Ferromagnetism and Kondo Insulator Behavior in the Disordered Periodic Anderson Model

Unjong Yu\textsuperscript{1}, Krzysztof Byczuk\textsuperscript{1,2}, and Dieter Vollhardt\textsuperscript{1}

\textsuperscript{1}Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany

\textsuperscript{2}Institute of Theoretical Physics, University of Warsaw, ul. Hoża 69, 00-681 Warszawa, Poland

(Dated: February 4, 2008)

The effect of binary alloy disorder on the ferromagnetic phases of \textit{f}-electron materials is studied within the periodic Anderson model. We find that disorder in the conduction band can drastically enhance the Curie temperature \(T_c\) due to an increase of the local \(f\)-moment. The effect may be explained qualitatively and even quantitatively by a simple theoretical \textit{ansatz}. The emergence of an alloy Kondo insulator at non-integer filling is also pointed out.

PACS numbers: 71.23.-k, 75.20.Hr, 75.30.Mb

Materials with \textit{f}-electrons such as the rare earths (e.g., cerium) or actinides (e.g., uranium) exhibit a wealth of highly unusual thermodynamic, magnetic and transport properties \cite{1}. The minimal microscopic model that can account for this diverse physical behavior is the periodic Anderson model (PAM) which describes a band of non-interacting electrons hybridizing with localized, interacting \textit{f}-electrons \cite{2}. Depending on the position of the \textit{f}-electron energy \(\varepsilon_i^f\) relative to the conducting band, and on the strength of the hybridization \(V\) and the local Coulomb interaction \(U\), the PAM is able to reproduce heavy fermion, intermediate valence, and local moment behavior. In the local moment regime and for large \(U\) the PAM reduces to the so called Kondo lattice model, which may be employed as an effective model for manganites exhibiting colossal magnetoresistance \cite{3}, or for diluted magnetic semiconductors which show promise for applications in spintronics \cite{4}. At low enough temperatures the PAM also describes magnetically ordered phases. While antiferromagnetic order is well-known to occur close to half-filling \cite{4}, ferromagnetic solutions are found far away from half-filling \cite{5}. Indeed, ferromagnetism has been observed in various \textit{f}-compounds \cite{4}.

Alloys of \textit{f}-electron materials also display intriguing properties. For example, by changing the stoichiometric composition of Ce(Pt\(_{1-x}\)Ni\(_x\))\(_2\)Si\(_2\) the systems can be tuned from the local moment regime at \(x = 0\) to the intermediate valence regime at \(x = 1\) \cite{6}. Alloying inevitably introduces disorder into the system. In general, disorder is expected to reduce the tendency towards ferromagnetic long-range order of the \textit{f}-electrons and thus lower the Curie temperature \(T_c\). On the other hand, in certain cases disorder is even known to improve the stability of ferromagnetism. For example, disorder in the conduction electron band caused by the substitution of Rh by Co in URh\(_{1-x}\)Co\(_x\)Ge leads to a maximum in \(T_c\) at \(x \approx 0.6\) \cite{8}. Similarly, a maximum in \(T_c\) is observed in CeCu\(_2\)Si\(_2-x\)Ge\(_x\) at \(x \approx 1.5\) which may be attributed to an enhanced exchange interaction between the \textit{f}-electron moments induced by the diffusive motion of the Cu electrons \cite{9}. Finally, alloying Ce with La as in (Ce\(_{1-x}\)La\(_x\))\(_3\)Bi\(_4\)Pt\(_3\) introduces disorder into the \textit{f}-electron system, which can trigger a transition from a Kondo insulator to a dirty metal \cite{10}. Clearly disorder is an important feature of many \textit{f}-electron alloys and must therefore be included in any comprehensive theoretical study of such compounds.

Previous investigations of the disordered PAM focussed, in particular, on the effect of nonmagnetic impurities on the heavy Fermi liquid or the Kondo insulating state \cite{11}, and on the disorder-driven non-Fermi liquid behavior in Kondo alloys \cite{12}. Grenzebach \textit{et al.} \cite{13} recently presented a detailed study of transport properties of the disordered PAM within the dynamical mean-field theory (DMFT) \cite{14} together with a thorough discussion of the development of the field. The effect of disorder in the \textit{f}-electrons on the ferromagnetic phase was investigated by Meyer \cite{15}, who found that the Curie temperature is always reduced.

