

Ferromagnetism in the large- U Hubbard model

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We study the Hubbard model on a hypercubic lattice with regard to the possibility of itinerant ferromagnetism. Dynamical mean-field theory is used to map the lattice model on an effective local problem, which is treated with the help of the noncrossing approximation. By investigating spin-dependent one-particle Green's functions and the magnetic susceptibility, a region with nonvanishing ferromagnetic polarization is found in the limit $U \rightarrow \infty$. The δ - T phase diagram as well as thermodynamic quantities are discussed. The dependence of the Curie temperature on the Coulomb interaction and the competition between ferromagnetism and antiferromagnetism are studied in the large- U limit of the Hubbard model. [S0163-1829(97)51338-5]

The microscopic description of ferromagnetism in narrow-band metals like Fe, Ni, Co, and others is one of the most interesting problems in solid state physics. Since the electrons in these systems are mobile one cannot use localized-spin models with effective interactions like, e.g., the Heisenberg model, but has to take into account this itinerancy together with the electron-electron interaction on a more fundamental level. The first model set up to describe such a system is the Hubbard model¹

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

However, it was realized relatively early that the Hubbard model rather seems to be a generic model for antiferromagnetism² and a correlation driven metal-insulator transition instead. Just these properties made it an early and rather successful candidate for the description of the high- T_c compounds.³

Nevertheless the question about ferromagnetism in the Hubbard model was never abandoned, since one of the few rigorous theorems about this model definitely proves its existence. In 1965 Nagaoka showed that for $U = \infty$ and one hole doped into the half-filled band the state with a fully polarized background is the ground state for several lattice structures due to a gain of kinetic energy for the hole.⁴ This theorem initiated a large amount of work on questions like the stability of the Nagaoka state with respect to doping δ , finite U , etc.⁵ Moreover, even after 30 years of research the situation appears to be rather controversial, especially for bipartite lattices: One obtains critical dopings in the range δ_c from 0 to 0.3, depending on the method used.^{6,7} Only for the infinite dimensional hypercubic lattice the situation seems to be clear: The work by Fazekas *et al.* suggests that the Nagaoka state is unstable for any finite doping,^{8,9} unless explicitly favored by long-range Coulomb interactions¹⁰ or band structure effects.¹¹

Most of the above studies are based on a variational ansatz and are thus restricted to the Nagaoka—i.e., fully polarized—state and its stability as the ground state. There is still the possibility of partially polarized ferromagnetism and in any case the necessity to calculate T_c as function of δ and U

etc. Generally speaking the question to what extent ferromagnetism is a generic feature of the Hubbard model or not is still unanswered.

In this paper we discuss the magnetic phase diagram of the Hubbard model on a hypercubic lattice for large Coulomb repulsion U . In the latter limit the ground-state and low-energy properties of the model are well captured by a t - J model with an effective antiferromagnetic exchange $J = 2t^2/U$.¹² To solve the t - J model or, more precisely, the underlying Hubbard model at $U = \infty$ we use the dynamical mean field theory (DMFT).¹³ This theory leads to purely local dynamical renormalizations of one-particle properties, which can be obtained from an effective impurity problem coupled to a self-consistent medium.^{14,15}

In addition to the one-particle properties the DMFT also allows us to calculate two-particle correlation functions and thermodynamic quantities consistently.^{16,17} Especially in the limit of large U one obtains¹⁷

$$\chi_F^U(T) = \chi_F^\infty(T) \left/ \left(1 + 2d \frac{2t^2}{U} \chi_F^\infty(T) \right) \right. \quad (2)$$

and

$$\chi_{AF}^U(T) = \chi_{AF}^\infty(T) \left/ \left(1 - 2d \frac{2t^2}{U} \chi_{AF}^\infty(T) \right) \right. \quad (3)$$

for the homogeneous $[\chi_F^U(T)]$ and staggered $[\chi_{AF}^U(T)]$ susceptibilities of the Hubbard model, respectively. The quantity $\chi_\alpha^\infty(T)$ denotes the susceptibility for $U = \infty$ and d is the spatial dimension of the system. These expressions allow us to discuss the influence of finite U once the $\chi_\alpha^\infty(T)$ are known.

