Precursor of Non-Fermi Liquid Behaviour in the
One-Dimensional Periodic Anderson Model with Disorder

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Abstract

We have studied the one-dimensional periodic, symmetric Anderson model at half filling in the presence of disorder using finite-temperature quantum Monte Carlo techniques. We have examined for the first time the disorder both in hybridization between the local \( f \)-orbitals and the conduction electrons and in the local \( f \)-site energy, using a uniform distribution of width \( \Delta \). The \( f \)-orbital local magnetic moment, the uniform magnetic susceptibility, the charge compressibility, and the nearest-neighbor magnetic correlation function have been calculated as a function of the disorder distribution width \( \Delta \). We find that the disorder in hybridization has a dramatic effect on the low-temperature magnetic properties exhibiting a non-Fermi-liquid behaviour, and that for the range of temperature studied the magnetic susceptibility can be scaled by a power law with an exponent that is in agreement with recent experiments. On the other hand, disorder in the local \( f \)-orbital energy level does not show a non-Fermi liquid behaviour.

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The last several years have witnessed dramatic growth in both the experimental [1–4] and theoretical [3,12] activity in a new class of heavy fermion materials which exhibit non-Fermi-liquid (NFL) behaviour in their physical properties at low temperatures. Some of the heavy fermion NFL metals, such as CeCu$_6-x$Au$_x$, have been associated with the proximity to a quantum critical point. [13,14] However, in several other cases of heavy-fermion compounds, such as Y$_{1-x}$U$_x$Pd$_3$, UCu$_{5-x}$Pd$_x$, and Ce$_{1-x}$Th$_x$RhSb, NFL behaviour occurs only when the $f$-electron materials, consisting primarily of Ce or U intermetallics, have been alloyed with a nonmagnetic element. The NFL behaviour in these compounds is characterized by a linear resistivity at low T, a logarithmic low temperature divergence of the specific heat coefficient and a logarithmic or weak power law of the susceptibility. [1–4]

Several models have been proposed to explain these experimental results. These include exotic single-impurity models, such as the quadrapolar Kondo model, [3] various multi-channel Kondo models [4] and the “compactified” Anderson impurity model. [5] Bhatt and Fischer [8] and Dobrosavljević et al [9] have examined the single-impurity Kondo problem in the presence of a random distribution of nonmagnetic impurities. However, all these calculations strictly apply to systems with a dilute collection of Kondo centres. The inclusion of lattice effects in the presence of disorder presents an additional challenge that has only recently started to be addressed. [10] Tešanović employed a slave boson technique. [10] More recently, Miranda et al [11] and Chattopadhyay and Jarrell [12] have analyzed the effects of disorder on concentrated Kondo alloys in the limit of infinite spatial dimensions and of infinite U using the dynamical mean field theory [13]. However, this approach does not take into account the RKKY interactions between the $f$-sites, which are pertinent to the formation of the singlet ground state in the periodic Anderson model (PAM) [14]. Another mechanism proposed as a possible cause of the NFL behaviour is a disordered distribution of Kondo temperatures [4]. Castro et al [17] have attributed the NFL behaviour to the existence of Griffiths singularities close to a quantum critical point. These singularities arise from the interplay between the RKKY and Kondo interactions in the presence of magnetic anisotropy and disorder.
In this Letter, we present the first investigation of the effects of disorder on the magnetic properties of the one-dimensional periodic Anderson model (PAM) at half filling using quantum Monte Carlo techniques. The quantum Monte Carlo calculations treat both the RKKY and the Kondo interactions on an equal footing, and allow one to treat both the weak and strong disorder regime. We have studied the effects of disorder both in hybridization, $V$, between the local $f$-orbitals and the conduction electrons and in the local $f$-site energy, $E_f$, using a uniform distribution of width $\Delta$. The former case corresponds to substitution in the ligand sites with the $f$ sublattice remaining unchanged, whereas the latter case corresponds to doping directly on the $f$-sites. We present results for the $f$-orbital local magnetic moment, the static uniform magnetic susceptibility, the charge compressibility, and the nearest-neighbor magnetic correlation function as a function of the disorder distribution width $\Delta$ for both types of disorder. The interplay of correlation and disorder can lead to different types of ground states. In the case of disorder in hybridization, we find that the magnetic susceptibility exhibits a NFL behaviour, and that it can be scaled at low temperatures with a power law with an exponent that is in excellent agreement with experiment. [4] On the other hand, disorder in the local $f$-site energy leads to a Fermi-liquid like behaviour.

