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 ($La_{1-x}Sr_xMnO_3$) 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) [4–6]. 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) $n = N_e/N_a$, where N_e (N_a) 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

$$H = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i\sigma} \epsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \qquad (1)$$

where t_{ij} is the hopping matrix element and U is the local Coulomb interaction. The disorder is represented by the ionic energies ϵ_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 Δ 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 $2xN_a$ and $2(1-x)N_a$, 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 $G_{\sigma n}$ is given by the bare density of states (DOS) $N^0(\epsilon)$ and the local self-energy $\Sigma_{\sigma n}$ as $G_{\sigma n} = \int d\epsilon N^0(\epsilon)/(i\omega_n + \mu - \Sigma_{\sigma n} - \epsilon)$. 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 μ is the chemical potential. Within DMFT the local Green function $G_{\sigma n}$ is determined self-consistently by

$$G_{\sigma n} = -\left\langle \frac{\int D[c_\sigma, c_\sigma^\star] c_{\sigma n} c_{\sigma n}^\star e^{\mathcal{A}_i\{c_\sigma, c_\sigma^\star, \mathcal{G}_\sigma^{-1}\}}}{\int D[c_\sigma, c_\sigma^\star] e^{\mathcal{A}_i\{c_\sigma, c_\sigma^\star, \mathcal{G}_\sigma^{-1}\}}} \right\rangle_{\text{dis}}, \qquad (2)$$

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

$$\mathcal{A}_i\{c_\sigma, c_\sigma^\star, \mathcal{G}_\sigma^{-1}\} = \sum_{n,\sigma} c_{\sigma n}^\star \mathcal{G}_{\sigma n}^{-1} c_{\sigma n} - \epsilon_i \sum_\sigma \int_0^\beta d\tau n_\sigma(\tau) - \frac{U}{2}\sum_\sigma \int_0^\beta d\tau c_\sigma^*(\tau) c_\sigma(\tau) c_{-\sigma}^*(\tau) c_{-\sigma}(\tau), \qquad (3)$$

where we used a mixed time/frequency convention for Grassmann variables c_σ, $c_\sigma^\star$. In the presence of binary-alloy disorder the single impurity problem has to be solved twice in each self-consistency loop. Averages over the disorder are obtained by $\langle \cdots \rangle_{\text{dis}} = \int d\epsilon P(\epsilon)(\cdots)$.

Since an asymmetric DOS is known to stabilize ferromagnetism in the one-band Hubbard model for moderate values of U [17–19], we use the DOS of the fcc lattice in infinite dimensions, $N^0(\epsilon) = \exp[-(1+\sqrt{2}\epsilon)/2]/\sqrt{\pi(1+\sqrt{2}\epsilon)}$ [20]. 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 [22]. 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 Δ 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 Δ 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 Δ at small U, but *increases* with Δ 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) $T_c^{\text{p}} \equiv T_c(\Delta = 0)$, the Curie temperature in the pure case, depends nonmonotonically on band filling n. Namely, $T_c^{\text{p}}(n)$ has a maximum at some filling $n = n^*(U)$, which increases as U is increased [17]; see Fig. 2.

(ii) In the alloy disordered system the band is split [16] when $\Delta \gg W$. As a consequence, for $n < 2x$ and $T \ll \Delta$ 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 $T_c^{\text{p}}(n_{\text{eff}})$ by a factor x; i.e., we find

$$T_c(n) \approx x T_c^{\text{p}}(n/x) \qquad (4)$$

when $\Delta \gg W$ [24]. Hence, as illustrated in Fig. 2, T_c can be determined by $T_c^{\text{p}}(n_{\text{eff}})$. 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).

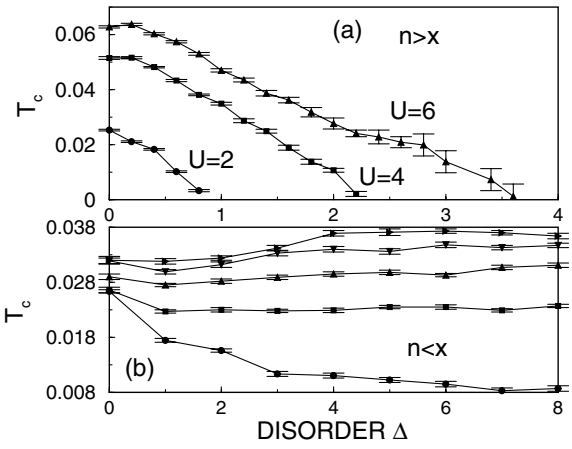

FIG. 1. Curie temperature T_c as a function of disorder strength Δ for band filling n larger (a) and smaller (b) than the ionic concentration x (here $x = 0.5$): (a) $n = 0.7$, $U = 2$, 4, and 6; (b) $n = 0.3$, $U = 2$, 3, 4, 5, and 6 (U increases from bottom to top). Note the different range of Δ in both figures.