In this Letter we report results of a detailed study of ferromagnetism in the PAM in the presence of alloy disorder. In particular, we show that \(T_c\) can be substantially enhanced by disorder in the \textit{conduction electrons}. We also predict Kondo insulator behavior away from half-filling at particular values of the alloy concentration. Quite generally, the Hamiltonian of the PAM in the presence of local disorder has the form

\begin{equation}
H = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i,\sigma} \left( \varepsilon_i^f f_{i\sigma}^{\dagger} f_{i\sigma} + \varepsilon_i^c c_{i\sigma}^{\dagger} c_{i\sigma} \right) + \sum_{i,\sigma} \left( V c_{i\sigma}^{\dagger} f_{i\sigma} + V^* f_{i\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow},
\end{equation}

where \(c_{i\sigma}^{\dagger} (c_{i\sigma})\) and \(f_{i\sigma}^{\dagger} (f_{i\sigma})\) are creation (annihilation) operators of conduction \((c)\) and localized \((f)\) electrons with spin \(\sigma\) at a lattice site \(i\). Here the on-site energies \(\varepsilon_i^f\) and \(\varepsilon_i^c\) are random variables and \(V\) is the local hybridization between \(f\)- and \(c\)-electrons. The hopping amplitude of the \(c\)-electrons is given by \(t_{ij}\). The Coulomb interaction \(U\) acts only between \(f\)-electrons on the same
The local self-energies appear in the physics described by the PAM it is instructive to investigate the case of the non-interacting bath electrons, with the lattice Green function, i.e., the averaged local Green function (4) to be the same as the function (3) depends on the same for all random variables \( \eta_{\sigma} \) is a natural parameter for the \( -\)electron system.

The function \( \eta_{\sigma} \) describes an effective dynamical hybridization of the c-electrons with the bath. It is the same for all random variables \( \{ y_i \} \) and is determined by the self-consistency equations to be discussed below. We start with the local matrix Green function

\[
G_{\sigma}^{\text{loc}}(\tau; \{ y_i \}) = \sum_{\sigma_n} \left( \begin{array}{cc} T_{++} f_{\sigma}(\tau) f_{\sigma}^\dagger(0) & T_{+,c}(\tau) c_{\sigma}^\dagger(0) \\ T_{c,\sigma}(\tau) c_{\sigma}^\dagger(0) & T_{cc,\sigma}(\tau) c_{\sigma}^\dagger(0) \end{array} \right),
\]

where \( T_{+} \) is the time-ordering operator. Since the Green function (3) depends on \( \{ y_i \} \) it is a random function. Here we perform arithmetic averaging, i.e., the averaged Green function is given by

\[
G_{\sigma}^{\text{loc}} = \int \prod_{\{ y_i \}} dy_i P(y_i) G_{\sigma}^{\text{loc}}(\tau; \{ y_i \}).
\]

In the absence of interactions one then obtains the results of the well-known coherent potential approximation (CPA) \([\text{17}]\). Effects of Anderson localization are neglected in this case but can be incorporated by employing the geometric average \([\text{18}]\). The self-consistency requires the averaged local Green function (4) to be the same as the lattice Green function, i.e.,

\[
G_{\sigma} = \sum_k \left( \begin{array}{cc} i\omega_n + \mu - \Sigma_{\sigma}^f & V^* \\ V & i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma}^c \end{array} \right)^{-1}.
\]

The local self-energies appear in the \( k \)-integrated Dyson equation \( \Sigma_{\sigma} = G_{\sigma}^{-1} - G_{\sigma} \), where \( G_{\sigma} \) is the local Green function of the non-interacting bath electrons, with

\[
G_{\sigma}^{-1} = \left( \begin{array}{cc} i\omega_n + \mu - \epsilon_0 & V^* \\ V & i\omega_n + \mu - \epsilon_0 - \eta_{\sigma} \end{array} \right).
\]

Eqs. (2-6) form a general, closed set of equations, which determine all local, dynamical correlation functions of the disordered PAM.

To understand the effect of alloy disorder on the physics described by the PAM it is instructive to investigate the case \( U = 0 \) first, since alloy disorder affects a hybridized two-band system in several interesting ways. To this end we consider the disorder to act only on the c-electrons or the f-electrons, respectively. In the case of c-electron disorder the diagonal elements of the local Green function (4) are given by

\[
G_{cc}^{\text{loc}} = \frac{x}{(G_{cc}^{\text{loc}})^{-1} - |V|^2 G_{ff}^{\text{loc}}} + \frac{1-x}{(G_{cc}^{\text{loc}})^{-1} - |V|^2 G_{ff}^{\text{loc}}} - \Delta^c,
\]

\[
G_{ff}^{\text{loc}} = \frac{x}{(G_{ff}^{\text{loc}})^{-1} - |V|^2 G_{cc}^{\text{loc}}} + \frac{1-x}{(G_{ff}^{\text{loc}})^{-1} - |V|^2 G_{cc}^{\text{loc}}}.
\]

The case of f-electron disorder is obtained by exchanging \( f \leftrightarrow c \) in Eq. (7). Large energy splitting \( \Delta^c \) leads to a band splitting of the conduction electrons as in the single band model \([\text{10}]\), i.e., each alloy subband contains \( 2N_L \) and \( 2(1-x)N_L \) states, respectively, where \( N_L \) is the number of lattice sites. At the same time, the f-level does not split. Altogether the alloy with hybridized c- and f-electrons can therefore be a band insulator even for total densities different from integer values (2 or 4) \([\text{19}]\).

