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D-Wave Kondo Problem in a Square Tight-Bounding Lattice *

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A Kondo model in a square tight-bonding lattice of conduction electrons is considered. The Kondo interaction takes a d-wave. Using mean-field theory and numerical simulations, it is found that there is a pseudo-gap for the impurity density of states at the Fermi level. Numerical results also show that the exponents of the low-temperature thermodynamic quantities are non-universal but dependent on the interaction.

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The Kondo problem is one of the most important problems in condensed matter physics. It represents almost the simplest strongly correlated electron system. The Kondo problem in ordinary three-dimensional metals has been extensively studied with the numerical renormalization group method,[1] the Bethe ansatz method,[2] and phenomenological local-Fermi-liquid method.[3] All the results show that a spin-1/2 impurity can be completely screened by the conduction electrons at low temperature and exhibits the local Fermi liquid behaviour. Recently, the Kondo problem in low-dimensional electronic systems has received much attention in the context of mesoscopic systems, quasi-one-dimensional compounds and high-T_c superconductors. Many interesting phenomena have been discovered in a Luttinger liquid, such as the power-law dependent Kondo temperature,[4] the ferromagnetic Kondo screening,[5] and the spin-splitting effect[6]. In high-T_c superconductors, substitution by divalent ions (Zn and Ni)[7] for Cu in the CuO_2 plane offers an important way to test the Kondo effect in such a host. This problem has been studied both experimentally[7] and theoretically[8] to obtain the local nature of the electronic states near the impurity.

Most of the current studies have been focused on the on-site Kondo coupling and have seldom considered an off-on site Kondo interaction. In this letter, we study the Kondo problem in a square tight-bonding lattice of conduction electrons. The Kondo coupling in the present model is assumed to take the d-wave form describing one magnetic impurity interacting interaction with the four surrounding conduction electrons. The configuration is shown in Fig. 1. The d-wave interacting interaction Hamiltonian is given by

$$H_{\rm I} = J(f^{\dagger}_{\sigma} f_{\sigma'} \boldsymbol{\tau}_{\sigma\sigma'} \cdot \boldsymbol{S}), \tag{1}$$

where

$$f^{\dagger}_{\sigma} = \frac{1}{2}(c^{\dagger}_{1\sigma} + c^{\dagger}_{3\sigma} - c^{\dagger}_{2\sigma} - c^{\dagger}_{4\sigma}), \tag{2}$$

creates an electron in the d channel and $\tau_{\sigma\sigma'}$ is the Pauli matrix. Note that the spin exchange involves processes in which the electrons can hop and flip between neighbouring orbits. Here $\boldsymbol{S}$ is the spin operator of the impurity

$$\begin{aligned} S^{+} &= d^{\dagger}_{\uparrow} d_{\downarrow}, \\ S^{-} &= d^{\dagger}_{\downarrow} d_{\uparrow}, \\ S^{z} &= \frac{1}{2}(d^{\dagger}_{\uparrow} d_{\uparrow} - d^{\dagger}_{\downarrow} d_{\downarrow}), \end{aligned} \tag{3}$$

with $d^{\dagger}_{\sigma}$ the creation operator of the impurity electron and the constraint $\sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} \leq 1$. The total Hamiltonian we shall consider reads

$$\begin{aligned} H = & -t \sum_{\sigma i} c^{\dagger}_{i\sigma} c_{i+\delta,\sigma} + \text{H.c.} + \epsilon_d \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} \\ & + H_{\rm I} - \mu \sum_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} - \nu \sum_{\sigma} (d^{\dagger}_{\sigma} d_{\sigma} - \frac{1}{2}). \end{aligned} \tag{4}$$

