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Non-Fermi-liquid properties in disordered Kondo systems

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Abstract
We investigate the Kondo effect in disordered electron systems using a finite-temperature quantum Monte Carlo method. Depending on the position of a magnetic impurity, the local moment is screened or unscreened by the spin of the conduction electron. The results indicate that the Kondo temperature has a spatial distribution. We show that the distribution of the Kondo temperature becomes wide and the weight at $T_K = 0$ becomes large as randomness increases. When randomness increases, the average susceptibility exhibits a logarithmic divergence, indicating that the observable susceptibility shows a non-Fermi-liquid behaviour at low temperatures.

Recently, non-Fermi-liquid behaviours in heavy-fermion systems have attracted a great amount of attention both theoretically and experimentally [1]. Several mechanisms have been proposed to explain thermodynamic and transport properties [1]. Effects of randomness constitute one of such mechanisms. The Kondo effect in strongly disordered systems was studied by taking account of the Coulomb interaction among conduction electrons [2]. On the basis of a slave-boson approach, it was shown that, as a result of the localization and interaction effects, the Kondo temperature has a spatial distribution, which leads to divergence behaviours of physical quantities such as the susceptibility of a magnetic impurity $\chi(T)$ and the coefficient of the linear specific heat C/T as temperature approaches zero. Such a spatial distribution in the Kondo temperature was suggested from experimental results on strong broadening of the Cu NMR line of $UCu_{5-x}Pd_x$ [3]. Furthermore, for $UCu_{5-x}Pd_x$ logarithmic and weak power-law divergences of $\chi(T)$ and C/T were observed experimentally at low temperatures [4–6]. The results show that the system $UCu_{5-x}Pd_x$ exhibits non-Fermi-liquid behaviours caused by randomness at low temperatures. In spite of these findings, the effects of strong randomness itself on the behaviour of a magnetic impurity have not yet been fully investigated from a microscopic viewpoint.

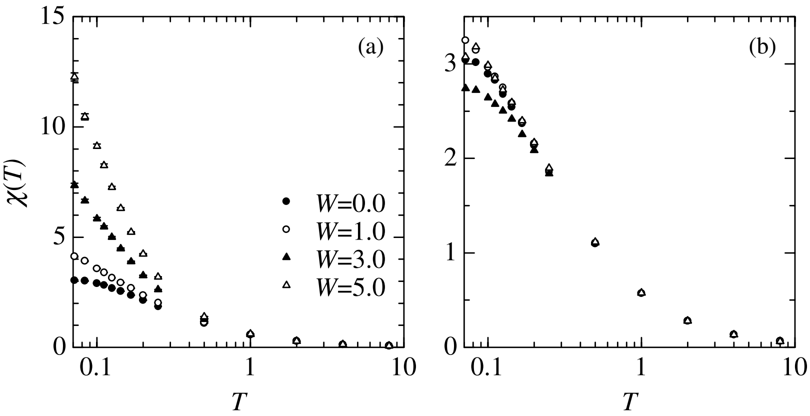

Figure 1. Susceptibility at the two different sites for $0 \leqslant W \leqslant 5.0$.

In this paper, we study the Kondo effect in strongly disordered electron systems using a finite-temperature quantum Monte Carlo (QMC) method [7]. Let us consider the single-impurity Anderson model with on-site random potentials described by the Hamiltonian

$$H = \sum_{i\sigma} \epsilon_i c_{i\sigma}^{\dagger} c_{i\sigma} - t \sum_{\langle ij\rangle\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \epsilon_d \sum_{\sigma} n_{d\sigma} + V \sum_{\sigma} (d_{\sigma}^{\dagger} c_{0\sigma} + \text{H.c.}) + U n_{d\uparrow} n_{d\downarrow}, \tag{1}$$

where random on-site potentials ϵ_i are chosen to be a flat distribution in the interval $[-W, W]$ under the condition $\sum_i \epsilon_i = 0$, $\langle i, j\rangle$ denotes the summation of the nearest-neighbour sites, and $n_{d\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$. The system consists of a $17 \times 17 \times 17$ simple cubic lattice with a magnetic impurity. We set the condition $\epsilon_d + (1/2)U = 0$ and use the parameters $U = 1.25$ and $V = -1.0$ in units of t. When $W = 0$, the Wilson ratio takes the value $\sim$1.75 at $T = 0.05$. Thus, the system is in the Kondo regime in the case without randomness.

