)$$

$$T\sum_n \frac{G_c(\mathbf{R}, \mathbf{R}, i\omega_n)}{i\omega_n - \epsilon_f - s^2 G_c(\mathbf{R}, \mathbf{R}, i\omega_n)} = \frac{1}{J}. \quad (2b)$$

G_c, the conduction electrons' Green's function in the presence of the corral only, is given by [15]

$$G_c(\mathbf{r}, \mathbf{r}', i\omega_n) = G_0(\mathbf{r} - \mathbf{r}', i\omega_n) + \sum_{j,l}{}' G_0(\mathbf{r} - \mathbf{r}_j, i\omega_n) \times T_{jl}(i\omega_n) G_0(\mathbf{r}_l - \mathbf{r}', i\omega_n), \quad (3)$$

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

$$T_{ij}(i\omega_n) = U\delta_{ij} + U\sum_l{}' G_0(\mathbf{r}_i - \mathbf{r}_l, i\omega_n) T_{lj}(i\omega_n). \quad (4)$$

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

$$G_c^{\text{tot}}(\mathbf{r}, \mathbf{r}', i\omega_n) = G_c(\mathbf{r}, \mathbf{r}', i\omega_n) + s^2 G_c(\mathbf{r}, \mathbf{R}, i\omega_n) F(i\omega_n) G_c(\mathbf{R}, \mathbf{r}', i\omega_n), \quad (5)$$

where $F = [i\omega_n - \epsilon_f - s^2 G_c(\mathbf{R}, \mathbf{R}, i\omega_n)]^{-1}$ is the Green's function of the f electrons. In the presence (absence) of the magnetic impurity, the host system's LDOS N_c^{tot} (N_c) is obtained from Eq. (5) [Eq. (3)] via $N_c^{(\text{tot})}(\mathbf{r}, \omega) = -2\text{Im}[G_c^{(\text{tot})}(\mathbf{r}, \mathbf{r}, \omega + i\delta)]/\pi$, with $\delta = 0.0025E_0$. Our results are expected to remain unchanged by electron-electron interactions in the host material as long as the relevant eigenmodes are located near the Fermi energy.

We consider a circular quantum corral of radius $r = 10$ consisting of $M = 80$ nonmagnetic impurities with $U = 2.5E_0$ [Fig. 1(b)]. In the absence of the magnetic impurity, the LDOS N_c exhibits well separated eigenmodes [Fig. 1(a)] that possess distinct spatial patterns, as shown in Figs. 1(b) and 1(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 $\mu = 0.077E_0$, such that the mode shown in Fig. 1(b) is located at the Fermi energy.

In Fig. 2, we present J_{cr} as a function of temperature for two positions $\mathbf{R}_{1,2}$ of the magnetic impurity, corresponding to the minimum [$\mathbf{R}_1 = (0, 0)$] and maximum [$\mathbf{R}_2 = (5, 0)$] in the LDOS of the zero-energy mode. For $T \to 0$, the behavior of J_{cr} at $\mathbf{R}_{1,2}$ is qualitatively different: While $J_{\text{cr}} \sim T$ at $\mathbf{R}_2$, J_{cr} saturates to a finite value at $\mathbf{R}_1$. This result can be understood by considering a model in which the eigenmodes are discrete and described by $G_c(\mathbf{r}, i\omega_n) = \sum_l \varphi_l(\mathbf{r})/(i\omega_n - \Omega_l)$. Ω_l and $\varphi_l(\mathbf{r})$ are the energy and the spectral weight of the l'th mode at position $\mathbf{r}$, respectively.

