Ferromagnetism and Metal-Insulator Transition in the Disordered Hubbard Model

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A detailed study of the paramagnetic to ferromagnetic phase transition in the one-band Hubbard model in the presence of binary alloy disorder is presented. The influence of the disorder (with concentration \( x \) and \( 1-x \) of the two alloy ions) on the Curie temperature \( T_c \) is found to depend strongly on electron density \( n \). While at high densities, \( n > x \), the disorder always reduces \( T_c \), at low densities, \( n < x \), the disorder can even enhance \( T_c \) if the interaction is strong enough. At the particular density \( n = x \) (i.e. not necessarily at half filling) the interplay between disorder-induced band splitting and correlation induced Mott transition gives rise to a new type of metal-insulator transition.

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In correlated electron materials it is a rule rather than an exception that the electrons, apart from strong interactions, are also subject to disorder. The disorder may result from non-stoichiometric composition, as obtained, for example, by doping of manganites \((La_{1-x}Sr_xMnO_3)\) and cuprates \((La_{1-x}Sr_xCuO_4)\) [1], or in the disulfides \(Co_{1-x}Fe_xS_2\) and \(Ni_{1-x}Co_xS_2\) [2]. In the first two examples, the Sr ions create different potentials in their vicinity which affect the correlated \( d \) electrons/holes. In the second set of examples, two different transition metal ions are located at random positions, creating two different atomic levels for the correlated \( d \) electrons. In both cases the random positions of different ions break the translational invariance of the lattice, and the number of \( d \) electrons/holes varies. As the composition changes so does the randomness, with \( x = 0 \) or \( x = 1 \) corresponding to the pure cases. With changing composition the system can undergo various phase transitions. For example, \( FeS_2 \) is a pure band insulator which becomes a disordered metal when alloyed with \( CoS_2 \), resulting in \( Co_{1-x}Fe_xS_2 \). This system has a ferromagnetic ground state for a wide range of \( x \) with a maximal Curie temperature \( T_{C} \) of 120 K. On the other hand, when \( CoS_2 \) (a metallic ferromagnet) is alloyed with \( NiS_2 \) to make \( Ni_{1-x}Co_xS_2 \), the Curie temperature is suppressed and the end compound \( NiS_2 \) is a Mott-Hubbard antiferromagnetic insulator with Néel temperature \( T_N = 40 \) K.

Our theoretical understanding of systems with strong interactions and disorder is far from complete. For example, it was realized only recently that in gapless fermionic systems the soft modes couple to order parameter fluctuations, leading to different critical behavior in the pure and the disordered cases [3]. A powerful method for theoretical studies of strongly correlated electron systems is the dynamical mean-field theory (DMFT) [4, 5, 6]. The DMFT is a comprehensive, conserving, and thermodynamically consistent approximation scheme which emerged from the infinite dimensional limit of fermionic lattice models [7]. During the last ten years the DMFT has been extensively employed to study the properties of correlated electronic lattice models. Recently the combination of DMFT with conventional electron structure theory in the local density approximation (LDA) has provided a novel computational tool, LDA+DMFT [8, 9], for the realistic investigation of materials with strongly correlated electrons, e.g. itinerant ferromagnets [10].

The interplay between local disorder and electronic correlations can also be investigated within DMFT [11, 12, 13, 14, 15]. Although effects due to coherent backscattering cannot be studied in this way [1], since the disorder is treated on the level of the coherent potential approximation [1], there are still important physical effects remaining. In particular, electron localization, and a disorder-induced metal-insulator transition (MIT), can be caused by alloy-band splitting. In the present paper we study the influence of disorder on the ferromagnetic phase. We will show that in a correlated system with binary-alloy disorder the Curie temperature depends non-trivially on the band filling. In the disordered one-band Hubbard model we find that for a certain band filling (density) \( n = N_e/N_o \), where \( N_e \) (\( N_o \)) is the number of electrons (lattice sites), disorder can weakly increase the Curie temperature provided the interaction is strong enough. A simple physical argument for this behavior is presented. We also find that at special band fillings \( n \neq 1 \) the system can undergo a new type of Mott-Hubbard MIT upon increase of disorder and/or interaction.

In the following we will study itinerant electron ferromagnetism in disordered systems, modeled by the Anderson-Hubbard Hamiltonian with on-site disorder

\[
H = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i\sigma} \epsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}
\]
where \( t_{ij} \) is the hopping matrix element and \( U \) is the local Coulomb interaction. The disorder is represented by the ionic energies \( \epsilon_i \), which are random variables. We consider binary alloy disorder where the ionic energy is distributed according to the probability density \( P(\epsilon) = x6(\epsilon + \Delta/2) + (1 - x)3(\epsilon - \Delta/2) \). Here \( \Delta \) is the energy difference between the two ionic energies, providing a measure of the disorder strength, while \( x \) and \( 1 - x \) are the concentrations of the two alloy ions. For \( \Delta \gg B \), where \( B \) is the band-width, it is known that binary alloy disorder causes a band splitting in every dimension \( d \geq 1 \), with the number of states in each alloy subband equal to \( 2xN_0 \) and \( 2(1 - x)N_0 \), respectively [14].