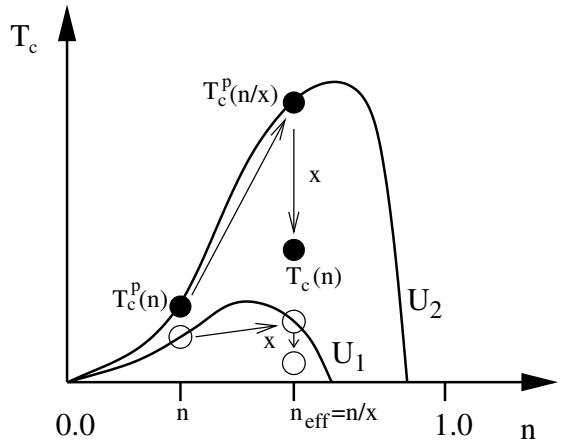

FIG. 2. Schematic plot explaining the filling dependence of T_c for interacting electrons with strong binary alloy disorder. Curves represent T_c^{p}, the Curie temperature for the pure system, as a function of filling n at two different interactions $U_1 \ll U_2$ (cf. [17]). For $n \lesssim x$, T_c of the disordered system can be obtained by transforming the open (for U_1) and the filled (for U_2) point from n to n_{eff}, and then multiplying $T_c^{\mathrm{p}}(n/x)$ by x as indicated by arrows. One finds $T_c(n) < T_c^{\mathrm{p}}(n)$ for U_1, but $T_c(n) > T_c^{\mathrm{p}}(n)$ for U_2. This difference originates from the nonmonotonic dependence of T_c^{p} on n.

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

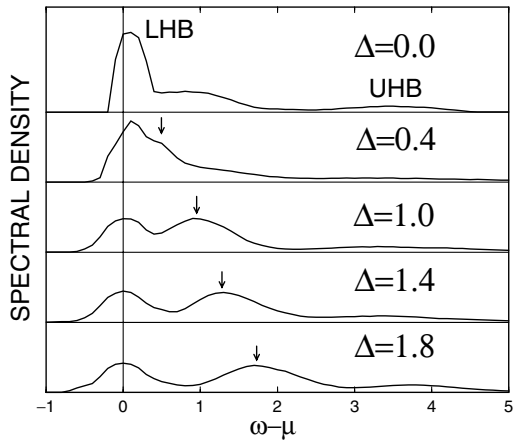

FIG. 3. Spectral density for different disorder strengths Δ at $n = 0.3$ and $U = 4$ as obtained by MEM from QMC data at $T = 0.071$. The position of the lower/upper Hubbard subbands (LHB/UHB) are almost unaffected by the disorder, while the upper alloy subband shifts to the right as indicated by arrows.

the correlated electron system for increasing Δ 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 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 Δ 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 $n_{\mathrm{eff}} = n/x > 1$ 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 Δ 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 ($n_{\mathrm{eff}} = 1$). 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 $T \lesssim T^* \approx 0.02W^*$, and a smooth crossover for $T \gtrsim T^*$. 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 $\Delta \approx 1.7$, 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 $\Sigma_{\sigma n} \sim 1/(i\omega_n)$ 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

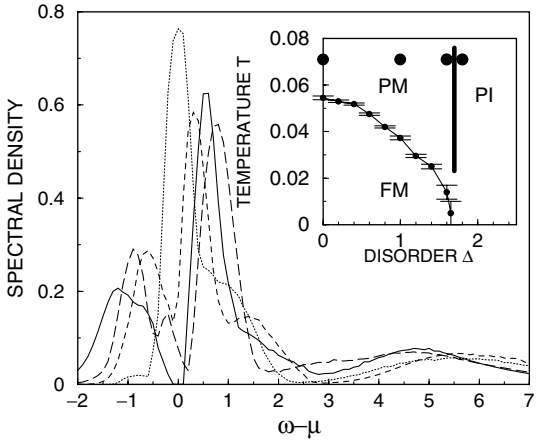

FIG. 4. Spectral density for disorder strengths $\Delta = 0$, 1, 1.6, and 1.8 (dotted, dashed, long-dashed, and solid curves, respectively) at $n = 0.5$ and $U = 6$ as obtained by MEM from QMC data at $T = 0.071$ with Trotter slice $\Delta\tau = 0.125$. For $\Delta \gtrsim 1.7$ a Mott-Hubbard gaplike 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 insulatorlike 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 (Δ, 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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