In the absence of disorder, the PAM is an interesting model since it exhibits various types of insulating states ranging from an antiferromagnetic insulator to a Kondo insulator or, if the $f$-$c$ hybridization dominates, a simple band insulator. [16] It is believed that the PAM describes the competition between magnetic ordering and singlet formation in a number of the heavy fermion systems. [16] The Hamiltonian for the one-dimensional PAM is

$$H = -t \sum_{i,\sigma} (c_{i,\sigma}^+ c_{i+1,\sigma} + H.c.) + E^c \sum_{i,\sigma} n_{i,\sigma}^c + \sum_{i,\sigma} V_i (f_{i,\sigma}^+ c_{i,\sigma} + H.c.)$$
$$+ U_f \sum_i n_i^f n_i^\downarrow + \sum_{i,\sigma} E_i^f n_i^\sigma. \quad (1)$$

Here, $t$ is the hopping parameter in the $c$ band, $U_f$ is the Coulomb repulsion on the $f$ band, $V_i$ is the hybridization energy between the two bands, $E_i^f$ and $E^c$ are the energy levels of the local $f$ and $c$ band, respectively, and $n_i^f \equiv f_{i,\sigma}^+ f_{i,\sigma}$ and $n_i^c \equiv c_{i,\sigma}^+ c_{i,\sigma}$ are the density operators for the $f$ and conduction electrons at site $i$ with spin $\sigma$. In the following we will
set $t = 1$ and consider the case at half filling ($E^c = 0$).

The important thing to notice in Eq. (1) is that, unlike the usual periodic Anderson model, the local $f$-site parameters $V_i$ or $E_{fi}$ are taken here to be random numbers (static, uncorrelated disorder) distributed according to uniform distributions $P_1(V_i)$ or $P_2(E_{fi})$, respectively. Namely,

$$P_1(V_i) = \frac{1}{2\Delta} \Theta(\Delta - |V_i - V_0|).$$  \hspace{1cm} (2)$$

$$P_2(E_{fi}) = \frac{1}{2\Delta} \Theta(\Delta - |E_{fi} - E_{f0}|).$$  \hspace{1cm} (3)$$

Here, $2\Delta$ denotes the width of the uniform distribution for each type of disorder, and $V_0$ and $E_{f0}$ are the average values of $V_i$ and and $E_{fi}$, respectively. We set $E_{f0} = -U_f/2$ (symmetric case in the absence of disorder) and $V_0 = U_f = 1$ (intermediate parameter regime). In the intermediate coupling regime Monte Carlo simulations provide essentially exact results, whereas analytic approaches are most likely to fail or are inaccurate.

We have employed a finite-temperature quantum Monte Carlo technique with an exact updating procedure. \textsuperscript{18} \textsuperscript{19} The calculated physical observables of the finite disordered system depend strongly on the particular realization of the disorder. Therefore, we have to average all quantities over a sufficient number of disorder realizations and calculate the averaged expectation values,

$$\langle \langle A \rangle \rangle_V = \int_{-\infty}^{+\infty} \prod dV_i P_1(V_i) \langle \hat{A} \rangle(\{V_i\}),$$  \hspace{1cm} (4)$$

for the case of disorder in hybridization or

$$\langle \langle A \rangle \rangle_E = \int_{-\infty}^{+\infty} \prod dE_{fi} P_2(E_{fi}) \langle \hat{A} \rangle(\{E_{fi}\}),$$  \hspace{1cm} (5)$$

for the case of disorder in the local $E_f$ energy level. Here, $\langle \hat{A} \rangle$ denotes the thermal expectation value of the operator $\hat{A}$ for a given disorder configuration, which is calculated using the grand-canonical quantum Monte Carlo method developed by Fye. \textsuperscript{20} We have carried out simulations on an eight-site chain and $\beta = \frac{1}{T} \leq 8$. We have made several checks for sixteen-site chains. The calculated results for the magnetic moment, the uniform $f$ susceptibility,
and the correlations functions agree with those of the 8-site calculations within the QMC statistical errors. This is due to the fact that the calculated observables are local and the size effects are quite small. For the case of the uniform $f$ susceptibility the main contribution arises from the local on-site $f-f$ contribution.

The distribution of tasks (disorder realizations) and the subsequent averaging procedure over disorder configurations was carried out in an IBM SP2 parallel machine using the Message-Passing Interface (MPI). We found that the statistical error is within 5% when the number of disorder configurations is above thirty. Thus, the measured quantities were averaged over thirty different disorder configurations.