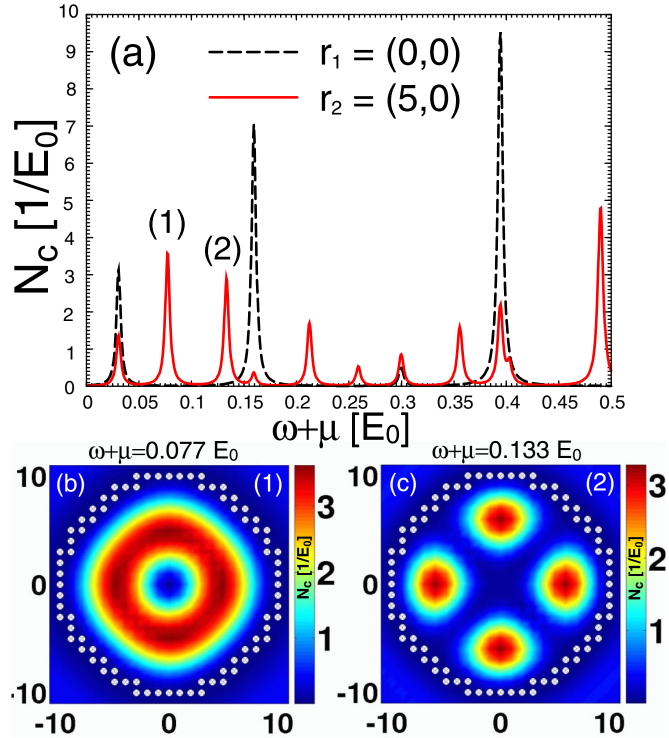

FIG. 1 (color online). (a) LDOS N_c as a function of $\omega + \mu$ at $\mathbf{r}_1 = (0, 0)$ and $\mathbf{r}_2 = (5, 0)$. (b),(c) Spatial plot of N_c at $\omega + \mu = 0.077E_0$ and $0.133E_0$, corresponding to modes (1) and (2) in (a), respectively. The solid white circles represent the nonmagnetic impurities forming the quantum corral.

Equation (2b) then yields [17]

$$\frac{1}{J_{\text{cr}}} = -\sum_l \frac{\varphi_l(\mathbf{R})}{\Omega_l}\left[n_F\left(\frac{\Omega_l}{T}\right) - \frac{1}{2}\right]. \quad (6)$$

Taking one mode to be located at zero energy $\Omega_p = 0$, while for all other modes $|\Omega_l| \gg T$, one finds in the low-temperature limit $\varphi_p(\mathbf{R})/4T \gg \sum_{l\neq p}\varphi_l(\mathbf{R})/2|\Omega_l|$ that $J_{\text{cr}} \approx 4T/\varphi_p(\mathbf{R})$. For fixed J, one has $T_K \approx J\varphi_p(\mathbf{R})/4$, implying that T_K scales linearly with the spectral weight of the zero-energy mode at $\mathbf{R}$—a result that is qualitatively

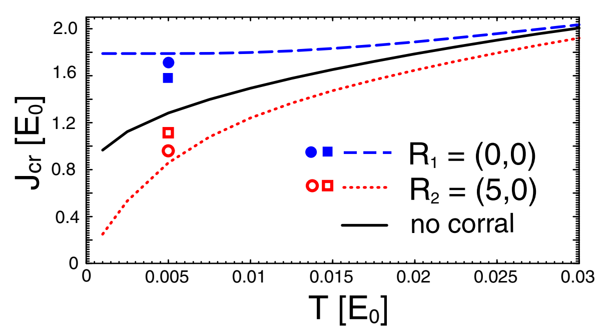

FIG. 2 (color online). J_{cr} at $\mathbf{R}_{1,2}$ as a function of T. The solid line represents J_{cr}^u for a system without a corral. The solid (open) square and circle represent J_{cr} at $\mathbf{R}_1$ ($\mathbf{R}_2$) for a quantum corral with $U = 0.2E_0$ and $0.5E_0$, respectively.

different from the single-impurity Kondo problem where T_K depends exponentially on the DOS [13]. This low-temperature behavior of J_{cr} is observed at $\mathbf{R}_2$ since $\varphi_p(\mathbf{R}_2) \neq 0$ for the mode shown in Fig. 1(b). In contrast, $\varphi_p(\mathbf{R}_1) = 0$, implying that for $T \to 0$, $J_{cr}(\mathbf{R}_1)$ saturates to a nonzero value given by $J_{cr}^{-1} \approx \sum_{l\neq p} \varphi_l(\mathbf{R}_l)/2|\Omega_l|$. In Fig. 2, we also plot the temperature dependence of J_{cr} for a system without quantum corral J_{cr}^u, which is qualitatively similar to that of $J_{cr}(\mathbf{R}_2)$ due to the nonzero DOS of the unperturbed, metallic host at $\omega = 0$. Since J_{cr}^u lies between $J_{cr}(\mathbf{R}_1)$ and $J_{cr}(\mathbf{R}_2)$, a quantum corral can either facilitate (at $\mathbf{R}_2$) or suppress (at $\mathbf{R}_1$) the screening of a magnetic impurity. Finally, the difference in J_{cr} between $\mathbf{R}_1$ and $\mathbf{R}_2$ is quite substantial already for rather weak scattering potential U, as follows from Fig. 2 where the solid [open] square and circle represent J_{cr} at $\mathbf{R}_1$ [$\mathbf{R}_2$] for a corral with $U = 0.2E_0$ and $0.5E_0$, respectively. This demonstrates the robustness of the spatially dependent Kondo effect even for small U.

