Derivation of the Curie-Weiss law in dynamical mean-field theory

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We present an analytic derivation of the linear temperature dependence of the inverse static susceptibility $\chi^{-1}(T,U)\sim T-T_c(U)$ near the transition from a paramagnetic-to-ferromagnetic correlated metal within the dynamical mean-field theory for the Hubbard model. The equations for the critical temperature and interaction strength of the transition are also determined.

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I. INTRODUCTION

The dynamical mean-field theory (DMFT) is a nonperturbative and thermodynamically consistent approximation scheme for quantum-mechanical many-body problems on a lattice (for reviews, see Refs. 1–3) which becomes exact in the limit of large coordination numbers.[4] In contrast to the static Hartree-Fock mean-field theory the dynamics of the quantum-mechanical correlation problem is fully included in the DMFT. In the last few years the DMFT proved to be a powerful tool for the investigation of fermionic lattice models with local Coulomb interaction such as the Hubbard model and the periodic Anderson model.[1,2] It is particularly useful in the case of intermediate-coupling problems such as the Mott-Hubbard metal-insulator transition or itinerant ferromagnetism where perturbative techniques fail (for reviews, see Refs. 1, 5 and 6). In the DMFT the lattice problem is mapped onto an effective single-site problem whose self-energy $\Sigma(\omega)$ and Green function $G(\omega)$ have to be calculated self-consistently with the $\mathbf{k}$-integrated Dyson equation. The theory is therefore purely local, i.e., the self-energy $\Sigma(\omega)$ is $\mathbf{k}$ independent and the propagator $G_{\mathbf{k}}(\omega)=G^0_{\mathbf{k}}[\omega-\Sigma(\omega)]$ may be represented by the noninteracting propagator $G^0_{\mathbf{k}}$ at shifted frequency, at least in the paramagnetic case. Here the mean-field character of the theory becomes particularly evident. The local nature of the theory implies that short-range order in position space is missing.

Numerical solutions of the DMFT equations, in particular by quantum Monte Carlo simulations, revealed that in the case of continuous phase transitions (e.g., from a paramagnetic metal to an antiferromagnetic insulator,[7] or to a ferromagnetic metal[8]) the static susceptibility $\chi(T)$ shows a Curie-Weiss behavior above T_c, i.e., $\chi^{-1}\propto T-T_c$, implying that $\chi\propto(T-T_c)^{-\gamma}$ diverges with a critical exponent $\gamma=1$. Furthermore, the order parameter was found to vanish with an exponent $\beta=1/2$.[8,9] In view of the mean-field nature of the DMFT these numerical findings did not come as a surprise. However, considering the dynamics of the quantum-mechanical problem the situation is not as self-evident as it may seem. At a continuous phase transition between two phases in high dimensions, a mean-field behavior is naturally expected if the low-energy excitation spectrum of both phases has a gap. In this case, the fermions may be integrated out, leading to an effective Ginzburg-Landau-Wilson field theory.[10] This applies to transitions in the Heisenberg spin model. By contrast, if the transition occurs between two *metallic* phases, e.g., from a paramagnetic-to-ferromagnetic metal, or between a metallic and an insulating phase, the result is far from trivial since the low-lying excitations in the metallic phases may couple to the order parameter and thereby lead to divergences in the effective field theory at $T=0$ or even at very low temperatures.[11] At present, the consequences of this feedback are still not entirely understood. It is therefore worthwhile to further investigate the transition between two metallic phases, also within the DMFT, using *analytical* methods.

Curie-Weiss behavior of the magnetic susceptibility is traditionally associated with *localized* magnetic moments, and, indeed, is readily obtained for Heisenberg-type spin models in mean-field approximations. Nevertheless, it is also a characteristic of interacting itinerant electrons as described, for example, by the Hubbard model. In particular, a Curie-Weiss behavior may be obtained within the Hartree-Fock approximation which yields $\chi^{-1}_{HF}(T)\sim T^2-T_c^2$ above T_c.[5,12] However, since this result is derived for interaction strengths where the Hartree-Fock approximation is not controlled by perturbation theory, its qualitative and quantitative validity is questionable.[13] The same criticism applies to the Stoner criterion for the onset of ferromagnetism.[14]

To calculate the static magnetic susceptibility in the vicinity of a continuous phase transition from the paramagnetic-to-ferromagnetic metallic state where electronic correlations are explicitly included we will use the one-band Hubbard model

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

on an arbitrary lattice and employ the DMFT. In particular, we will show that the critical exponent is indeed $\gamma=1$.