In the following we use $4dt^2 = 1$ as an energy unit. With this choice the bare density of states for the hypercubic lattice is of Gaussian form for large d : $\rho_0(\varepsilon) = 1/\sqrt{\pi} \exp(-\varepsilon^2)$. The effective impurity problem of the DMFT is solved within the NCA (Refs. 18 and 19) and for $U = \infty$ we furthermore do the calculations with spin-dependent quantities to explicitly look at the properties in the symmetry-broken phase. An extension of these calculations to finite U is extremely tedious and studies along this line are in progress.²⁰

We begin the discussion of our results with the case $U = \infty$. Figure 1 shows the inverse susceptibility (homogeneous

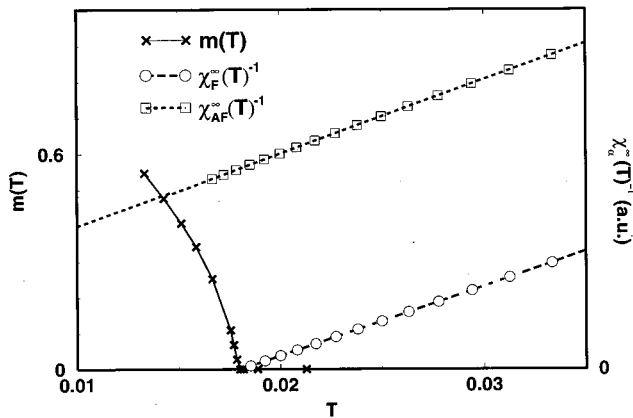


FIG. 1. Magnetization $m(T)$ (crosses), inverse homogeneous susceptibility $\chi_F^\infty(T)^{-1}$ (circles) and staggered susceptibility $\chi_{AF}^\infty(T)^{-1}$ (squares) for $\delta=0.03$ as a function of temperature.

and staggered) as a function of temperature T for a doping $\delta=1-\langle n \rangle=0.03$. While $\chi_{AF}^\infty(T)^{-1}$ remains finite for all T , $\chi_F^\infty(T)^{-1}$ vanishes linearly for a $T_C > 0$ and below T_C we observe a finite magnetization $m=n_\uparrow-n_\downarrow$ with $m(T)=c\sqrt{|T-T_C|}$. Note that the critical points found from $m(T)$ and $\chi_F^\infty(T)$ coincide indicating a second-order transition (see Fig. 1). Unfortunately our data are not sufficient to extrapolate for $m(T=0)$, which according to the results by Fazekas, Menge, and Müller-Hartmann⁸ we would expect to have a value $m(T=0) < n$. Clearly, this point needs further investigation.

Repeating the above calculation for different dopings we obtain the δ - T phase diagram in Fig. 2, which shows a fairly extended region of ferromagnetism with a maximum in T_c at δ between 0.07 and 0.08. Although the NCA in principle does not allow us to do calculations down to T_c beyond $\delta=0.1$, the observed Curie-Weiss form of $\chi_F^\infty(T)$ enables us to obtain data points in this region of the phase diagram from

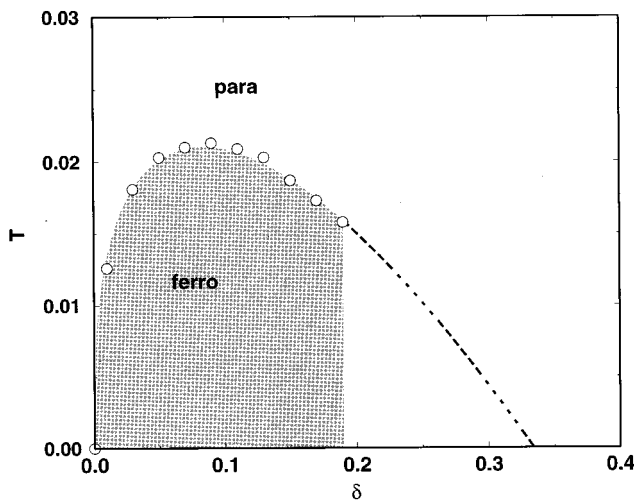


FIG. 2. Magnetic phase diagram for the Hubbard model on a hypercubic lattice. The dashed line represents a fit to the last data points and predicts a critical doping $\delta_c \approx 0.33$ beyond which $T_C=0$.

