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Two Kondo impurities in nanoscopic systems

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Abstract. We study the problem of two Kondo impurities in a small system. Using a slave boson approach we investigate the effect on the electron confinement of the Kondo physics of the two impurity problem. We show that the confinement splits the symmetric and antisymmetric channels and for small systems weakly coupled to a reservoir this gives two well defined behaviors: For the Fermi energy lying at a resonant state, the two impurities are Kondo screened with two characteristic energy scales. For the Fermi energy between two resonances, the inter-impurity interaction destroys the Kondo effect.

PACS. 72.10.Fk Scattering by point defects, dislocations, surfaces, and other imperfections (including Kondo effect) – 72.15.Qm Scattering mechanisms and Kondo effect

The problem of Kondo like impurities in nanoscopic systems has been the subject of a number of recent works. A Kondo impurity in the bulk of a metallic material can be viewed, in its simple form, as a single quantum spin interacting with an ideal electron gas via an antiferromagnetic coupling J_K. This interaction gives rise to a singular scattering at the Fermi surface and the simultaneously screening of the impurity spin by the conduction electrons spins [1]. Consequently, at low temperatures, the impurity contribution to the resistivity increases logarithmically and the magnetic susceptibility saturates. There is a characteristic temperature, known as the Kondo temperature $T_K \sim De^{-1/\lambda}$, with D the free electron band width and $\lambda = J_K/D$ a dimensionless coupling constant, that separates the low temperature from the high temperature regimes. While for $T \gg T_K$, the impurity spin is essentially free and the problem can be treated by perturbations in λ, for $T \ll T_K$ the impurity spin is screened and the system can be described by an effective strong coupling Hamiltonian. The two-impurity problem in bulk materials has also been studied in detail due to the interesting interplay between the Kondo effect and the inter-impurity correlations [2]. In systems with electron hole symmetry two impurities with two channels, symmetric and antisymmetric, present a quantum phase transition between two different ground states: a non-Kondo state with strong inter-impurity correlations for weak coupling and a Kondo regime for strong coupling. When the electron-hole symmetry is broken, the transition becomes a crossover.

During the last years, new realizations of the Kondo problem have been achieved by artificially designing quantum dots embedded in circuits [3]. In these cases, the quantum dot may act as a magnetic impurity and the contacts or leads as the host metal. The possibility of observing the Kondo physics in quantum dots triggered a number of experiments and theoretical works [4,5]. In this context, the two quantum dots system has attracted recent interest [6,7]. Although the problem studied in this work is relevant for quantum dots in mesoscopic systems, for the sake of clarity, in what follows, we refer to atomic Kondo-like impurities.

Recent experiments posed the question of what happens with the Kondo effect when the metallic host is reduced to sizes so small that the conduction electron spectrum becomes discrete with an average level spacing $\Delta \sim T_K$ [8–11]. The problem has been analyzed using different techniques including numerical renormalization group [9] and slave boson approaches [8,11]. The one impurity problem in nanoscopic systems presents new regimes induced by the electron confinement. This suggest that the old two impurity problem could be also subject to important effects if the impurities are embedded in a small sample. In the present work we analyze what happens with the two-impurity problem in a nanoscopic system and show how the confinement of conduction electrons changes the Kondo physics. We show that in nanoscopic

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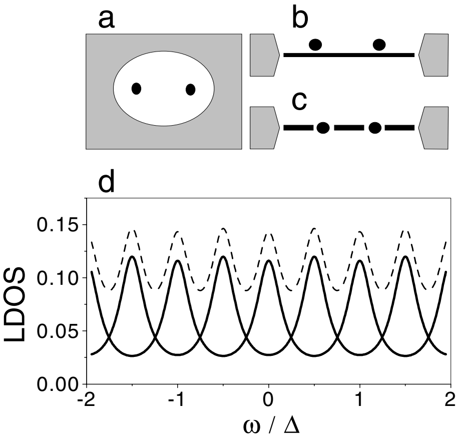

Fig. 1. (a), (b) and (c) show three possible geometrical configurations of the system, the gray areas represent reservoirs to which the nanoscopic system is weakly coupled. In (a) two impurities are at the foci of an elliptical sample; (b) and (c) represent two quantum dots connected to finite wires, the dots are outside (b) or inside the wires, the wires are coupled to the reservoirs. In (d) we show in solid lines the LDOS of the symmetric ($\eta = +$) and antisymmetric ($\eta = -$) states, in dashed lines the sum of both.

systems, the confinement of the electronic states separates the even and odd channels and in some sense greatly simplifies the physics of the two-impurity problem.