We solve (1) within DMFT. The local nature of the theory implies that short-range order in position space is missing. However, all dynamical correlations due to the local interaction are fully taken into account.

In the DMFT scheme the local Green function \( G^{\sigma}_{\alpha n} \) is given by the bare density of states (DOS) \( N^0(\epsilon) \) and the local self-energy \( \Sigma_{\alpha n} \) as \( G^{\sigma}_{\alpha n} = \int d\epsilon N^0(\epsilon)/(\imath \omega_n + \mu - \Sigma_{\alpha n} - \epsilon) \). Here the subscript \( n \) refers to the Matsubara frequency \( \omega_n = \imath(2n + 1)\pi/\beta \) for the temperature \( T \), with \( \beta = 1/k_BT \), and \( \mu \) is the chemical potential. Within DMFT the local Green function \( G^{\sigma}_{\alpha n} \) is determined self-consistently by

\[
G^{\sigma}_{\alpha n} = -\left( \int \frac{D[c_\sigma, c_\sigma^*]}{D[c_\sigma, c_\sigma^*]} c_\sigma^* G^{-1}_{\alpha n} c_\sigma \right) \ , \quad (2)
\]

together with the \( k \)-integrated Dyson equation \( G^{-1}_{\alpha n} = G^{\sigma}_{\alpha n} + \Sigma_{\alpha n} \). The single-site action \( A_i \) for a site with the ionic energy \( \epsilon_i = \pm \Delta/2 \) has the form

\[
A_i(c_\sigma, c_\sigma^*, \delta G_{\alpha n}^{-1}) = \sum_{n, \sigma} c_\sigma^* \delta G^{-1}_{\alpha n} c_\sigma - \epsilon_i \sum_\sigma \int_0^\beta d\tau n_\sigma(\tau) \delta G_{\alpha n}(\tau) - U \sum_\sigma \int_0^\beta d\tau c_\sigma(\tau) c_\sigma^*(\tau) c_{\sigma - \sigma}(\tau), \quad (3)
\]

where we used a mixed time/frequency convention for Grassmann variables \( c_\sigma, c_\sigma^* \). Averages over the disorder are obtained by \( \langle \cdots \rangle_{\text{dis}} = \int d\epsilon P(\epsilon) \langle \cdots \rangle \).

Since an asymmetric DOS is known to stabilize ferromagnetism in the one-band Hubbard model for moderate values of \( U \) [17, 18, 19] we use the DOS of the fcc-lattice in infinite dimensions, \( N^0(\epsilon) = \exp[-(1 + \sqrt{2}\epsilon)/2] / \sqrt{\pi(1 + \sqrt{2}\epsilon)} \) [24]. This DOS has a square root singularity at \( \epsilon = -1/\sqrt{2} \) and vanishes exponentially for \( \epsilon \to \infty \). In the following the second moment of the DOS, \( W \), is used as the energy scale and is normalized to unity [21]. The one-particle Green function in Eq. (2) is determined by solving the DMFT equations iteratively [17, 18] using Quantum Monte-Carlo (QMC) simulations [24]. Curie temperatures are obtained by the divergence of the homogeneous magnetic susceptibility [17, 23].

We find a striking difference in the dependence of the Curie temperature \( T_c \) on disorder strength \( \Delta \) for different band fillings \( n < x \) and \( n > x \) (we chose \( x = 0.5 \) for numerical calculations). At \( n = 0.7 \), the critical temperature \( T_c(\Delta) \) decreases with \( \Delta \) for all values of \( U \) and eventually vanishes at sufficiently large disorder [Fig. 1(a)]. By contrast, at \( n = 0.3 \), \( T_c(\Delta) \) weakly decreases with \( \Delta \) at small \( U \), but increases with \( \Delta \) at large values of \( U \) [Fig. 1(b)].

As will be explained below, this striking difference originates from three distinct features of interacting electrons in the presence of binary alloy disorder:

i) The disorder leads to a reduction of the Curie temperature \( T_c \) in the pure case, depends non-monotonically on band filling \( n \) (here \( x = 0.5 \) for numerical calculations). At \( n = 0.7 \), the critical temperature \( T_c(\Delta) \) decreases with \( \Delta \) for all values of \( U \) and eventually vanishes at sufficiently large disorder [Fig. 1(a)]. By contrast, at \( n = 0.3 \), \( T_c(\Delta) \) weakly decreases with \( \Delta \) at small \( U \), but increases with \( \Delta \) at large values of \( U \) [Fig. 1(b)].