II. DERIVATION OF THE SUSCEPTIBILITY

We wish to calculate the magnetization density

$$m=(1/2\beta)\sum_n \sigma G_{\sigma n}, \tag{2}$$

where the local Green function $G_{\sigma n}$ in DMFT is given by the bare density of states $N^0(\epsilon)$ and the local self-energy $\Sigma_{\sigma n}$ as

$$G_{\sigma n}=\int d\epsilon \frac{N^0(\epsilon)}{i\omega_n+\mu+\sigma h-\Sigma_{\sigma n}-\epsilon}. \tag{3}$$

Here the subscript n refers to the Matsubara frequency $i\omega_n = i(2n+1)\pi/\beta$ for the temperature T, with $\beta=1/k_BT$, and h is the external magnetic field in energy units. Within the DMFT the local Green function $G_{\sigma n}$ is determined self-consistently through Eq. (3) and

$$G_{\sigma n}=-\frac{\int D[c_\sigma,c_\sigma^*]c_{\sigma n}c_{\sigma n}^* e^{\mathcal{A}\{c_\sigma,c_\sigma^*,\mathcal{G}_\sigma^{-1}\}}}{\int D[c_\sigma,c_\sigma^*]e^{\mathcal{A}\{c_\sigma,c_\sigma^*,\mathcal{G}_\sigma^{-1}\}}}, \tag{4}$$

by the **k**-integrated Dyson equation

$$\mathcal{G}_{\sigma n}^{-1}=G_{\sigma n}^{-1}+\Sigma_{\sigma n}. \tag{5}$$

The single-site action $\mathcal{A}$ has the form

$$\mathcal{A}\{c_\sigma,c_\sigma^*,\mathcal{G}_\sigma^{-1}\}=\sum_{n,\sigma} c_{\sigma n}^*\mathcal{G}_{\sigma n}^{-1}c_{\sigma n} - U\int_0^\beta d\tau c_\sigma^*(\tau)c_\sigma(\tau)c_{-\sigma}^*(\tau)c_{-\sigma}(\tau), \tag{6}$$

where we used a mixed time/frequency convention for Grassman variables c_σ, c_σ^*.

We first separate the self-energy $\Sigma_{\sigma n}$ into its static (i.e., Hartree-Fock) part and its explicitly dynamical contribution $\tilde{\Sigma}_{\sigma n}$ as

$$\Sigma_{\sigma n}=U\frac{n_0}{2}-\sigma Um+\tilde{\Sigma}_{\sigma n}. \tag{7}$$

Here n_0 is the density of particles. The Hartree-Fock approximation corresponds to neglecting $\tilde{\Sigma}_{\sigma n}$. Since we are interested in the behavior of the susceptibility close to a continuous transition, i.e., in the limits $T\to T_c$, $h\to 0$, and $m\to 0$, where T_c is the, yet unknown, Curie temperature, we write

$$\begin{aligned} G_{\sigma n}&=G_n+\delta G_{\sigma n},\\ \mathcal{G}_{\sigma n}&=\mathcal{G}_n+\delta\mathcal{G}_{\sigma n},\\ \tilde{\Sigma}_{\sigma n}&=\tilde{\Sigma}_n+\delta\tilde{\Sigma}_{\sigma n}, \end{aligned} \tag{8}$$

where $\delta G_{\sigma n}$, $\delta\mathcal{G}_{\sigma n}$, and $\delta\tilde{\Sigma}_{\sigma n}$ are spin-dependent corrections to the respective paramagnetic (i.e., spin-independent) parts. In the next step we expand Eqs. (3) and (5) up to first order in these corrections. Using Eqs. (3) and (7) we find

$$\delta G_{\sigma n}=-[\sigma h+\sigma Um-\delta\tilde{\Sigma}_{\sigma n}]F_n, \tag{9}$$

where we introduced the function

$$F_n=\int d\epsilon \frac{N^0(\epsilon)}{\left[i\omega_n+\mu-U\frac{n_0}{2}-\tilde{\Sigma}_n-\epsilon\right]^2}. \tag{10}$$

