Ferromagnetism and disorder: A dynamical mean-field study

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Abstract

We investigate ferromagnetism in the periodic Anderson model with diagonal disorder. Using dynamical mean-field theory in combination with the modified perturbation theory, the disorder can be included in the calculation consistently, which turns out to be equivalent to the CPA method. Disorder generally reduces the Curie temperature and can for certain configurations completely suppress ferromagnetic order. This can be ascribed to the enhanced quasiparticle damping and the special structure of the density of states.

PACS 71.10.Fd, 71.28+d, 75.30.Md

Keywords

Periodic Anderson Model, Ferromagnetism, Disorder, Dynamical Mean-Field Theory

The investigation of models for strongly correlated electron systems has made significant progress in recent years due to the introduction of the dynamical mean-field theory \[1, 2\] which is based on the non-trivial limit of infinite spatial dimensions \[3, 4\]. In this limit, the lattice self-energy becomes wave-vector independent and the problem can be mapped onto a single-site problem \[5\]. Many questions concerning strongly correlated electron systems such as the Mott-Hubbard metal-insulator transition could be answered by this approach \[3, 4\]. Also important insight into the physics of band-ferromagnetism could be gained \[5\].

The treatment of disorder also simplifies in the limit of infinite spatial dimensions \[10\]: The well-known CPA method \[11\], which has to be seen as the best single-site approximation for solving disorder problems \[12\], becomes exact here.

As first shown by Ulmke et al. \[13\], the dynamical mean-field theory therefore allows to investigate the interplay of disorder and strong electron correlations by taking into account both problems on the same level of approximation (see also \[14, 15, 16\]).

In this paper we want to focus on the influence of disorder on band-ferromagnetism, in particular the ferromagnetic phase of the periodic Anderson model in the intermediate-valence regime \[17, 18, 19\]. The periodic Anderson model is defined by its Hamiltonian:

\[
H = \sum_{\vec{k},\sigma} \epsilon(\vec{k}) s^\dagger_{\vec{k}\sigma} s_{\vec{k}\sigma} + V \sum_{i,\sigma} (f^\dagger_{i\sigma} s_{i\sigma} + s^\dagger_{i\sigma} f_{i\sigma}) + \\
+ \sum_{i,\sigma} \epsilon_{f} f^\dagger_{i\sigma} f_{i\sigma} + \frac{1}{2} U \sum_{i,\sigma} n_{i\sigma} n_{i\sigma}^\dagger
\]

Here, \( s^\dagger_{\vec{k}\sigma} \) (\( f^\dagger_{i\sigma} \)) and \( s_{\vec{k}\sigma} \) (\( f_{i\sigma} \)) are the creation and annihilation operators for a conduction electron with Bloch vector \( \vec{k} \) and spin \( \sigma \) (a localized electron on site \( i \) and spin \( \sigma \)) and \( n_{i\sigma}^\dagger = f^\dagger_{i\sigma} f_{i\sigma} \) (\( s^\dagger_{\vec{k}\sigma} = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k}\vec{R}_i} s_{\vec{k}\sigma} \)). The dispersion of the conduction band is \( \epsilon(\vec{k}) \) and \( \epsilon_{f} \) is the position of the localized level. The hybridization strength \( V \) is taken to be \( \vec{k} \)-independent, and finally \( U \) is the on-site Coulomb interaction strength between two \( f \)-electrons. Throughout this paper, the conduction band will be described by a free (Bloch) density of states, \( \rho_0(E) = \frac{1}{W} \sum_{\vec{k}} \delta(E - \epsilon(\vec{k})) \), of semi-elliptic shape. Its width \( W = 1 \) sets the energy scale, and its center of gravity the energy zero: \( T_{ii} = \frac{1}{W} \sum_{\vec{k}} \epsilon(\vec{k})^\dagger \epsilon(\vec{k}) \approx 0 \). To obtain the single-electron Green’s function for this model, we apply dynamical mean-field theory (DMFT) in combination with the modified perturbation theory (MPT) \[20\] to solve the associated impurity problem. The DMFT approach becomes exact for \( Z \to \infty \) (\( Z \) being the coordination number) and
represents a well-defined local approximation for finite dimensions (finite $Z$). The DMFT-MPT approach recovers the high-energy features of the Green’s function up to order $(1/Z)$. Furthermore, its low-energy behavior is at least qualitatively correct. The investigation of ferromagnetism in the Hubbard model \cite{21, 22} as well as the Mott-Hubbard transition \cite{3, 23} have shown that this method is able to predict qualitatively correct phenomena of strongly correlated systems. Numerical results are obtained using a standard DMFT algorithm which basically consists of a self-consistency loop as follows: Starting with an initial guess for the self-energy for the lattice, the conduction electron bath of an associated impurity problem is defined using the self-consistency equation \cite{3}. Then this impurity problem is solved by some means, and its self-energy extracted. The latter is then taken to be the lattice self-energy and a new impurity model is defined via the self-consistency equation. This loop is iterated until self-consistency is achieved. More details on practical calculations can be found in \cite{2, 24}.