In Fig. 3, we present J_{cr} (at $T = 0.005E_0$), T_K, and the LDOS of the zero-energy mode inside the corral along $\mathbf{R} = (x, 0)$. The maximum of the LDOS at $\mathbf{R} = (5, 0)$ coincides with a minimum in J_{cr} and a maximum in T_K, and a more detailed analysis yields that T_K scales linearly with the mode's spectral weight at $\mathbf{R}$. For a given J, a magnetic impurity exhibits characteristic signatures of Kondo screening only for those locations inside the corral for which $T < T_K(\mathbf{R})$—a result that remains qualitatively unaffected by the interpretation of T_K as a crossover. A comparison of $T_K(\mathbf{R})$ with the spatially uniform T_K for $J = 1.3E_0$ in the absence of a corral [see Fig. 3(b)] shows that $T_K(\mathbf{R})$ 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 Fig. 4, we present N_c^{tot} and the f electrons' LDOS $N_f = -N\text{Im}[F(\mathbf{R}, \omega)]/\pi$ for an impurity at $\mathbf{R} = (5, 0)$ with $J = 1.45E_0$. Kondo screening results in multiple Kondo resonances, a phenomenon characteristic of a discrete excitation spectrum in a host system [7,9]. 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 zero-energy eigenmode leads to two Kondo resonances almost symmetrically located around $\omega = 0$ [9]. Note that, because of 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. 1(b) and 5(a) shows that Kondo screening of the impurity strongly suppresses the LDOS of the zero-energy eigenmode at the impurity position $\mathbf{R}$ and its mirror site $-\mathbf{R}$. The same result holds for eigenmodes away from zero energy [see, e.g., Figs. 1(c) and 5(b)]. In contrast, the LDOS of the Kondo resonance at $\omega = -0.019E_0$ possesses a peak around $\mathbf{R}$ with a weaker image at the mirror site $-\mathbf{R}$, while the resonance at $\omega = 0.018E_0$ exhibits a peak in the LDOS only at the

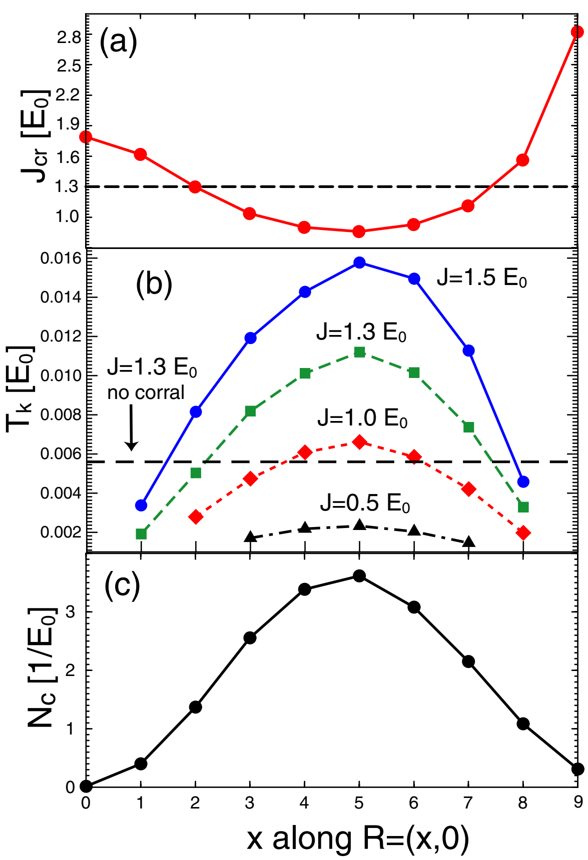

FIG. 3 (color online). (a) J_{cr} along $\mathbf{R} = (x, 0)$ for $T = 0.005E_0$. (b) T_K for several J along the same path as in (a). The black dashed line shows T_K for a magnetic impurity with $J = 1.3E_0$ in the absence of a corral. If no value for T_K is given, T_K is smaller than the lowest temperature we considered, $T = 10^{-3}E_0$. (c) N_c at $\omega = 0$ along the same path as in (a).