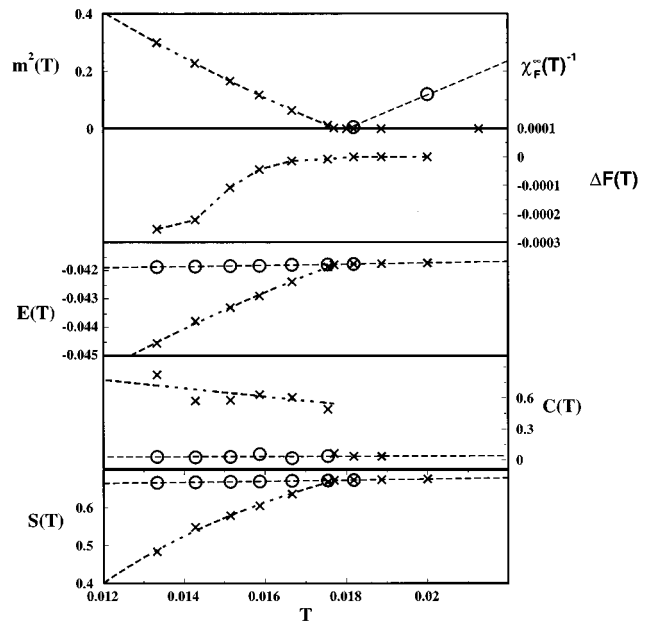


FIG. 3. Squared magnetization $m(T)^2$, inverse homogeneous susceptibility $\chi_F^\infty(T)^{-1}$, difference in free energies $\Delta F(T)=F_{FM}(T)-F_{PM}(T)$, internal energy $E(T)$, specific heat $C(T)$ and entropy $S(T)$ for $\delta=0.03$ in the paramagnetic (circles) and ferromagnetic phase (crosses) close to T_C . From $\Delta F(T < T_C) < 0$ it is clear that below T_c the ferromagnetic solution is stable.

$\chi_F^\infty(T)$ at high temperatures. Obviously this procedure becomes less accurate for increasing doping so that the behavior of the phase line $T_c(\delta)$ currently remains unknown for $\delta > 0.2$. The extrapolation of the available data nevertheless indicates that a critical doping δ_c between 0.3 and 0.4 exists beyond which $T_C=0$.

The stability of the ordered phase depends on the interplay of internal energy $E(T)$ and entropy $S(T)$ entering the free energy $F=E-TS$. In Fig. 3 we thus show the difference in free energies $\Delta F(T)=F_{FM}(T)-F_{PM}(T)$ together with the internal energy, specific heat and entropy for the ferromagnetic and paramagnetic state. To relate the data to the preceding discussion the magnetization and inverse susceptibility from Fig. 1 are shown again in the upper part of Fig. 3. Below T_C the difference $\Delta F(T)$ becomes negative, i.e., the ferromagnetic state is indeed thermodynamically stable.