Next we need to specify how the impurity model is solved. For this we employ the modified perturbation theory. This method is based on the following ansatz for the self-energy \cite{25, 26}:

$$\Sigma_{\sigma}(E) = U n_{\sigma}^{(f)} + \frac{\alpha_{\sigma} \Sigma_{\sigma}^{(SOC)}(E)}{1 - \beta_{\sigma} \Sigma_{\sigma}(E)} \tag{2}$$

$\alpha_{\sigma}$ and $\beta_{\sigma}$ are introduced as parameters to be determined later. $\Sigma_{\sigma}^{(SOC)}(E)$ is the second-order contribution to perturbation theory around the Hartree-Fock solution \cite{27}. Equation (2) can be understood as the simplest possible ansatz which can, on the one hand, reproduce the perturbational result in the limit $U \to 0$, and, on the other hand, recovers the atomic limit for appropriately chosen $\alpha_{\sigma}$ and $\beta_{\sigma}$ \cite{23}.

Using the perturbation theory around the Hartree-Fock solution introduces an ambiguity into the calculation. Within the self-consistent Hartree-Fock calculation, one can either choose the chemical potential to be equivalent to the chemical potential of the full MPT calculation, or take it as parameter $\tilde{\mu}$ to be fitted to another physically motivated constraint. In reference \cite{23}, the Luttinger theorem \cite{28}, or equivalently the Friedel sum rule \cite{28, 30}, was used to determine $\tilde{\mu}$. As discussed in Ref. \cite{17}, we use the physically motivated condition of identical impurity occupation numbers for the Hartree-Fock and the full calculation ($n_{\sigma}^{(f, HF)} = n_{\sigma}^{(f)}$) to determine $\tilde{\mu}$, which also allows for a consistent extension of the method to finite temperatures \cite{31, 14}. Except for symmetric parameters this will lead to an approximate fulfillment of the Luttinger theorem only \cite{20}. Bearing in mind that for disordered systems, the Luttinger theorem does not apply, this should not be a decisive disadvantage for this study. A more detailed analysis of the different possibilities to determine $\tilde{\mu}$ is found in reference \cite{12} where the DMFT-MPT was applied to the single-band Hubbard model. Finally, the parameters $\alpha_{\sigma}$ and $\beta_{\sigma}$ have to be determined. Instead of using the “atomic” limit of $V = 0$ as was done for example in references \cite{22, 23, 26}, we make use of the moments of the spectral density. This procedure is described in detail in references \cite{32, 20}. The result not only fulfills the $V = 0$ limit, but also recovers the high-energy behavior of the Green’s function up to the order $(1/Z)$.

The results concerning ferromagnetism in the periodic Anderson model have been discussed elsewhere \cite{7, 8, 22}. For the following it is important to note that in the intermediate-valence regime, more precisely for $-W/2 \lesssim \epsilon_{i} \lesssim -W/4$, a ferromagnetic solution with finite $T_c$ exists for a range of electron densities. The $T = 0$ phase diagram is plotted in Fig. 1. In this area of the phase diagram, the ferromagnetic solution shows typical features of a band-ferromagnet \cite{33, 3}. The origin of the ferromagnetic order lies in the competition of kinetic and potential energy. Ferromagnetic order is stabilized by high values of the density of states (DOS) close to the lower band edge. The electron density needs to be chosen that the chemical potential lies in this region of large DOS. So although Stoner’s theory \cite{24} does not capture the right physics, his criterion for the occurrence of

![Figure 1: Zero-temperature phase diagram for the periodic Anderson model without disorder from $\text{[17]}$. $U = 4$ and $V = 0.2$. In the shaded region, the system is ferromagnetic, elsewhere paramagnetic.](image-url)
band-ferromagnetism ($U\rho(\mu) \gg 1$) turns out to remain valid [3, 13].