The motion of the conduction electrons is confined in a square tight-bonding lattice. Here μ is the chemical potential, ν is the Laplacian multiplier, and $\epsilon_d < 0$ is the bare level of the impurity. The two subsystems couple with each other by the local exchange (the third term). In order to obtain the physical properties of the system, now we use a mean-field theory[9] to deal with the magnetic interaction between the localized spin and itinerant electron. Letting

$$\Delta_{df} = \langle f^{\dagger}_{\sigma} d_{\sigma} \rangle, \tag{5}$$

then we obtain the mean-field Hamiltonian

$$\begin{aligned} H = & -t \sum_{\sigma i} c^{\dagger}_{i\sigma} c_{i+\delta\sigma} + \text{H.c} + \epsilon_d \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} \\ & + \frac{3J}{2} \Delta_{df} \sum_{\sigma} f_{\sigma} d^{\dagger}_{\sigma} + \text{H.c.} - \mu \sum_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} \\ & - \nu \sum_{\sigma} (d^{\dagger}_{\sigma} d_{\sigma} - \frac{1}{2}) - 3J|\Delta_{fd}|^2. \end{aligned} \tag{6}$$

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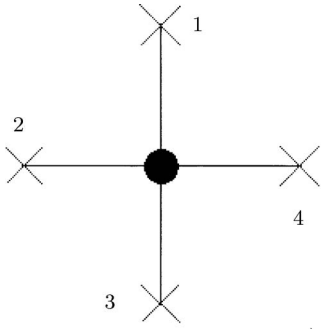


Fig. 1. Kondo coupling configuration in a square lattice. Here dots denotes the impurity site and crosses indicate the conduction electron site.

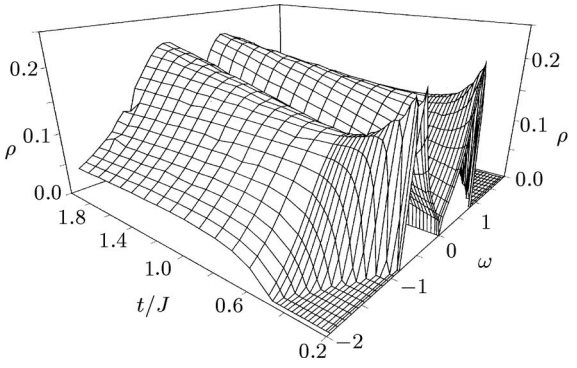


Fig. 2. Density of state of the impurity for the d-wave Kondo coupling. Here ω ranges from -2 to 2 and t/J ranges from 0.0 to 2.0.

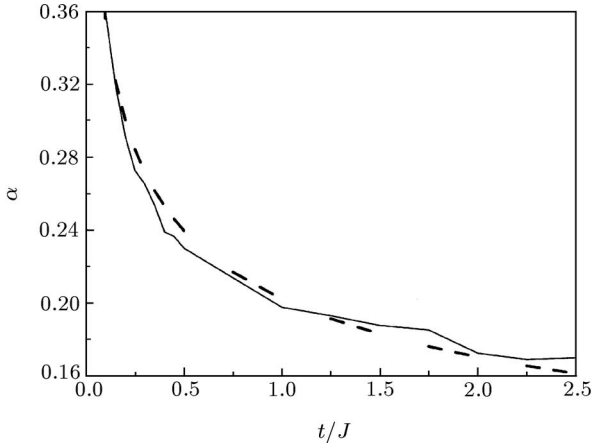


Fig. 3. Exponent α versus t/J. The solid line is the numerical result and the dashed line is the fit.

In the k space it reads

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \epsilon'_d \sum_\sigma d^\dagger_\sigma d_\sigma + \sum_{k,\sigma} V_k c_{k\sigma} d^\dagger_\sigma + \sum_{k\sigma} V^*_k d_\sigma c^\dagger_{k\sigma} + \text{const}, \tag{7}$$

where

$$V_k = \frac{3J}{2}\Delta_{df}(\cos k_y - \cos k_x),$$
$$\epsilon_k = -2t(\cos k_x + \cos k_y) - \mu, \epsilon'_d = \epsilon_d - \nu.$$