We now include the interaction \( U \) between the f-electrons and investigate its influence on the alloy subbands. The effective two-orbital impurity problem in the presence of disorder, Eqs. (20), is solved by finite temperature determinant quantum Monte-Carlo (QMC) simulations. Ferromagnetic instabilities are detected by the divergence of the static spin susceptibility and by a non-vanishing value of the magnetization \([\text{20}]\). In the numerical examples presented below the DOS for the non-interacting c-electrons has the model form \( N_0(\varepsilon) = \sqrt{4 - \varepsilon^2/2\pi} \), where the energy unit is \( t = 1 \). In the following we fix the interaction and the hybridization at \( U = 1.5 \) and \( V = 0.6 \), respectively, and include disorder either in the f-electron or c-electron system.

As shown in Fig. (11) the computed Curie temperature for the transition to the ferromagnetic state is a non-monotonic function of the alloy concentration \( x \). In par-
ticular, the behavior is quite different for disorder acting on the \( f \)- or the \( c \)-electrons.

**\( f \)-electron disorder:** In agreement with Meyer \[13\] the presence of \( f \)-electron disorder always reduces the Curie temperature relative to its non-disordered values at \( x = 0 \) or 1. For strong enough disorder \( T_c \) eventually vanishes, e.g., at \( x = 0.28 \) and \( x = 0.75 \), respectively, for \( \Delta' = 1.7 \) (left panel of Fig. 1). This is due to the splitting of the \( f \)-electron band at large \( \Delta' \) which increases the double occupation of the lower alloy subband; this reduces the local moment of the \( f \)-electrons and thereby \( T_c \).

**\( c \)-electron disorder:** By contrast, \( c \)-electron disorder leads to a much more subtle dependence of \( T_c \) on concentration \( x \). Namely, for increasing energy splitting \( \Delta^c \) there are, in general, three different features observed, the physical origin of which will be discussed in more detail later: (i) at \( x = 1 \), i.e., in the non-disordered case, \( T_c \) is reduced; (ii) a minimum develops in \( T_c \) at \( x = n_{\text{tot}} - 1 > 0 \); (iii) \( T_c \) is enhanced over its non-disordered values at \( x = 0 \) or 1. Altogether this leads to a global maximum in \( T_c \) vs. \( x \). While the decrease of \( T_c \) at \( x = 1 \) is a simple consequence of the reduction of the energy difference between the \( f \)-level and the \( c \)-electron band, \( \varepsilon^c - \varepsilon^f = \varepsilon^c - \varepsilon^f_0 - \Delta^c \), for increasing \( \Delta^c \), the latter effects are more subtle.

To understand the minimum in \( T_c \) vs. \( x \) we computed the evolution of the spectral functions \( N^c(\omega) \) at \( x = 0.3 \) for \( \Delta^c \) increasing from 0 to 6 (Fig. 2). There is an opening of a gap at the chemical potential signalling a metal-insulator transition in this system. This is caused by the splitting of the \( c \)-electron band due to binary alloy disorder and the correlations between the \( f \)-electrons. Namely, for energy splittings \( \Delta^c \) much larger than the width of the \( c \)-electron band the total number of available low-energy states is reduced from \( 4N_L \) to \( 4 - 2(1 - x)N_L = 2(1 + x)N_L \), whereby the filling effectively increases by a factor of \( 4/(2(1 + x)) \), such that \( n_{\text{eff}} = 2n_{\text{tot}}/(1 + x) \), if \( n_{\text{tot}} < 2(1 + x) \). For the filling \( n_{\text{tot}} = 1.3 \) studied in the Figs. 1 and 2 the concentration \( x = 0.3 \) is a special case since then \( n_{\text{eff}} = 2 \). The system is then effectively at half-filling and behaves as a Kondo insulator at large \( U \), \( \Delta^c \), and low temperatures. In particular, itinerant ferromagnetism is unfavorable in this case, i.e., \( T_c \) \( = 0 \) in the vicinity of \( x = 0.3 \) at \( \Delta^c = 2 \), cf. Fig. 1. The metal to Kondo insulator transition at non-integral filling in the PAM predicted here is a counterpart of the Mott-Hubbard metal to insulator transition at non-integral fillings in the one-band Hubbard model found in \[13\] and \[21\].