Shifting the position of a magnetic impurity 16 times around the centre in the same realization of the random potential, we calculate $\chi(T)$ for $0 \leqslant W \leqslant 5.0$. In figure 1, we show the typical results. At the site shown in figure 1(a), $\chi(T)$ shows logarithmic divergence for $W = 3.0$ and power-law divergence with the exponent -0.93 for $W = 5.0$. At the site shown in figure 1(b), in contrast, $\chi(T)$ shows a local Fermi-liquid behaviour for $0 \leqslant W \leqslant 5.0$. Depending on the position of a magnetic impurity for given W, the local moment of a magnetic impurity can be screened or unscreened by the spin of the conduction electron. In the former case $\chi(T)$ shows a local Fermi-liquid behaviour, while in the latter case $\chi(T)$ shows power-law or logarithmic divergence. For $W = 5.0$, $\chi(T)$ shows a local Fermi-liquid behaviour at 11 positions among 17 positions. At two positions $\chi(T)$ shows logarithmic divergence, at the other two positions $\chi(T)$ shows weak power-law divergence with the exponents -0.76 and -0.85, and at the remaining two positions the local moment behaves as a free spin; $\chi(T) \sim T^{-1}$.

The behaviours of $\chi(T)$ indicate that the Kondo temperature T_K has a spatial distribution down to $T_K = 0$, since $T_K = [2\pi\chi(0)]^{-1}$ [8]. We extrapolate $\chi(0)$ and evaluate the distribution of the Kondo temperature. The results are summarized in figure 2. As W increases, the distribution of the Kondo temperature becomes wider and the weight at $T_K = 0$ increases considerably. We have thus shown that the spatial distribution of the Kondo temperature can be caused only by the effects of a random potential.

In the disordered systems with dilute magnetic impurities, where each magnetic impurity acts as a single magnetic impurity, the observable susceptibility can be obtained by averaging

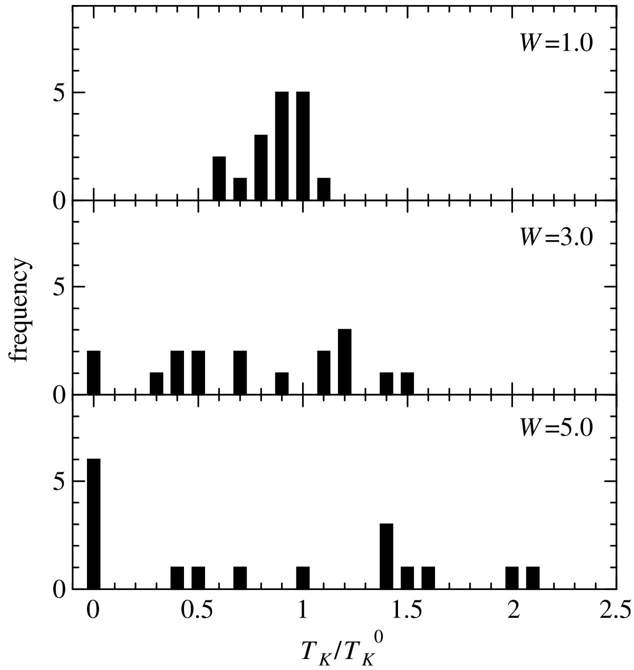

Figure 2. Distributions of the Kondo temperature for $W = 1.0$, 3.0, and 5.0. Seventeen positions of a magnetic impurity are used around the centre. The Kondo temperature without randomness ($W = 0$) is denoted as T_K^0.

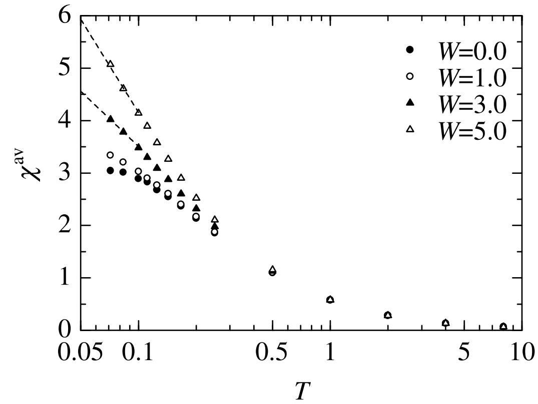

Figure 3. Average susceptibilities for $W = 1.0$, 3.0, and 5.0. The broken lines are fitted by the least-squares method.

over the susceptibility at each position of a magnetic impurity. We thus take an average over the susceptibilities at 17 positions around the centre of the system. The results are shown in figure 3. For $W = 3.0$ and 5.0 the average susceptibility $\chi_{\mathrm{av}}(T)$ exhibits logarithmic divergence for $0.05 \leqslant T \leqslant 0.1$, while for $W = 1.0$ the average susceptibility $\chi_{\mathrm{av}}(T)$ exhibits a local Fermi-liquid behaviour. Therefore, in strongly disordered electron systems with dilute magnetic impurities, the observable susceptibility shows a non-Fermi-liquid behaviour at low temperatures.

We have investigated the Kondo effect in strongly disordered systems. The results in this study are qualitatively the same as those for the two-dimensional disordered systems [9]. Therefore, the characteristics of the Kondo effect in strongly disordered systems may be insensitive to the dimensionality of the system. This feature is in contrast with the case for the Kondo effect in the weakly localized regime, where the anomalous temperature dependence depending on the dimensionality appears in physical quantities [10, 11]. To confirm this argument, a further study has to be developed.

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