The internal energy $E(T, n)$ is given by the expectation value of H , which for $U=\infty$ is equivalent to the kinetic energy. As is evident from Fig. 3, $E(T)$ for the ferromagnetic solution is lower than the corresponding values in the paramagnet below T_c . Therefore the transition to the ferromagnetic phase is obviously connected with a gain in kinetic energy. This leads to the conjecture that the physics underlying the stability of the ferromagnetic state should be roughly the same as in the particular case studied within the Nagaoka theorem. Since at T_c the slope of the internal energy $E(T)$ changes for the ferromagnetic solution the specific heat $C(T)=\partial E/\partial T$ shows a jump characteristic for a second-order phase transition. Note that only a very small temperature region around T_C is shown in Fig. 3 and that $C(T)$ decreases again for lower temperatures. Finally, the

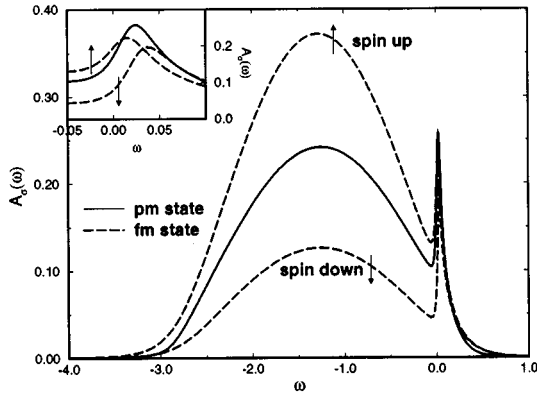


FIG. 4. Spectral functions for $\delta=0.03$ and $\beta=70$ for both spins. The temperature is well below T_c , so that the spin-dependent solution (dashed line) shows a difference in the spectral weight for the two spin directions. The inset shows details near the Fermi energy.

entropy $S(T)$ is obtained from $F=E-TS$. Just above T_C its value is very close to $\ln 2$, the value expected for a spin 1/2 system, while below T_C the increasing spin order leads to a strong decrease of $S(T)$.

The ordered state of course also shows up in the dynamical properties such as the one-particle Green's function. In Fig. 4 we show the density of states (DOS) for a doping $\delta=0.03$ at a temperature $T=1/70 < T_C$ for both the paramagnetic (full line) and ferromagnetic solution (dashed lines). The basic features in the ferromagnetic phase are similar to those of the paramagnet. One finds the lower Hubbard band represented by a broad peak and a quasiparticle resonance near the Fermi energy.^{14,15} Due to $U=\infty$ the upper Hubbard band does not appear.

Depending on temperature and doping spectral weight is transferred between the states with spin σ and that of $-\sigma$, most prominent in the charge-fluctuation peaks, which results in differences in the occupation numbers n_σ and in a finite magnetization $m=n_\uparrow - n_\downarrow$. Note that this does not occur due to any explicit magnetic exchange but rather to the fact that the energy loss by increasing the population of the σ band is outweighed by the gain in kinetic energy from the holes in the $-\sigma$ states.⁴ In addition the peak positions for the minority and/or majority spins are shifted to a somewhat higher and/or lower energy. In terms of a band picture this means a slight splitting of the lower Hubbard band.

The energy splitting is observed for the quasiparticle resonance near the Fermi energy as well (see inset of Fig. 4). In contrast to the lower Hubbard band *both peaks* show a loss of spectral weight compared to the paramagnetic state. This reflects the suppression of the Kondo-like effect underlying the quasiparticle resonance by ferromagnetism, analogous to the effect of an external magnetic field in conventional Kondo physics. With increasing magnetization the resonances will continuously decrease in height and eventually vanish for very low temperatures.

Let us now turn to the interesting question of the dependence of these results on U . Generally speaking we expect that with decreasing U the Curie temperature T_C should be suppressed and, due to the antiferromagnetism favored by a finite U ,²¹ a competition between ferromagnetic and antifer-

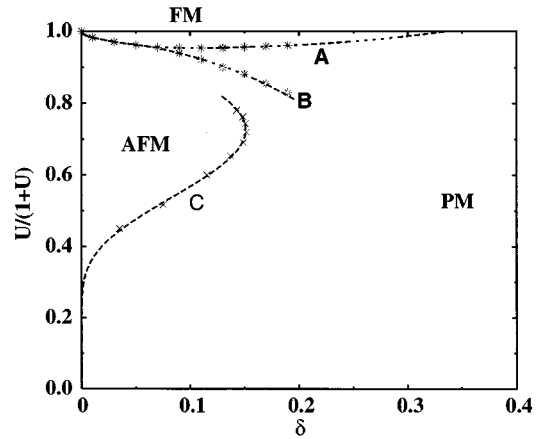


FIG. 5. δ - U phase diagram of the Hubbard model from the large- U limit (curves A and B). We find a region with ferromagnetism above curve A. Below curve B antiferromagnetism is predicted. The phase line at small U (curve C) is taken from Ref. 16 and extrapolates to our phase line for $U \rightarrow \infty$.