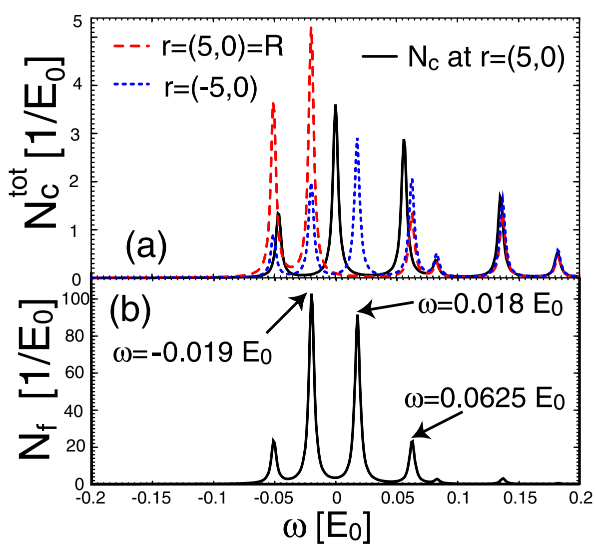

FIG. 4 (color online). (a) N_c^{tot} and (b) N_f as a function of frequency for $\mathbf{R} = (5, 0)$, $J = 1.45E_0$, $T_K = 0.0145E_0$, $T = 0.005E_0$, $\epsilon_f = 0.02E_0$, and $s^2 = 0.03E_0^2$.

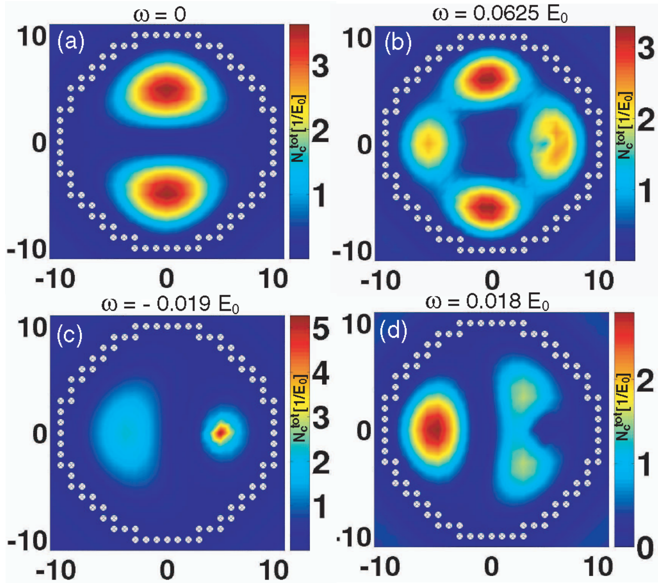

FIG. 5 (color online). Spatial form of N_c^{tot} at (a) $\omega = 0$ and at three of the Kondo resonances shown in Fig. 4: (b) $\omega = 0.0625E_0$, (c) $\omega = -0.019E_0$, and (d) $\omega = 0.018E_0$.

mirror site but not at **R**. We find that similarly strong signatures of Kondo screening in the LDOS exist for all locations of the magnetic impurity with $T < T_K(\mathbf{R})$.

2D metallic host materials are the primary candidate systems for the observation of the spatially dependent Kondo effect discussed above. Such systems, which could be realized, for example, by growing ultrathin films of only a few atomic layers on insulating or semiconducting substrates [18], would avoid several disadvantages arising from the coupling of surface and bulk states in 3D host metals, such as a decrease in the spatial variation and the lifetime of the corral's eigenmodes. These effects are similar to those observed when U is decreased (see Fig. 2), and we therefore conclude that the qualitative features of our results remain unchanged as long as the coupling is such that the separation between the zero-energy eigenmode and all other eigenmodes remains larger than T_K. Moreover, it was argued for the specific case of a single Co atom on a Cu(111) surface [19,20] that the hybridization of the Kondo impurity to the bulk states is larger than that of the impurity to the surface states. Whether this result holds in quantum corrals is presently unclear, in particular, since the hybridization between impurity and surface states was shown to be experimentally relevant in Ref. [11]. In any case, a coupling between impurity and bulk states would weaken the spatial variation of T_K due to the less pronounced spatial and frequency variation of the bulk LDOS near the corral.

In summary, we studied the Kondo screening of a magnetic impurity inside a nonmagnetic 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 LDOS 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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