The single-particle Green function can be derived as

$$\langle\langle d_\sigma \mid d^\dagger_\sigma\rangle\rangle = \frac{1}{\omega - \epsilon_d - \sum_k |V_k|^2/(\omega - \epsilon_k)},$$
$$\langle\langle d_\sigma \mid c^\dagger_{k\sigma}\rangle\rangle = \frac{V_k}{\omega - \epsilon_k}\langle\langle d_\sigma \mid d^\dagger_\sigma\rangle\rangle, \tag{8}$$

where $\Delta_{df} = \sum_k (\cos k_y - \cos k_x)\langle c^\dagger_{k\sigma} d\rangle$ can be determined self-consistently

$$\Delta_{df} = \sum_k (\cos k_y - \cos k_x) \int_{-\infty}^{\infty} \mathrm{d}\omega f(\omega) \cdot \left\{ \frac{V_k \Gamma}{(\omega - \epsilon_k)[(\omega - \epsilon_d - \sum_k \frac{|V_k|^2}{\omega - \epsilon_k})^2 + (\pi\Gamma)^2]} - \frac{V_k \delta(\omega - \epsilon_k)(\omega - \epsilon_d - \sum_k \frac{|V_k|^2}{\omega - \epsilon_k})}{(\omega - \epsilon_d - \sum_k \frac{|V_k|^2}{\omega - \epsilon_k})^2 + (\pi\Gamma)^2} \right\}, \tag{9}$$

where $f(\omega)$ is the Fermi distribution function. $\Gamma = \sum_k |V_k|^2 \delta(\omega - \epsilon_k)$. The density of state (DOS) of the impurity is given by the following formula

$$\rho(\omega) = \frac{\mathrm{i}}{2\pi} \int_{-\infty}^{\infty} \frac{\langle\langle d|d^\dagger\rangle\rangle_{\omega+\mathrm{i}\eta} - \langle\langle d|d^\dagger\rangle\rangle_{\omega-\mathrm{i}\eta}}{\mathrm{e}^{\beta\omega} + 1} \mathrm{d}\omega. \tag{10}$$

Here $\rho(\omega)$ for $T = 0$ is calculated numerically. For the d-wave Kondo coupling, there is a pseudo-gap at the Fermi surface. Accompanying this pseudo-gap, there are also two peaks sited aside the Fermi level symmetrically. The $\rho^d_{\mathrm{imp}}(\omega) \sim \omega$ curve is shown in Fig. 2 for some t/J values. At the low-energy scales, the DOS of the impurity can be expressed approximately as

$$\rho_d(\omega) \approx \rho^d_0 |\omega|^\alpha, \tag{11}$$

where α is a positive constant, which is not universal but changes with t/J as shown in Fig. 3. ρ^d_0 is also a t/J dependent constant (for example, $\rho^d_0 = \mathrm{e}^{-0.65}$ at $t/J = 0.5$). The low-temperature specific heat and the magnetic susceptibility of the impurity can be easily derived as

$$C^d_{\mathrm{imp}} = (\alpha + 2)\rho^d_0 T^{\alpha+1} \int_{-\infty}^{\infty} \mathrm{d}x \frac{x^{\alpha+1}}{\mathrm{e}^{\,x} + 1}. \tag{12}$$

$$\begin{aligned}\chi^d_{\rm imp} &= \lim_{h\to 0}\sum_{\sigma}\frac{\mu_{\rm B}\sigma}{h}\langle d_\sigma d^\dagger_\sigma\rangle \\ &= \lim_{h\to 0}\frac{\mu_{\rm B}}{h}\Big\{\int_{-\infty}^{\infty}\frac{\rho_\uparrow(\omega)}{{\rm e}^{\,\omega/T}+1}{\rm d}\omega \\ &\quad -\int_{-\infty}^{\infty}\frac{\rho_\downarrow(\omega)}{{\rm e}^{\,\omega/T}+1}{\rm d}\omega\Big\} \\ &= \rho_0^d T^\alpha\int_{-\infty}^{\infty}\frac{x^\alpha}{{\rm e}^{\,x}+1}{\rm d}x. \qquad (13)\end{aligned}$$

For $T\to 0, \chi^d_{\rm imp}\to 0$, which indicates that the impurity is completely compensated in the ground state.

In conclusion, we have studied the Kondo problem in a square tight-bonding lattice of conduction electrons. The Kondo coupling in our model takes the d-wave form which describes the impurity interaction with the conduction electrons on the four surrounding sites. The model was solved with a mean-field method. With numerical simulations, it is found that there is a pseudo-gap for the d-wave Kondo coupling case. The low-temperature thermodynamics of the impurity deviates from that of a local Fermi liquid, but the impurity moment can also be completely compensated in the ground state. Here the exponent of thermodynamic quantities is non-universal but coupling dependent.

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