As in the Weiss molecular-field theory, the particles may be interpreted as moving in an *effective* magnetic field

$$h_{eff}\equiv h+Um-\sigma\delta\tilde{\Sigma}_{\sigma n}. \tag{11}$$

However, in the case of interacting electrons considered here this effective field is, in general, found to be dynamic, i.e., it fluctuates in time due to the local correlations which lead to an exchange of energy between the particles. Neglecting the dynamical term $\delta\tilde{\Sigma}_{\sigma n}$ we recover the usual static mean-field expression for the effective magnetic field. Similarly, expanding Eq. (5) and using Eq. (7) we obtain

$$\mathcal{G}_n^{-1}=G_n^{-1}+\tilde{\Sigma}_n+U\frac{n_0}{2}, \tag{12}$$

and

$$\frac{\delta\mathcal{G}_{\sigma n}}{\mathcal{G}_n^2}=\frac{\delta G_{\sigma n}}{G_n^2}+\sigma Um-\delta\tilde{\Sigma}_{\sigma n}. \tag{13}$$

Our goal is to find $\delta\tilde{\Sigma}_{\sigma n}$ and then, with the help of Eq. (9), to calculate the magnetization m. Since Eq. (13) still contains the two unknown functions $\delta\tilde{\Sigma}_{\sigma n}$ and $\delta\mathcal{G}_{\sigma n}$, an additional condition is required to close the set of equations. This condition is provided by the fact that the self-energy is a functional of $\mathcal{G}_{\sigma n}$ in perturbation theory, i.e., $\tilde{\Sigma}_{\sigma n}=\tilde{\Sigma}_\sigma[\mathcal{G}_{\sigma n}]$, to infinite order. Hence, we can formally expand as

$$\tilde{\Sigma}_\sigma[\mathcal{G}_{\sigma n}]=\tilde{\Sigma}_\sigma[\mathcal{G}_n+\delta\mathcal{G}_{\sigma n}]\approx\tilde{\Sigma}[\mathcal{G}_n]+\sum_{n'}\frac{\delta\tilde{\Sigma}[\mathcal{G}_n]}{\delta\mathcal{G}_{n'}}\delta\mathcal{G}_{\sigma n'}. \tag{14}$$

Using Eq. (12) relating $\mathcal{G}$ and G we find the functional derivative

$$\frac{\delta\tilde{\Sigma}}{\delta\mathcal{G}}=\frac{\delta\tilde{\Sigma}}{\delta G}\cdot\frac{\delta G}{\delta\mathcal{G}}=\frac{1}{F}\frac{\delta G}{\delta\mathcal{G}}, \tag{15}$$

where $F\equiv F_n$ is given by Eq. (10). Employing Eq. (4) in the paramagnetic phase and using Eq. (13), we obtain the spin-dependent correction to the self-energy $\tilde{\Sigma}_{\sigma n}$ as

$$\delta\tilde{\Sigma}_{\sigma n}=\sigma h\sum_{n'}M_{nn'}^{-1}\sum_{n''}\frac{\Gamma_{n'n''}F_{n''}}{F_{n'}G_{n''}^2} + \sigma Um\sum_{n'}M_{nn'}^{-1}\sum_{n''}\frac{\Gamma_{n'n''}}{F_{n'}}\left(\frac{F_{n''}}{G_{n''}^2}-1\right), \tag{16}$$

where $M_{nn'}^{-1}$ is the inverse of the matrix $M_{nn'}$ defined as

$$M_{nn'} \equiv \delta_{nn'} + \frac{\Gamma_{nn'}}{F_n}\left(\frac{F_{n'}}{G_{n'}^2} - 1\right), \tag{17}$$

and

$$\Gamma_{nn'} \equiv \frac{1}{2}\sum_{\sigma\sigma'}\left[\langle c_{\sigma n} c_{\sigma n}^* c_{\sigma' n'} c_{\sigma' n'}^*\rangle - \langle c_{\sigma n} c_{\sigma n}^*\rangle\langle c_{\sigma' n'} c_{\sigma' n'}^*\rangle\right] \tag{18}$$

is the two-particle density-density correlation function calculated in the paramagnetic phase. We note that in the Hartree-Fock approximation the two-particle correlations are neglected, i.e., $\Gamma_{nn'}^{HF}=0$, and therefore $\tilde{\Sigma}_{\sigma n}=0$.