The system is described by the following two-impurity Anderson Hamiltonian [1]:

$$H_{AM} = \sum_{\alpha,\sigma} \varepsilon_d d^\dagger_{\alpha\sigma} d_{\alpha\sigma} + \sum_{\alpha} U d^\dagger_{\alpha\uparrow} d_{\alpha\uparrow} d^\dagger_{\alpha\downarrow} d_{\alpha\downarrow} + \sum_{\nu,\sigma} \varepsilon_\nu c^\dagger_{\nu\sigma} c_{\nu\sigma} + \sum_{\alpha,\nu,\sigma} (V^*_{\nu,\alpha} c^\dagger_{\nu\sigma} d_{\alpha\sigma} + V_{\nu,\alpha} d^\dagger_{\alpha\sigma} c_{\nu\sigma}), \quad (1)$$

here the subindex $\alpha = 1, 2$ identifies the impurity, the operator $d^\dagger_{\alpha\sigma}$ creates an electron with spin σ and energy ε_d at the α impurity, U is the intra-atomic Coulomb repulsion, $c^\dagger_{\nu\sigma}$ creates an electron in an extended state with quantum numbers ν and σ and energy ε_ν. In this notation, the nano-structure of the system is hidden in the structure of the one-electron extended states with energies ε_ν and wavefunctions $\psi_\nu(\mathbf{r})$. In equation (1) the hybridization matrix elements are taken proportional to the extended state wavefunctions at the impurity position, i.e. $V_{\nu,\alpha} = V_0\psi_\nu(R_\alpha)$ where R_α is the coordinate of the α impurity. For simplicity, in what follows we consider symmetric samples as those illustrated in Figure 1 with the two impurities placed at equivalent points. Figure 1a is an elliptical sample with the impurities at the foci, Figures 1b and c represent two quantum dots connected to finite wires. The gray areas represent reservoirs to which the systems are weakly coupled. The exact form of the host density of states in the impurities sites is not relevant here, thus it is included in a somehow idealized way. Figure 1d shows the local density of states (LDOS) used in the calculations. If the system is decoupled from the reservoirs, the energy spectrum of the finite host consist of a collection of levels separated by a characteristic energy Δ. As the system is weakly coupled to the reservoirs, these states acquire a width that gives the life time for electrons in the finite sample. Then the spectral density of the host sample is characterized by two energy scales: Δ that gives the energy separation of the resonant states and decreases as the system increases, and the width of the resonances γ, that decreases as the coupling with the reservoir decreases. For small systems weakly coupled to the reservoirs $\Delta \gg \gamma$ and in what follows we consider only this case. In any real system, all resonances do not have the same width γ and their energy separation Δ is not constant. However the Kondo physics is dominated by the behavior of the host spectral density at the Fermi level and in our case, the parameters Δ and γ refer to the characteristic separation and width of the resonances centered close to the Fermi energy. The calculation does not require all Δ's and γ's to be the same. Note that the relevant states are in general only one sector of the total Hilbert space: if for symmetry reasons $V_{\nu,\alpha} = 0$, the state with quantum numbers ν is not to be included in our analysis. A schematic picture of the host spectral density is shown in Figure 1d, due to the symmetry of the problem the local density of states at the coordinates of the two impurities is the same, only the relative phase of the hybridization matrix element may depend on α. As indicated in the figure the spectral density can be separated in the contributions from symmetric (with $V_{\nu,1} = V_{\nu,2}$) and antisymmetric (with $V_{\nu,1} = -V_{\nu,2}$) states. This completely defines the properties of the host and we analyze the cases in which the Fermi energy lies at a resonance (at resonance case) or between two resonances (off resonance case). For one impurity, it has been shown that these two cases present quite different behaviors [9]. The structure in the local density of states becomes important only when $T \sim \Delta$. For the at resonance case the universal Kondo behavior is recovered at low temperature with a Kondo temperature that may be much larger than the bulk Kondo temperature T^0_K corresponding to a system with the average density of states ρ_0. For the off resonance case the screening takes place in two steps leading to new partially screened regimes.

