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 concentrations \(x\) 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 nonstoichiometric composition, as obtained, for example, by doping of manganites (La\(_{1-x}\)Sr\(_x\)MnO\(_3\)) and cuprates (La\(_{1-x}\)Sr\(_x\)CuO\(_4\)) [1], or in the disulfides Co\(_{1-x}\)Fe\(_x\)S\(_2\) and Ni\(_{1-x}\)Co\(_x\)S\(_2\) [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\(_x\)S\(_2\). 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\(_x\)S\(_2\), 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) [4–6]. 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 [11–15]. Although effects due to coherent backscattering cannot be studied in this way [11], since the disorder is treated on the level of the coherent potential approximation [16], 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 this Letter we study the influence of disorder on the ferromagnetic phase. We show that in a correlated system with binary-alloy disorder the Curie temperature depends nontrivially 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

\[
H = \sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} \epsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{1}
\]
where $t_{ij}$ is the hopping matrix element and $U$ is the local Coulomb interaction. The disorder is represented by the ion energies $\epsilon_i$, which are random variables. We consider binary-alloy disorder where the ionic energy is distributed according to the probability density $P(\epsilon) = x\delta(\epsilon + \Delta/2) + (1 - x)\delta(\epsilon - \Delta/2)$. 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 bandwidth, 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 $2nx_{\text{Na}}$ and $2(1 - x)N_{\text{Na}}$, respectively [16].

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

$$G_{\alpha\gamma} = -\left\{ \frac{\int D[c_{\alpha}, c_{\alpha}^*)] \delta[c_{\alpha}, c_{\alpha}] \mathcal{A}_i[c_{\alpha}, c_{\alpha}^*, G_{\alpha\gamma}^{-1}] \right\}_{\text{dis}},$$

(2)

together with the k-integrated Dyson equation $G_{\alpha\gamma}^{-1} = G_{\alpha\gamma}^{-1} + \Sigma_{\alpha\gamma}$. The single-site action $\mathcal{A}_i$ for a site with the ionic energy $\epsilon_i = \pm \Delta/2$ has the form

$$\mathcal{A}_i[c_{\alpha}, c_{\alpha}^*, G_{\alpha\gamma}^{-1}] = \sum_{n,\sigma} c_{\alpha n}^* G_{\alpha\gamma}^{-1} c_{\alpha n} - \epsilon_i \sum_{\sigma} \int_0^\beta d\tau n_{\sigma}(\tau) - U/2 \sum_{\sigma} \int_0^\beta d\tau c_{\sigma}^*(\tau)c_{\sigma}(\tau)c_{-\sigma}(\tau)c_{-\sigma}(\tau).$$

(3)

electrons occupy only the lower alloy subband while the upper subband is empty. Effectively, one can therefore describe this system by a Hubbard model mapped onto the lower alloy subband. Hence, it corresponds to a single band with the effective filling $n_{\text{eff}} = n/x$. It is then possible to determine $T_c$ from the phase diagram of the Hubbard model without disorder [17].

(iii) The disorder leads to a reduction of $T_c^0(n_{\text{eff}})$ by a factor $x$; i.e., we find

$$T_c(n) = xT_c^0(n/x)$$

(4)

when $\Delta \gg W$ [24]. Hence, as illustrated in Fig. 2, $T_c$ can be determined by $T_c^0(n_{\text{eff}})$. Surprisingly, then, it follows that, if $U$ is sufficiently strong, the Curie temperature of a disordered system can be higher than that of the corresponding pure system (cf. Fig. 2).

**FIG. 1.** Curie temperature $T_c$ as a function of disorder strength $\Delta$ for band filling $n$ larger (a) and smaller (b) than the ionic concentration $x$ (here $x = 0.5$). (a) $n = 0.7$, $U = 2$, 4, and 6; (b) $n = 0.3$, $U = 2$, 3, 4, 5, and 6 ($U$ increases from bottom to top). Note the different range of $\Delta$ in both figures.
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 maximum entropy method (MEM). 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 splitting of the alloy subbands and, as a result, the changing of the band filling in the effective Hubbard model imply 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. 1(a)]. Our conclusion that $T_c$ vanishes for $n_{\text{eff}} = n/x > 1$ when $\Delta \gg W$ is consistent with the observation in [17] 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 noninteracting band splits, leaving $2xN_a$ states in the lower and $2(1 - x)N_a$ states in the upper alloy subbands. 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 $U$ [25]. In fact, for $\Delta \gg U$ we may infer a critical value $U_c = 1.47W^*$ at $T = 0$ from the results of Refs. [26,27], where $W^*$ is the renormalized bandwidth of the lower alloy subband. Furthermore, from the analogy of this MIT with that in the pure case [28] we can expect a discontinuous transition for $T \leq T' = 0.02W^*$, and a smooth crossover for $T \geq T'$. From the results shown in Fig. 4 it follows that $T' < 0.071$, since for $T = 0.071$ and $U = 6$ a gaplike structure develops in the spectrum at $\Delta = 1.7$, implying a smooth but rapid crossover from a metallic to an insulatorlike phase [29]. Indeed, as the gap opens, the form of the self-energy changes into $\Sigma_{\text{eff}} \sim 1/(i\omega_n)$ which is characteristic for an insulator [4].

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 actual boundary between the paramagnetic metal (PM) and the paramagnetic insulatorlike phase (PI) has not yet been determined. The thick line in the inset of Fig. 4 indicates the approximate position of the phase boundary between the PM and PI phases. A ferromagnetic polarization exists only in the metallic phase.

In summary, we showed within DMFT that the interplay between binary-alloy disorder and electronic correlation can result in unexpected effects, such as the enhancement of the transition temperature $T_c$ for itinerant ferromagnetism by disorder, and the occurrence of a Mott-Hubbard type MIT off half filling. An observation
FIG. 4. Spectral density for disorder strengths $\Delta = 0, 1, 1.6,$ and $1.8$ (dotted, dashed, long-dashed, and solid curves, respectively) at $n = 0.5$ and $U = 6$ as obtained by MEM from QMC data at $T = 0.071$ with Trotter slice $\Delta \tau = 0.125$. For $\Delta \approx 1.7$ a Mott-Hubbard gaplike structure develops around the Fermi level. Inset: $\Delta - T$ 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). Circles: parameter values ($\Delta, T$) corresponding to the spectral densities shown in the main panel.

of these effects requires good control of the system parameters over a wide range as was recently shown to be possible in experiments with optical lattices [30].

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[21] Exponential tails in the DOS prohibit the formation of a genuine disorder and/or correlation induced gap in the spectrum. However, a “soft gap,” where the spectrum vanishes at a single point, is permitted.
[24] Equation (4) can be derived within Hartree-Fock theory. We find it to be valid even at strong interactions.
[25] The same holds true when $n = 1 + x$, i.e., when the upper alloy subband is half filled.
[29] We are currently investigating this transition scenario at $T = 0$ using the numerical renormalization group. [K. Byczuk, W. Hofstetter, and D. Vollhardt (unpublished)].