In the present study we present results of the effect of the two different kinds of disorder on the following observables: (i) The square of the $f$-orbital local moment $\sigma$,

$$\sigma = \frac{1}{N} \sum_i \langle \langle (n_{i\uparrow}^f - n_{i\downarrow}^f)^2 \rangle \rangle,$$  

where $N$ is the total number of lattice sites; (ii) The static $f$ component of the uniform magnetic susceptibility $\chi_f$,

$$\chi_f = \frac{1}{N} \sum_{i,j} \int_0^\beta d\tau \langle \langle [n_{i\uparrow}^f(\tau) - n_{i\downarrow}^f(\tau)] [n_{j\uparrow}^f(0) - n_{j\downarrow}^f(0)] \rangle \rangle;$$  

(iii) The charge compressibility $\kappa$,

$$\kappa = \frac{1}{N} \sum_{i,j} \int_0^\beta d\tau \{ \langle \langle [n_{i\uparrow}^f(\tau) + n_{i\downarrow}^f(\tau)] [n_{j\uparrow}^f(0) + n_{j\downarrow}^f(0)] \rangle \rangle \} - \langle \langle n_{i\uparrow}^f + n_{i\downarrow}^f \rangle \rangle \langle \langle n_{j\uparrow}^f + n_{j\downarrow}^f \rangle \rangle;$$  

and (iv) The nearest-neighbor magnetic correlation function $C(i, i + 1)$,

$$C(i, j) = \langle \langle [n_{i\uparrow}^f - n_{i\downarrow}^f] [n_{j\uparrow}^f - n_{j\downarrow}^f] \rangle \rangle,$$  

with $j = i + 1$.

In the absence of disorder, the ground state of the one-dimensional PAM exhibits short-range magnetic correlations; the local $f$-electron spin moments are compensated by correlations with those of other $f$-electrons, as well as with those of the conduction electrons leading to a nonmagnetic ground state. The charge gap in the PAM is due to hybridization in
the absence of the Coulomb interaction $U_f$ and is due to the on-site Coulomb interaction when $U_f$ is larger than the band width of the conduction electrons, since the $f$-electron decouples from the conduction electrons. \[21\] For the parameter set used in this work the single-impurity Kondo temperature ($T_K \approx 0.182U[8\Delta\pi U]^{1/2}e^{-\frac{8\Delta}{\pi U}}$) is $T_K/t = 0.096$ and the Kondo gap ($\Delta_K \approx T_ke^{1/2\rho J}$) \[22\] is $\Delta_K/t = 0.21$.

We first present results for the case of disorder in hybridization which couples the $f$-orbital and the conduction electrons. In Fig.1 we plot the impurity magnetic moment $\sigma$, the susceptibility $T\chi_f$, the charge compressibility $T\kappa$, and the nearest-neighbor spin correlation function $C(i, i+1)$ as a function of the disorder width $\Delta$ at low temperatures, $\beta = 8$. We find that the average of the square of the $f$-orbital local magnetic moment, $\sigma$, increases as the disorder width $\Delta$ increases. This result shows that the number of the unquenched local spins at low temperatures increases with disorder. Similarly, the low-temperature magnetic susceptibility $T\chi_f$, which measures the “effective” magnetic moment, increases with increasing disorder width. The low value of the effective moment for $\Delta = 0$ at low temperatures indicates that the magnetic correlations act to screen the $f$-site moment leading to a singlet ground state. Turning on the disorder in hybridization results in a destruction of the singlet ground-state and a reduction of the spin gap between the singlet ground state and the lowest lying excited triplet state. \[21\] Fig. 1 shows also that the nearest-neighbor spin correlation function $C(i, i+1)$ increases monotonically with $\Delta$. These short-range $f$-$f$ antiferromagnetic correlations have been found to be as important as the $f$-$c$ correlations in the formation of the singlet state in the PAM. \[16,20\] Consistent with the above results, we find that increase of disorder in hybridization tends to suppress these short-range antiferromagnetic $f$-$f$ correlations, resulting in non-compensated $f$ moments. On the other hand, the charge compressibility $T\kappa$, shown also in Fig. 1, is almost unchanged by disorder in hybridization. This suggests that the charge gap might be due to correlation effects rather than hybridization effects.