Using the slave boson theory at the saddle point approximation, we show that for the two-impurity problem, the at resonance and the off resonance cases also give quite different behaviors. To do so we proceed as in references [12] and [13]. First we assume a large Coulomb repulsion ($U \to \infty$) and neglect double occupation of the impurity orbital. The fermionic operator $d_{\alpha\sigma}$ is then decomposed in a slave boson operator $b^\dagger_\alpha$ that creates an empty state and a fermionic operator $f_{\alpha\sigma}$ that destroys a singly occupied state: $d_{\alpha\sigma} = b^\dagger_\alpha f_{\alpha\sigma}$. In terms of these operators, the physical Hilbert space corresponds to the sector with $b^\dagger_\alpha b_\alpha + \sum_\sigma f^\dagger_{\alpha\sigma} f_{\alpha\sigma} = 1$ that guarantees that the impurity orbital is either empty or singly occupied with a spin up or a spin down fermion. The Hamiltonian can be put as:

$$H = \sum_{\alpha,\sigma} \varepsilon_d f^\dagger_{\alpha\sigma} f_{\alpha\sigma} + \sum_{\nu,\sigma} \varepsilon_\nu c^\dagger_{\nu\sigma} c_{\nu\sigma} + \sum_{\nu,\sigma} (V^*_{\nu,\alpha} c^\dagger_{\nu\sigma} f_{\alpha\sigma} b^\dagger_\alpha + V_{\nu,\alpha} b_\alpha f^\dagger_{\alpha\sigma} c_{\nu\sigma}) + \sum_\alpha \lambda_\alpha (b^\dagger_\alpha b_\alpha + \sum_\sigma f^\dagger_{\alpha\sigma} f_{\alpha\sigma} - 1) \quad (2)$$

where the last term represents the constrain that projects the Hilbert space into the physical sector with the Lagrange multipliers λ_α. The saddle point approximation corresponds to neglect the dynamics of the boson field and replace $b^\dagger_\alpha$ and b_α by c-numbers. Due to the symmetry of the problem – the impurities are placed at equivalent points – we can take $\lambda_1 = \lambda_2 \equiv \lambda$ and $b_1 = b_2 \equiv b$. It is known that the RKKY inter-impurity interaction mediated by the conduction electrons is not obtained with the saddle point approximation, it is recovered only when the fluctuations around the saddle point are properly included [12]. When working at a mean field level, it is a standard procedure to add to the Hamiltonian an inter-impurity interaction:

$$H' = I/2 \sum_{\sigma,\sigma'} f^\dagger_{1\sigma} f_{1\sigma'} f^\dagger_{2\sigma'} f_{2\sigma} \quad (3)$$

that has the same form as the RKKY interaction, $I < 0$ ($I > 0$) corresponds to a ferromagnetic (antiferromagnetic) interaction between the impurities. At the end of the calculation the parameter I can be put in terms of the microscopic parameters of the original Hamiltonian to reproduce the RKKY exchange. The RKKY interactions of magnetic impurities in nanoscopic systems has been studied in some detail [14]. It has been shown that, in the limit $\Delta \gg \gamma$, the interaction between impurities at equivalent positions is ferromagnetic or antiferromagnetic depending on whether the system is at-resonance or off-resonance. In what follows we discuss the two cases.

The at resonance case: This case corresponds to the Fermi level lying at one of the resonant states of the host. Regardless of the symmetry of this state [14], the inter-impurity interaction is ferromagnetic, $I < 0$. Contrary to the case of antiferromagnetic interactions, a ferromagnetic interaction between impurities is irrelevant, it does not change the properties of the ground state and we can safely ignore it. More over, a mean field treatment of this term with a link variable as is done below, does not change the results. It is convenient to write the Hamiltonian in terms of the symmetric and antisymmetric states characterized by the index $\eta = \pm$, with the plus and minus signs corresponding to the symmetric and antisymmetric states respectively.

$$H = \sum_{\eta,\sigma} \widetilde{\varepsilon}_d f^\dagger_{\eta\sigma} f_{\eta\sigma} + \sum_{\eta,\nu,\sigma} \varepsilon_{\eta\nu} c^\dagger_{\eta\nu\sigma} c_{\eta\nu\sigma} + \sum_{\eta,\nu,\sigma} b V_{\eta\nu} (c^\dagger_{\eta\nu\sigma} f_{\eta\sigma} + f^\dagger_{\eta\sigma} c_{\eta\nu\sigma}) + 2\lambda(b^2 - 1) \quad (4)$$

where $\widetilde{\varepsilon}_d = \varepsilon_d + \lambda$, $f_{\eta\sigma} = (f_{1\sigma} + \eta f_{2\sigma})/\sqrt{2}$ and we have included the index η in the extended states quantum numbers to explicitly indicate their parity. The LDOSs of the symmetric and antisymmetric extended states are shown in Figure 1d.