We now turn to the maximum in \( T_c \) vs. \( x \). It can be understood within the following model based on an \textit{ansatz} for the Curie temperature, \( T_c(U, V, \mu) = T_c^0(U, V, \mu) + F^c(\mu - \varepsilon^c_0) \) or \( F^f(\mu - \varepsilon^f_0) \), which implies that the formation of local \( f \)-electron moments \( (F^f) \) is assumed to be independent from the \( c \)-electron mediated ordering of these moments \( (F^c) \). In fact, for the RKKY model this \textit{ansatz} can be microscopically justified within a static mean-field theory \[22\]. The two functions \( F^c \), \( F^f \) are determined by \( T_c \) calculated within DMFT for the non-disordered case at fixed \( \mu - \varepsilon^c_0 \) or \( \mu - \varepsilon^f_0 \) respectively; they are shown in Fig. 3(a) and 3(b) for one set of parameters. The prefactor \( T_c^0 \) is determined by the requirement that the dimensionless functions \( F^f \) and \( F^c \) be equal to one at their maxima. We note that \( F^f(\mu - \varepsilon^f_0) \) has a maximum when the \( f \)-level is half-filled (\( \mu = \varepsilon^f_0 + U/2 \)), i.e., when the local moment is maximal.

The Curie temperature in the presence of \( c \)-electron disorder can now be estimated by averaging over the \( c \)-electron part, \( F^c \), giving rise to the disorder-dependent function \( F^c(x, \mu - \varepsilon^c_0) = [x F^c(\mu - \varepsilon^c_0 + \Delta^c) + (1 - x) F^c(\mu - \varepsilon^c_0 - \Delta^c)] / (x + (1 - x)) \).

![FIG. 1: Curie temperature \( T_c \) as a function of alloy concentration \( x \) and energy splitting \( \Delta^f \) (left column) and \( \Delta^c \) (right column) for \( n_{\text{tot}} = 1.3 \) and \( \varepsilon^c_0 - \varepsilon^f_0 = 3.25 \). Strong \( c \)-electron disorder enhances \( T_c \) compared to its values at \( x = 0 \) or 1.](image)

![FIG. 2: Spectral function of \( c \)-electrons for different \( \Delta^c \) at \( x = 0.3 \) (other parameters as in Fig. 1) obtained within QMC and maximal entropy at \( T = 1/60 \). By increasing \( \Delta^c \) a pseudogap opens which becomes a real gap for \( T \to 0 \).](image)
The linear dependence on the alloy concentration can again be justified microscopically within a static mean-field theory for the RKKY model, where $T_c$ depends linearly on the DOS at the chemical potential $\Delta^c = 0$. $T_c$ is now determined for each concentration $x$. We calculate $\mu$, which is an implicit function of $x$, in the non-hybridized limit ($V = 0$) within a rigid band approximation [23]. The dependence of the resulting functions $F^c(x, \mu - \epsilon_0^c)$ and $F^f(\mu - \epsilon_0^f)$ on $x$ are shown in Fig. 3(c). By contrast, $F^c(x, \mu - \epsilon_0^c)$ is characterized by a wide minimum, related to the formation of the pseudogap in the interacting DOS seen in Fig. 2. This minimum reaches zero, i.e., $F^c(x, \mu - \epsilon_0^c) = 0$, for a finite range of $x$ values as shown in Fig. 3(c). The resulting $T_c(x)$ obtained by the product of these two functions agrees remarkably well with the numerical result obtained by DMFT as shown in Fig. 3(d).

In conclusion, the interplay between the disorder induced splitting of the conduction band and many-body correlations among the $f$-electrons can lead to a remarkable enhancement of the Curie temperature in the periodic Anderson model. There are two competing effects determining $T_c$ as the alloy concentration $x$ is decreased from $x = 1$: (i) a rise due to an increase of the local moment, and (ii) a decrease due to the opening of a gap in the alloy Kondo insulator at non-integer filling. Altogether this leads to a global maximum in $T_c$ vs. $x$. Therefore experimental investigations of $f$-electron materials with alloy disorder in the conducting band are expected to be particularly rewarding.

This work was supported in part by the Sonderforschungsbereich 484 of the Deutsche Forschungsgemeinschaft (DFG).

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Approximating the chemical potential by $\mu = x\mu_{x=1} + (1-x)\mu_{x=0}$, leads to qualitatively similar results as long as $\Delta^c$ is smaller than the band width.