The spin-dependent correction to the local Green function $G_{\sigma n}$ can now be expressed as

$$\delta G_{\sigma n} = -\sigma[hH_n + Um(H_n + \Delta H_n)]F_n, \tag{19}$$

where

$$H_n \equiv 1 - \sum_{n'} M_{nn'}^{-1} \sum_{n''} \frac{\Gamma_{n'n''}F_{n''}}{F_{n'}G_{n''}^2}, \tag{20}$$

and

$$\Delta H_n \equiv \sum_{n'} M_{nn'}^{-1} \sum_{n''} \frac{\Gamma_{n'n''}}{F_{n'}}. \tag{21}$$

We see that the effective magnetic field (11) acting on an electron is given by

$$h_{eff} = hH_n + Um(H_n + \Delta H_n). \tag{22}$$

It is interesting to observe that the dynamics of the two terms is *different*, i.e., the correlation problem leads to an asymmetry between the external (h) and the induced (Um) effective magnetic fields. The origin of this asymmetry lies in the self-consistency Eq. (5), where h enters through $\delta G_{\sigma n}$, while Um enters both through $\delta G_{\sigma n}$ and $\Sigma_{\sigma n}$. In the Hartree-Fock approximation, the frequency-dependent factors H_n and ΔH_n reduce to unity and zero, respectively, such that $h_{eff}=h+Um$ becomes a *static* effective magnetic field.

We are now able to calculate the magnetic susceptibility $\chi^{DMFT}(T,U)$. Noting that the magnetization m, Eq. (2), has nonvanishing contributions only from $\delta G_{n\sigma}$, and using Eq. (19) one finds

$$m = -\frac{1}{\beta}\sum_n H_n F_n h - \frac{1}{\beta}\sum_n (H_n + \Delta H_n) F_n U m. \tag{23}$$

The linear magnetic susceptibility is then obtained from $m = \chi^{DMFT}(T,U)h$ as

$$\chi^{DMFT}(T,U) = \frac{\chi_0(T,U)}{1 - U[\chi_0(T,U) + \Delta\chi_0(T,U)]}, \tag{24}$$

where

$$\chi_0(T,U) = -\frac{1}{\beta}\sum_n H_n F_n, \tag{25}$$

and

$$\Delta\chi_0(T,U) = -\frac{1}{\beta}\sum_n \Delta H_n F_n. \tag{26}$$

Equation (24) with Eqs. (25) and (26) is one of the main results of our paper. We note that the expression for the static susceptibility $\chi^{DMFT}(T,U)$ in Eq. (24) is deceptively simple. Indeed, it has the *form* of the corresponding random phase approximation (RPA) expression, with the Pauli susceptibility $\chi_0(T)$ of the noninteracting system replaced by the susceptibilities $\chi_0(T,U)$ and $\Delta\chi_0(T,U)$ of the interacting system. If both $\tilde{\Sigma}_n$ and $\Gamma_{nn'}$ were neglected we would recover the well-known Hartree-Fock result. The result for the static susceptibility can be expressed in the RPA-like form

$$\chi^{DMFT}(T,U) = \frac{\chi(T,U)}{1 - U\chi(T,U)} \tag{27}$$

with

$$\chi(T,U) \equiv \frac{\chi_0(T,U)}{1 - U\Delta\chi_0(T,U)}. \tag{28}$$

This equation suggests that, as in RPA, the susceptibility can be written as an infinite series of bubble diagrams with (three-leg) vertex corrections. So far it was not possible to deconvolute the corresponding Bethe-Salpeter equation for the vertex corrections, since the scattering function (four-leg vertex), although **k** independent in the infinite dimensional theory, is still a complicated function of frequency. It should be noted, however, that our algebraic derivation of the static susceptibility is nonperturbative anyway since it is not based on direct diagrammatic resummations.

III. DISCUSSION

The transition point between the paramagnetic and ferromagnetic phases is determined by the divergence of the static susceptibility $\chi^{DMFT}(T,U)$ in Eq. (24),

$$1 - U[\chi_0(T_c,U) + \Delta\chi_0(T_c,U)] = 0. \tag{29}$$

Using the spectral representation for the summation over the Matsubara frequencies one can write Eq. (29) in a closed form as

$$1 - \int_{-\infty}^{\infty} d\epsilon \left(\frac{1}{e^{\beta_c\epsilon}+1}\right)\left\{-\frac{1}{\pi} Im[(H(\epsilon + i0^+) + \Delta H(\epsilon + i0^+))F(\epsilon + i0^+)]\right\} = 0, \tag{30}$$

where $H(\epsilon+i0^+)$ and $\Delta H(\epsilon+i0^+)$ are obtained by analytic continuation: $H_n \equiv H(i\omega_n) \to H(\epsilon+i0^+)$ and $\Delta H_n \equiv \Delta H(i\omega_n) \to \Delta H(\epsilon+i0^+)$. It should be noted that $H(\epsilon)$ and $\Delta H(\epsilon)$ are still functions of temperature because of the internal summations over Matsubara frequencies in Eqs. (20) and (21). For given U Eq. (30) determines the Curie temperature $T_c(U)$. Similarly, one may fix the temperature to determine the critical interaction strength $U_c(T)$. In this re-