The energy minimization with respect to b and λ gives:

$$\sum_{\eta,\sigma} \langle f^\dagger_{\eta\sigma} f_{\eta\sigma} \rangle + 2(b^2 - 1) = 0 \quad (5)$$

and

$$\sum_{\eta,\nu,\sigma} V_{\eta\nu} \langle f^\dagger_{\eta\sigma} c_{\eta\nu\sigma} \rangle + 2\lambda b = 0 \quad (6)$$

with

$$\langle f^\dagger_{\eta\sigma} f_{\eta\sigma} \rangle = -\frac{1}{\pi} \int^{\varepsilon_F} d\omega \mathrm{Im} \frac{1}{\omega - \widetilde{\varepsilon}_d - b^2 V_0^2 g_\eta(\omega)} \quad (7)$$

and

$$\sum_\nu V_{\eta\nu} \langle f^\dagger_{\eta\sigma} c_{\eta\nu\sigma} \rangle = - V_0^2 \frac{1}{\pi} \int^{\varepsilon_F} d\omega \mathrm{Im} g_\eta(\omega) \frac{1}{\omega + i0 - \widetilde{\varepsilon}_d - b^2 V_0^2 g_\eta(\omega)}. \quad (8)$$

In these equations the propagator $g_\eta(\omega)$ is given by:

$$g_\eta(\omega) = \sum_\nu \frac{|\psi_{\eta\nu}(R_1)|^2}{\omega - \varepsilon_{\eta\nu} + i0^+} = \int d\varepsilon \frac{\rho_\eta(\varepsilon)}{\omega - \varepsilon + i0^+} \quad (9)$$

where $\rho_\eta(\varepsilon)$ is the contribution of the symmetric ($\eta = 1$) and antisymmetric ($\eta = -1$) states to the local density of states as shown in Figure 1. $\widetilde{\varepsilon}_d$ gives the position of the Kondo resonance. Solving these equations we obtain the self consistent solution of the problem.

In terms of the auxiliary boson and fermion fields, the impurity spectral density $A_i(\omega)$ is given by

$$A_i(\omega) = -\frac{b^2}{2\pi} \sum_\eta \mathrm{Im} \frac{1}{\omega + i0 - \widetilde{\varepsilon}_d - b^2 V_0^2 g_\eta(\omega)} \quad (10)$$

and the self consistent solution is shown in Figure 2 for two sets of parameters. These results show that for small energies and for the bulk Kondo temperature $T_K^0 < \gamma < \Delta$, the spectral density of each impurity can be put as the sum of two resonances:

$$A_i(\omega) \approx -\frac{b^2}{2\pi} \mathrm{Im} \left(\frac{1}{\omega + iT_{K1}} + \frac{1}{\omega + iT_{K2}} \right) \quad (11)$$

with two energy scales T_{K1} and T_{K2} associated with the two channels with parity η_0 and $-\eta_0$ at the Fermi level. The ratio between these energy scales is not exponential, it is given by $T_{K2}/T_{K1} = N_{\eta_0}(\varepsilon_F)/N_{-\eta_0}(\varepsilon_F)$ where $N_{\eta_0}(\varepsilon_F)$ is the contribution to the local density of states of the states with parity η_0. This is so because the two channels are not independent, in our approach they are linked by the constrains.

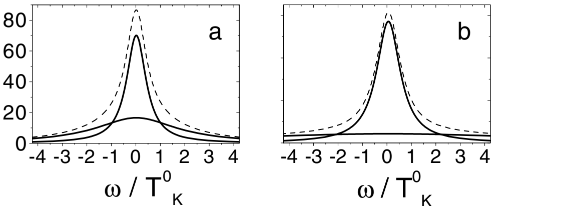

Fig. 2. Spectral density of the impurities in the *at resonance* case for two values of the width γ (a) $\gamma/T_K^0 = 320$, (b) $\gamma/T_K^0 = 170$. In solid lines is shown the symmetric and antisymmetric components and in dashed lines the total spectral densities. The energy scale T_K^0 is the Kondo temperature for one impurity evaluated with an average density of states.