romagnetic order should occur. This anticipated behavior can readily be read off the signs in Eqs. (2) and (3), i.e., $U < \infty$ tends to suppress $\chi_F^U(T)$ and enhance $\chi_{AF}^U(T)$. In addition, the Curie-Weiss form of $\chi_F^U(T)$ and $\chi_{AF}^U(T)$ (see Fig. 1) allows us to rewrite Eqs. (2) and (3) in such a way as to identify a Curie temperature $T_C(U, \delta) = T_C^\infty(\delta) - C(\delta)/U$ and a Néel temperature $T_N(U, \delta) = -\Theta(\delta) + \bar{C}(\delta)/U$, where $T_C^\infty(\delta)$ and $C(\delta)$ are the Curie temperature and Curie constant for $U = \infty$, while $\Theta(\delta)$ and $\bar{C}(\delta)$ denote the intercept and inverse slope of $\chi_{AF}^\infty(T)^{-1}$. A detailed discussion of $C(\delta)$, $\bar{C}(\delta)$, and $\Theta(\delta)$ will be given elsewhere.²⁰ Here we want to focus on the resulting δ - U phase diagram in Fig. 5, curves A and B, which were obtained by plotting $\max[T_C(U, \delta), T_N(U, \delta), 0]$.

One sees that for large U an extended region of ferromagnetism exists above curve A, which is completely suppressed for $U < U_c \approx 20$. For decreasing U the ferromagnetic order is eventually replaced by antiferromagnetism in the region below curve B. Note that up to $\delta \approx 0.07$ we find a direct transition from the ferromagnet to the antiferromagnet, which we would expect to be of first order ending in a second-order critical point. A more detailed investigation of the region would thus be of great interest. However, since the transition temperatures are already very small there we do not see any chance to achieve this with the methods currently available. Beyond $\delta \geq 0.07$ a paramagnetic region separates the two phases. In addition to our findings we also include results on the phase line between antiferromagnet and paramagnet for the full Hubbard model (1) at small U (curve C).¹⁶ The behavior for the largest- U values in this case extrapolates nicely to our phase line B for $U \rightarrow \infty$. For decreasing U and increasing δ , however, the approximation of the Coulomb term by an effective exchange becomes worse, i.e., the magnetic order is much stronger suppressed by doping for a given U .

To conclude, we have shown that the Hubbard model on a hypercubic lattice provides a scenario of ferromagnetism for finite doping and at finite temperatures. We were able to

obtain sensible results for T_C as function of δ and U for the strong-coupling case. As in Nagaoka's case the phase transition originates from a gain of kinetic energy, as we could see from thermodynamic quantities. The δ - T - U phase diagram shows a fairly extended region of ferromagnetism for large U that is completely suppressed for $U < U_c \approx 20$ and $\delta > \delta_c \approx 0.3$. For small doping and large U we observed in addition a direct transition from the ferromagnet into an antiferromagnet as a function of U .

Unfortunately our method to solve the DMFT does not allow us to study temperatures $T \ll T_c$. Thus several important questions have to remain unanswered: What is the

ground-state magnetization $m(T \rightarrow 0)$ (cf. Refs. 8 and 9) and of what nature is the ferromagnetic \leftrightarrow antiferromagnetic transition, for example. In future works one also must investigate the order of the transition paramagnet \leftrightarrow ferromagnet, which is under current discussion (cf. Ref. 22, where a first-order transition is stated within a different method), more closely.

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