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To illustrate the alloy band splitting in the presence of strong interactions discussed above [see (ii)] we calculate the spectral density from the QMC results by the maximal entropy method. The results in Fig. 3 show the evolution of the spectral density in the paramagnetic phase at $U = 4$ and $n = 0.3$. At $\Delta = 0$ the lower and upper Hubbard subbands can be clearly identified. The quasiparticle resonance is merged with the lower Hubbard subband due to the low filling of the band, and is reduced by the finite temperature. At $\Delta > 0$ the lower and upper alloy subbands begin to split off. A similar behavior was found at $n = 0.7$. The separation of the alloy subbands in the correlated electron system for increasing $\Delta$ is one of the preconditions [cf. (ii)] for the enhancement of $T_c$ by disorder when $n < x$, as discussed above.

The splitting of the alloy subbands and, as a result, the changing of the band filling in the effective Hubbard model implies that $T_c$ vanishes for $n > x$. Namely, in the ferromagnetic ground state each of the alloy subbands can accommodate only $xN_a$ and $(1-x)N_a$ electrons, respectively. Therefore, if the ground state of the system were ferromagnetic the upper alloy subband would be partially occupied for all $n > x$. This would, however, increase the energy of the system by $\Delta$ per particle in the upper alloy subband. Therefore, in the $\Delta \gg U$ limit the paramagnetic ground state is energetically favorable. This explains why $T_c$ vanishes at $n = 0.7$, as found in our QMC simulations [Fig. 2(a)]. Our conclusion that $T_c$ vanishes for $n_{\text{eff}} = n/x > 1$ when $\Delta \gg W$ is consistent with the observation in [7] that there is no ferromagnetism for $n > 1$ in the Hubbard model without disorder on fcc-lattice in infinite dimensions.

The filling $n = x$ is very particular because a new MIT of the Mott-Hubbard type occurs. Namely, when $\Delta$ increases (at $U = 0$), the non-interacting band splits, leaving $2xN_a$ states in the lower and $2(1-x)N_a$ states in the upper alloy subband. Effectively, it means that at $n = x$ the lower alloy subband is half filled ($n_{\text{eff}} = 1$). Consequently, a Mott-Hubbard MIT occurs in the lower alloy subband at sufficiently large interaction $U$. In fact, for $\Delta \gg U$ we may infer a critical value $U_c = 1.47W^*$ at $T = 0$ from the results of Refs. [27–28], where $W^*$ is the renormalized bandwidth of the lower alloy subband. Furthermore, from the analogy of this MIT with that in the pure case [22] we can expect a discontinuous transition for $T \lesssim T^* \approx 0.02W^*$, and a smooth crossover for $T \gtrsim T^*$. From the results shown in Fig. 2 it follows that $T^* < 0.071$, since for $T = 0.071$ and $U = 6$ a gap-like structure develops in the spectrum at $\Delta \approx 1.6$, implying a smooth but rapid crossover from a metallic to an insulator-like phase [8].

The MIT described above is not obscured by the onset of antiferromagnetic long-range order because in infinite dimensions the fcc-lattice is completely frustrated [20]. Hence the insulator is paramagnetic. The transition therefore occurs between a paramagnetic insulator (PI) at high $T$ and a ferromagnetic metal (FM) at low $T_c$ at least at large $U$, as shown in the inset of Fig. 2. The actual boundary between the paramagnetic metal (PM) and the paramagnetic insulator-like phase has not yet been determined. The thick line in the inset of Fig. 2 indicates the approximate position of the phase boundary between the PM and PI phases. We note that at the
of the Deutsche Forschungsgemeinschaft. von Humboldt-Foundation (KB), and through SFB 484 work was supported by a Fellowship of the Alexander sions, and to G. Keller for computer assistance. This rammeters over a wide range as was recently shown to be of these effects requires good control of the system pa-

Circles: parameter values (∆, T) changes. In summary, we showed within DMFT that the inter-

play between binary-alloy disorder and electronic corre-

lation can result in unexpected effects, such as the en-

hancement of the transition temperature Tc for itiner-

ant ferromagnetism by disorder, and the occurrence of a Mott-Hubbard gap-like structure develops around the Fermi level. Inset: ∆−T phase diagram of the binary alloy Hubbard model on the fcc-lattice in infinite dimensions at U = 6; PM - paramagnetic metal, PI - paramagnetic insulator-like phase, FM - ferromagnetic metal. Points with error bars represent the Curie temperatures obtained from QMC simulations; the solid line is a guide for the eye only. The thick line indicates the phase boundary between the PM and PI phases (see text). Point where this boundary meets the FM phase the slope of the transition line Tc(∆) changes.

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