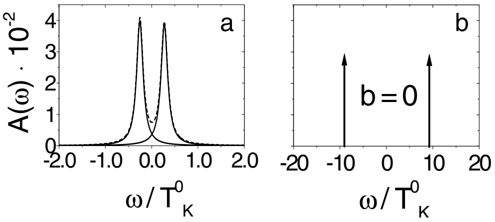

Fig. 3. Impurity spectral densities with the Fermi level placed off resonance. Parameters are like in Figure 2 with $\gamma/T_K^0 = 320$. In (a) the antiferromagnetic interaction I produces a split of the density in two narrow peaks. In (b), a value of I greater than a certain critical value decouples, in this approximation, the impurities from the reservoir.

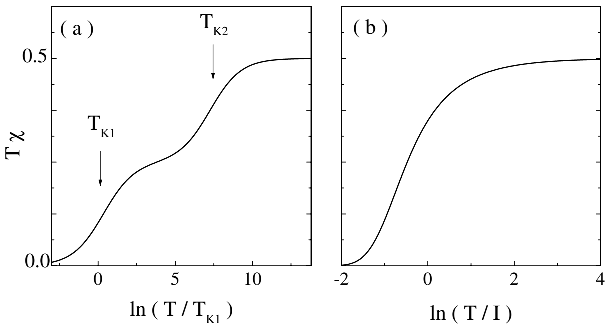

Fig. 4. Schematic form of the impurity susceptibility for (a) the *at resonance* case and (b) the *off resonance* case.

It is instructive to analyze the results in terms of a real space picture. For the at resonance situation, the expectation value of the number of extended electrons in the small system is close to an odd number. All resonances but the one that is centered at the Fermi energy, contribute with approximately zero or two electrons while the later with one. That means that in the small system there is a free spin 1/2. This spin can screen half of the localized spins, and defines a screening energy T_{K2}. The electrons of the macroscopic host, with wavefunctions that penetrate the small system with exponential tails, complete the screening within an energy scale $T_{K1} < T_{K2}$. As the temperature increases, first at $T \sim T_{K1}$ the correlation between the localized spins and the spins of the reservoir are destroyed and only for $T > T_{K2}$ the localized spins are free. The impurities magnetic moments are then screened in two steps. According to expression (11), in this limit ($T_K^0 < \gamma < \Delta$) the impurity spectral density, and all thermodynamic properties related to it, can be put as the sum of the even and odd channels contributions. In particular the low temperature susceptibility $\chi(T)$ is the sum of two Kondo-like susceptibilities with Kondo temperatures T_{K1} and T_{K2} respectively (see Fig. 4).

The off resonance case: This case corresponds to the Fermi level lying between two resonant states of the host. For this case and $\gamma < \Delta$ the RKKY interaction is antiferromagnetic and then we take $I > 0$. The antiferromagnetic interaction between impurities competes with the Kondo effect and the two effects are to be treated at equivalent footings. To do so we resort to a mean field approach as in reference [15] and introduce a link variable χ_{12} in terms of which the spin-spin interaction takes the form:

$$H' = -I/2 \sum_\sigma (\chi_{12} f_{1\sigma}^\dagger f_{2\sigma} + hc) + I\chi_{12}^2/2. \qquad (12)$$

We then proceed as in the previous case, the only difference is that now the diagonal energies of the symmetric and antisymmetric localized states are shifted by the spin-spin interaction: in Hamiltonian (4) the first term has $\widetilde{\varepsilon}_{d\eta} = \widetilde{\varepsilon}_d - \eta I \chi_{12}/2$. For the case we are discussing with $\gamma < \Delta$, the local density of states at the impurity sites is small, and we are then in the weak coupling limit. For very small inter-impurity interaction I, the Kondo resonance is splitted in two resonances corresponding to the symmetric and antisymmetric states. The impurity spectral density $A_i(\omega)$ for this case is shown in Figure 3a. These results were obtained assuming that the two host resonances that are close to the Fermi level have different symmetries. The reduction of $A_i(\varepsilon_F)$ is an indication of the weakening of a Kondo effect. As I increases, the splitting of the double structure of the Kondo resonance increases as the widths of the line decreases. For I larger than a critical value, the width becomes zero as in the homogeneous case [13]. In general, for $\gamma < \Delta$, at the off resonance case, we expect to be in this limit where the Kondo effect is completely destroyed by the inter-impurity exchange interaction. The impurity susceptibility is then given by:

$$k_B T \chi(T) = \frac{4\mu_B^2}{3 + e^{I/k_B T}} \qquad (13)$$

and its behaviour is shown in Figure 4, the change of behavior occurs for $k_B T \sim I$, indicating that the saturation of the susceptibility is not due to a Kondo screening.