In order to gain further insight into the effect of the hybridization-disorder on the magnetic properties of the $f$-electrons, we present in Fig. 2 the $f$ magnetic susceptibility $\chi_f$ as a
function of temperature for $\Delta = 0$ (PAM) and $\Delta = 1$. In agreement with a previous study for the PAM ($\Delta = 0$), we find that as the temperature is lowered $\chi_f$ saturates to a constant value. On the other hand, the total uniform magnetic susceptibility which contains both the $f$ and the conduction electron components goes to zero due to the presence of the spin gap. This Fermi liquid behaviour in the absence of disorder signals the compensation of the $f$ moment by the antiferromagnetic $f - f$ spin correlations in addition to the already-present Kondo-like fluctuations from the antiferromagnetic $c - f$ screening correlations. On the other hand, in the presence of disorder, $\chi_f$ exhibits a non-Fermi-liquid behaviour, diverging at low temperatures. We find that $\chi_f$ can be scaled at low temperatures by a power law, $\chi_f \sim T^{-\gamma}$, with the exponent $\gamma = 0.66$, which is comparable to recent experimental results. This result might be interpreted that the hybridization-disorder causes some of the local $f$ sites to possess low Kondo temperatures and consequently to behave as nearly free magnetic moments, leading to a NFL behaviour.

We next present results for the effect of disorder in the $f$-electron energy level, $E_f$, on the magnetic properties. In Fig. 3 we show the impurity local magnetic moment $\sigma$, the magnetic susceptibility $T\chi_f$, the charge compressibility $T\kappa$, and the nearest-neighbor $f - f$ spin correlation function $C(i, i+1)$ as a function of the $f$-energy-level disorder width $\Delta$ at temperature $T/t = 1/8$. Note, that the range of $\Delta$ values in Fig. 3 is larger than that in Fig. 1. In the weak-disorder regime, $\Delta/t \leq 1$, all quantities are almost unchanged by the disorder in $E_f$, in contrast to the corresponding results shown in Fig. 1 for the case of hybridization in $V$. This is due to the fact that the majority of the $f$ sites are occupied, since the average $f$-electron energy level is below the Fermi energy ($E^f_0 = -U/2$). On the other hand, in the strong-disorder regime, $\Delta/t > 1$, some of the local $f$-energy levels are distributed above the Fermi energy as $\Delta$ increases further. This in turn causes the average local magnetic moment $\sigma$ to decrease with $\Delta$ because some of the $f$-orbitals become empty. The “effective moment” $T\chi_f$ increases slightly with $\Delta$, indicating that even though a few diluted $f$ spins cease to contribute to the compensation state, the singlet ground state is not destroyed. The nearest-neighbor spin correlation function $C(i, i+1)$ is suppressed because
some of the effective $f$-electron orbitals are diluted by disorder. The low-temperature charge compressibility $\kappa$ increases with the disorder width in the strong-disorder regime. Strong disorder in the distribution of the $E_f$'s leads to a reduction of the charge gap and hence an increase of $\kappa$.

In conclusion, we have studied the effect of two kinds of disorder on the magnetic properties of the one-dimensional PAM using quantum Monte Carlo simulations. We find that disorder in hybridization modifies considerably the low-temperature properties due to the presence of unquenched local moments. The low-temperature susceptibility exhibits a NFL behaviour which is found to diverge with a power law with an exponent in agreement with experiment. On the other hand, disorder in the $f$-site energy level results in a conventional Fermi liquid behaviour.

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FIGURES

FIG. 1. The square of the $f$-orbital local moment $\sigma$ (open squares), the $f$ magnetic susceptibility $T\chi_f$ (solid squares), the charge susceptibility $T\kappa$ (solid triangles) and the nearest-neighbor $f-f$ spin correlation function $C(i,i+1)$ (open triangles) as a function of the hybridization-disorder width $\Delta$ at temperature $T/t = 1/8$ with $U_f/t = 1$ and $V/t = 1$. 
FIG. 2. The uniform $f$ magnetic susceptibility as a function of temperature for the hybridization-disorder width $\Delta = 0$ (triangles) and $\Delta = 1$ (circles) for $U_f/t = 1$ and $V/t = 1$. For $(T/t \leq 1)$, $\chi_f$ can be scaled by the power law, $\chi_f \sim T^{-\gamma}$, with $\gamma = 0.66$. 
FIG. 3. The square of the \( f \)-orbital local moment \( \sigma \) (open squares), the \( f \) magnetic susceptibility \( T\chi_f \) (solid squares), the charge susceptibility \( T\kappa \) (sold triangles) and the nearest-neighbor \( f-f \) spin correlation function \( C(i, i+1) \) (open triangles) as a function of the \( f \)-energy-level disorder width \( \Delta \) at temperature \( T/t = 1/8 \) with \( U_f/t = 1 \) and \( V/t = 1 \).