Let us now turn to the problem of disorder. A general extension of model [3] to include diagonal (on-site) disorder is

$$H \to H + H^{\text{dis}}$$

$$H^{\text{dis}} = \sum_{i,\sigma} \Delta V_i (f_{i\sigma}^\dagger n_{i\sigma} + n_{i\sigma}^\dagger f_{i\sigma}) +$$

$$+ \sum_{i,\sigma} \Delta \epsilon_i f_{i\sigma}^\dagger f_{i\sigma} + \frac{1}{2} \sum_{i,\sigma} \Delta U_i n_{i\sigma}^{(f)} n_{i-\sigma}^{(f)}$$

(4)

In this model, the $f$-electron energy ($\epsilon_f$), the on-site hybridization ($V$) and the interaction strength ($U$) can deviate from the value denoted before by $\Delta \epsilon_i, \Delta V_i$ and $\Delta U_i$, respectively. The distribution for each of these quantities can be defined by a probability distribution function $P(\Delta \epsilon_{f,i})$, $P(\Delta V_i)$ and $P(\Delta U_i)$.

A standard method to solve electron systems with disorder is the well-known coherent potential approximation (CPA) [11]. This method is considered the best single-site approximation and at least for one-particle properties, has proven to be remarkably successful [11]. It is known to become exact in a number of limiting cases, namely for small impurity concentration, small potential strengths, vanishing inter-site hopping, and as discussed by [23] also for $Z^{-1}$. This last limiting case suggests that CPA results could be obtained by an alternative (DMFT-like) algorithm employing a mapping onto an impurity model. This was shown to be the case [13], and allows for a systematic extension to include many-body interactions, which would be not possible within the standard CPA procedure [13, 30]. One has to bear in mind, however, that single-site approximations such as the one described here do have some limitations. A major limitation in regards to disorder is the inability to describe inhomogeneous, phase-separated systems which are discussed in the context of manganites [33].

To calculate the single-electron Green function for a (diagonally) disordered system using DMFT, the algorithm described above for pure systems needs to be modified in the following way: Instead of one, several impurity models need to be solved, one for each possible on-site configuration of the lattice model. The configurational averaging is then performed on the results for these impurity models, and the averaged self-energy extracted and taken as lattice self-energy. This self-energy is fed into the self-consistency equation to determine a new impurity bath function. This cycle is then iterated until self-consistency is obtained [13, 30].

In the following, we want to present and discuss numerical results for the periodic Anderson model with diagonal disorder. For simplicity, we have set all $\Delta U_i = 0$ and $\Delta V_i = 0$, including only disorder with respect to the $f$-level energy $\epsilon_f$. We further restrict ourselves to binary alloys, i.e. $P(\Delta \epsilon_{f,i}) = p\delta(\Delta \epsilon_f) + (1-p)\delta(0)$. The in general rather complex definition of the disorder is reduced to two parameters: the difference of $f$-level positions of the two components $\Delta \epsilon_f$, and the concentration $p$.

To examine the influence of disorder on ferromagnetic order, we investigate two different scenarios using this simple model of disorder: Selecting $U$, $V$ and the electron density $n^{(\text{tot})}$ so that a ferromagnetic solution is possible for a range of values of $\epsilon_f$, we can choose $\epsilon_f$ and $\Delta \epsilon_f$ so that one of the two alloy components would in a pure system be ferromagnetic, and the other not. We have taken $\epsilon_f = -0.4$ and $\Delta \epsilon_f = 0.2$. These parameters for the two alloy components are indicated in the phase diagram (Fig. 1) as solid circles. The other scenario corresponds to alloying two differ-