We have considered the case of small systems weakly coupled to reservoirs, the results presented above correspond to $T_K < \gamma < \Delta$. For a transition metal impurity in a noble metal, like Co in Cu, the Kondo temperature is of the order of 50 K. If we take $\Delta \sim \hbar v_F(\pi/L)$ with L a characteristic dimension of the sample, the condition $T_K < \Delta$ is fulfilled for L of the order of 100 Å. For a QD on GaAs a typical Kondo temperature is $T_K = 1$ K and for single channel wires this condition implies that L could be as large as 1 μm.

For $T_K \gg \Delta$ the confinement effects are not relevant and one should recover the behavior of the thermodynamic limit ($L \to \infty$) as described in reference [7].

In summary, we have analyzed the two-impurity problem in mesoscopic systems. We have shown that for $T_K < \gamma < \Delta$ the behavior of the system is very sensitive to the relative position of the Fermi level and the structure of the density of states. In particular we have analyzed the cases in which the Fermi level is aligned with a resonant state, or between two resonant states, of the mesoscopic sample. The difference in the behavior is due to two effects, on one hand the Kondo screening depends on the local density of states at ε_F and on the other the RKKY interaction is ferromagnetic for the at-resonance and antiferromagnetic for the off-resonant case. The condition $T_K < \gamma < \Delta$, that implies small samples, is appropriate to observe "quantum mirages" [16] with one impurity. The effects observed with two impurities for the "at resonance" case can be interpreted as a coherent interference of the Kondo effect of one impurity with the mirage of the other [14,17].

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References

1. For a review, see A.C. Hewson in *The Kondo problem to heavy fermions* (Cambridge Univ. Press, 1993)
2. B.A. Jones, C.M. Varma, Phys. Rev. Lett. **58**, 843 (1987); B.A. Jones, C.M. Varma, J.W. Wilkins, Phys. Rev. Lett. **61**, 125 (1988)
3. D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu, D. Abush-Magder, U. Meirav, M.A. Kaster, Nature **391**, 156 (1998)
4. Y. Ji, M. Heiblum, D. Sprinzak, D. Mahalu, H. Shtrikman, Science **290**, 779 (2000)
5. L.I. Glazman, M.E. Raikh, JETP Lett. **47**, 452 (1988); T.K. Ng, P.A. Lee, Phys. Rev. Lett. **61**, 1768 (1988)
6. A. Georges, Y. Meir, Phys. Rev. Lett. **82**, 3508 (1999)
7. T. Aomo, M. Eto, K. Kawamura, J. Phys. Soc. Jpn **67**, 1860 (1998)
8. W.B. Thimm, J. Kroha, J. von Delft, Phys. Rev. Lett. **82**, 2143 (1999)
9. P.S. Cornaglia, C.A. Balseiro, Phys. Rev. B **66**, 115303 (2002); Phys. Rev. B **66**, 174404 (2002)
10. I. Affleck, P. Simon, Phys. Rev. Lett. **86**, 2854 (2001)
11. H. Hu, G.-M. Zhang, L. Yu, Phys. Rev. Lett. **86**, 5558 (2001)
12. P. Coleman, Phys. Rev. B **35**, 5072 (1987)
13. B.A. Jones, B.G. Kotliar, A.J. Millis, Phys. Rev. B **39**, 3415 (1989)
14. A. Correa, K. Hallberg, C.A. Balseiro, Europhys. Lett. **58**, 899 (2002)
15. I. Affleck, J.B. Marston, Phys. Rev. B **37**, 3774 (1988)
16. H.C. Manoharan, C.P. Lutz, D.M. Eigler, Nature **403**, 512 (2000)
17. G. Chiappe, A.A. Aligia, Phys. Rev. B **66**, 075421 (2002)