spect Eqs. (29) and (30) are generalizations of the Stoner criterion[15] $U_c^{Stoner}=1/N^0(\epsilon_F)$ obtained in Hartee-Fock theory. In general Eq. (30) implies that, due to the inclusion of genuine correlations, the transition point to the ferromagnetic phase is not merely determined by the density of states (DOS) *at* the Fermi level but, rather, by the density of states at *all* energies. Due to the increase in the kinetic energy the value of U_c is reduced by an asymmetric DOS, especially if the DOS has a singularity at the lower band edge. This had already been found in the numerical solution of the DMFT equations for a model DOS using Monte Carlo simulations[8,14] and in the approximate treatment of DMFT within the modified perturbation theory.[16] Equation (30) confirms these numerical findings analytically and explains the origin as a correlation effect.

Expanding the static susceptibility (24) around $T_c(U)$ (for $T>T_c>0$) we find a Curie-Weiss law

$$\chi^{DMFT}(T,U)=\frac{C^{DMFT}[T_c(U),U]}{T-T_c(U)}, \tag{31}$$

with

$$C^{DMFT}[T_c(U),U]=-\frac{\chi_0[T_c(U),U]}{U\left\{\dfrac{d[\chi_0(T,U)+\Delta\chi_0(T,U)]}{dT}\right\}_{T_c(U)}}, \tag{32}$$

which is hence seen to be a genuine property of the DMFT. The critical exponent $\gamma=1$ is in accordance with the mean-field nature of the DMFT, which neglects short-range spatial correlations between the electrons.

In the similar manner one can show that at $T=0$, where the transition becomes a quantum phase transition, the static spin susceptibility diverges as the control parameter U approaches $U_c(T=0)$ from below,

$$\chi^{DMFT}(T=0,U)\sim\frac{1}{U_c(T=0)-U}, \tag{33}$$

with the mean-field exponent $\gamma=1$.

While the dynamics, i.e., the effect of temporal correlations, is found to be very important in determining nonuniversal quantities such as the critical temperature or the Curie constant, we conclude that it apparently does not affect the universal scaling properties of the paramagnetic-to-ferromagnetic phase transition within the DMFT.

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[1] A. Georges, G. Kotliar, W. Krauth, and M.J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[2] Th. Pruschke, M. Jarrell, and J.K. Freerick, Adv. Phys. **44**, 187 (1995).
[3] D. Vollhardt, *Correlated Electron Systems*, edited by V. J. Emery (World Scientific, Singapore, 1993), p. 57.
[4] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[5] P. Fazekas, *Lecture Notes on Electron Correlation and Magnetism* (World Scientific, Singapore 1999).
[6] D. Vollhardt, N. Blümer, K. Held, and M. Kollar, in *Band-Ferromagnetism*, edited by K. Baberschke *et al.*, Lecture Notes in Physics, Vol. 580 (Springer, Heidelberg, 2001), p. 191.
[7] M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992); M. Jarrell and Th. Pruschke, Z. Phys. B: Condens. Matter **B 90**, 1891 (1993).
[8] M. Ulmke, Eur. Phys. J. B **1**, 301 (1998).
[9] M. Jarrell, H. Akhlaghpar, and Th. Pruschke, *Quantum Monte Carlo Method in Condensed Matter Physics*, edited by M. Suzuki, (World Scientific, Singapore, 1993), p. 221.
[10] We are grateful to M. Vojta for an illuminating discussion of this point.
[11] D. Belitz, T.R. Kirkpatrick, and T. Vojta, Phys. Rev. Lett. **82**, 4707 (1999).
[12] E.P. Wohlfarth, Philos. Mag. **42**, 374 (1951); Rev. Mod. Phys. **25**, 211 (1953); M. Shimizu, Rep. Prog. Phys. **44**, 329 (1981); T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism* (Springer-Verlag, Berlin, 1985).
[13] For a discussion see, for example, V. Janiš, J. Mašek, and D. Vollhardt, Z. Phys. B: Condens. Matter **91**, 325 (1993).
[14] J. Wahle, N. Blümer, J. Schlipf, K. Held, and D. Vollhardt, Phys. Rev. B **58**, 12 749 (1998).
[15] E.C. Stoner, Philos. Mag. **15**, 1018 (1933).
[16] W. Nolting, *Lectures on the Physics of Highly Correlated Electron Systems IV*, edited by F. Mancini (AIP, Woodbury, 2000) pp. 118–225.