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2}
\caption{Curie temperatures for the PAM with disorder for $U = 4$, $n^{(\text{tot})} = 1.3$, $V = 0.2$. The $\epsilon_f$ and the disorder parameters are explained in the text.}
\end{figure}
ent ferromagnetic materials. It is realized by using $\epsilon_f = -0.5 \text{ and } \Delta \epsilon_f = 0.2$. The resulting components are shown by the crosses in Fig. 2. In Fig. 3 we have plotted the Curie temperature as function of $p$. As one would expect, $T_c$ decreases with increasing $p$, in the beginning linearly, and around $p \approx 0.28$, rather suddenly. With $p \gtrsim 0.29$, the system is paramagnetic already for $T = 0$.

The second scenario reveals more unexpected behaviour. For $p = 0$ as well as for $p = 1$ (corresponding to the two crosses in Fig. 3) the system is ferromagnetic and has finite $T_c$. In between these two pure limits, we find a strong reduction of the Curie temperature. Around $p \approx 0.7$, $T_c$ even becomes zero and the system is then paramagnetic. The reduction of $T_c$ can be ascribed to the additional quasiparticle damping induced by the disorder. This effect of quasiparticle damping was already noticed in previous studies investigating the role of quasiparticle damping in the Hubbard model [27] and in the PAM [18]. The cited works did not involve disorder, but tested the influence of quasiparticle damping by comparing different approximation schemes some of which neglected quasiparticle damping completely. A similar reduction of $T_c$ due to disorder was also found for a ferromagnetic Kondo-lattice model with classical spins [16].

To display the enhanced quasiparticle damping due to disorder, we have performed calculations for a weakly interacting ($U = 0.2$), paramagnetic system. In Fig. 3 the resulting $f$-density of states is plotted together with the imaginary part of the self-energy. These two quantities were calculated for $p = 0$, $p = 0.5$ and $p = 1$. Except for the smaller value of $U$, all other parameters were taken as in the lower panel of Fig. 2. For both pure situations, the self-energy vanishes quadratically at the Fermi energy which is indicated by the respective thin vertical line (note: the chemical potential is shifted by varying $p$ since we keep the total electron density $n^{(\text{tot})}$ constant). In the alloyed compound, the imaginary part of the self-energy remains finite at the Fermi energy. And over a large energy range it is strongly enhanced compared to the pure limits. This strong disorder-induced quasiparticle damping is independent of the interaction strength, and can have a suppressing effect on ferromagnetism [16].

Another effect is complementing the quasiparticle damping as mechanism to completely suppress ferromagnetism as seen in Fig. 2. As already mentioned before, the occurrence of band-ferromagnetism is linked to a Stoner-like criterion requiring a large density of states at or close to the Fermi energy [13, 20]. For both pure cases ($p = 0$ and $p = 1$), the Fermi energy lies within the charge excitation peak in the density of states as can be seen from Fig. 3 for the small $U$ case. In the disordered case, however, the structure of the DOS is dominated not by one, but two charge excitation peaks. The positions of these are given by the respective charge excitations in the pure limits. For intermediate values of $p$ ($p \approx 0.5$), the Fermi energy lies in between these two peaks, and the value of the density of states at this energy is relatively low. This should therefore reduce the tendency towards ferromagnetism. The special structure of the DOS for intermediate $p$ leads therefore to further suppression of ferromagnetism. Whether (and for which $p$) $T_c$ really vanishes, or not, now critically depends on the position of the Fermi energy, and therefore on the electron density.

To summarize, we have performed dynamical mean-field theory calculations for a periodic Anderson model (PAM) with disorder. The inclusion of disorder into these calculations follows a relatively simple and straightforward recipe [13, 28]. Our numerical analysis shows how even small amounts of disorder can reduce the Curie temperature of a ferromagnetically ordered PAM in the intermediate-valence regime significantly.
Stronger disorder can lead to a complete suppression of the ferromagnetic phase, even for a binary alloy of two ferromagnetically ordered components.

Acknowledgements
The author wants to thank K. Byczuk for introducing me to this topic, and D. Edwards, A. Hewson and W. Nolting for pleasant and helpful discussions.

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