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COMPREHENSIVE MEAN FIELD THEORY FOR THE HUBBARD MODEL

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ABSTRACT

We derive an exact expression for the grand potential of the Hubbard model in $d = \infty$ dimensions. By simplifying the energy transfer between up and down spins we obtain a comprehensive mean-field theory for this model. It is (i) thermodynamically consistent in the entire range of input parameters, (ii) conserving and, (iii) exact in several non-trivial limits, e. g. in the free ($U \to 0$), atomic ($t \to 0$) and Heisenberg ($U \gg t$, $n = 1$) limit.

1 Introduction

In condensed matter physics the Hubbard model[1] represents the generic lattice model for strongly correlated fermions with a local interaction. Most recently the questions arising in the context of high-T_c superconductivity have further stimulated intensive investigations of this model. However, in spite of undisputable progress a secured understanding of the model is still lacking. In statistical mechanics a first rough description of the properties of a model is often obtained within mean field theory (MFT). For example, the Weiss molecular field theory is a MFT for the Ising model,

which becomes exact in the limit of high dimensions ($d \to \infty$).[2] This MFT contains no unphysical singularities and is applicable for all values of the coupling, temperature and external field. It is also diagrammatically controlled.[2] The construction of a MFT for fermionic models with on-site interaction is made complicated by the additional energy transfer between particles. There *do* exist well-known mean-field-type approximation schemes (e. g. Hartree-Fock, RPA, saddle-point evaluations of path-integrals, decoupling of equations of motion, etc.). However, these approximations are not MFTs in the statistical mechanical sense, since they are not able to give a comprehensive description of the model (e. g. the phase diagram, thermodynamics, etc.) in the entire range of input parameters. Clearly, a MFT based on the exact solution of the Hubbard model in the limit $d = \infty$ would be desirable. For fermionic lattice models this limit has been introduced only recently.[3,4] In $d = \infty$ substantial simplifications occur in the *spatial* properties (reduction to an effective single site problem).[3,5] However, the *dynamics* of systems with an on-site interaction is not affected.[5] Hence so far only a simplified Hubbard model ("Falicov-Kimball model"), where one of the two spin components is static,[6–8] has been solved exactly in $d = \infty$.[9–11]

In this paper a local expression for the exact grand potential of the Hubbard model in $d = \infty$ will be derived. From this we construct an approximate theory for the Hubbard model with the comprehensive properties of a MFT in statistical mechanics.

2 The Hubbard model in high dimensions

The Hamiltonian

$$\hat{H} = \sum_{\langle \mathbf{ij} \rangle, \sigma} t_\sigma \hat{c}^+_{\mathbf{i}\sigma} \hat{c}_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}\uparrow} \hat{n}_{\mathbf{i}\downarrow} - \sum_{\mathbf{i},\sigma} \mu_\sigma \hat{n}_{\mathbf{i}\sigma} \,, \tag{1}$$

where $\mu_\sigma \equiv \mu + \sigma h$ is the chemical potential of σ-spins with h as the external magnetic field, represents both the Hubbard model ($t_\uparrow = t_\downarrow \equiv -t$) and its simplified version (e. g. $t_\uparrow = -t, t_\downarrow = 0$). Here $\hat{c}^+_{\mathbf{i}\sigma}, \hat{c}_{\mathbf{i}\sigma}$ and $\hat{n}_{\mathbf{i}\sigma} \equiv \hat{c}^+_{\mathbf{i}\sigma} \hat{c}_{\mathbf{i}\sigma}$ are the usual fermion operators.

For fermionic models to remain non-trivial in the limit $d = \infty$ the hopping amplitude has to be scaled as

$$t \to \bar{t}/\sqrt{2d}\,, \tag{2}$$

with $\bar{t} = const.$[3] This square-root scaling law follows from the fact that the free energy, and all measurable quantities, are determined by *even* powers of the hopping amplitude, the lowest power being 2 for single-particle quantities. (The same scaling applies in the case of the classical spin glass problem where the average $\langle J_{ij}^n \rangle$ of the spin-spin coupling is only non-zero for even n.[12]) By contrast, the Hubbard interaction, being purely local, is completely independent of the surrounding of a given lattice site. Hence the dimensionality of a lattice does not enter at all. Therefore the Hubbard interaction U does *not* have to be scaled in the limit $d \to \infty$. This property distinguishes the Hubbard interaction from all other interactions. In particular, non-local interactions of the type $V_{ij}^{\sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'}$ have to be rescaled as in classical models, e.g. the Ising model, namely $V_{ij}^{\sigma\sigma'} \to \bar{V}_{ij}^{\sigma\sigma'}/2d$ for nearest neighbor interactions. Hence they reduce to the corresponding Hartree approximation.[5] This implies that of all interactions it is *only* the Hubbard interaction that remains dynamical in the limit $d \to \infty$. Note that the scaling (2) does not imply particles to be localized in $d = \infty$. Particles still move, but they hop with a reduced amplitude to very many possible sites so that the overall kinetic energy E_{kin} remains finite

$$E_{kin} = -\frac{t}{2\pi i} \sum_{(ij),\sigma} \int_{-\infty}^{\infty} d\omega G_{\sigma ij}(\omega) \propto L\bar{t}\,, \tag{3}$$

where L is the number of lattice sites. Here $G_{\sigma,ij}(\omega)$ is the propagator, which obviously is of order $1/\sqrt{d}$ small, since $t \sim 1/\sqrt{d}$ and the sum over nearest neighbors gives a factor $\sim d$. We see that, although we calculate the kinetic energy strictly in $d = \infty$, we have to include contributions of order $1/\sqrt{d}$!

As a consequence of the scaling (2) the proper self-energy $\Sigma_{\sigma ij}(\omega)$ becomes site-diagonal,[3,5] i.e. its Fourier transform becomes a **k**-independent quantity $\Sigma_\sigma(\omega)$. This result may be understood as follows. Let us consider the motion of a particle on a lattice. The interaction between particles will affect the motion. This change is described by a complex, spatially dependent, dynamical field — the self-energy $\Sigma_{\sigma ij}(\omega)$.

In the case where a lattice site has a very large number of nearest neighbors the *spatial* dependence of this field becomes increasingly unimportant and vanishes completely for $d \to \infty$. So the field becomes a *mean field* in position space, while retaining its full dynamics. (In the case of a broken symmetry in position space this picture has to be slightly modified , but still holds). There is a direct analogy with the problem of non-interacting electrons in a random medium: in the limit $d \to \infty$ the self-energy becomes a purely local, i.e. **k**-independent, quantity, sometimes called "coherent potential".[13] In this limit the coherent potential approximation (CPA) becomes exact.[14] CPA is a single-site theory where a particle moves through an *effective medium* described by a self-energy $\Sigma_\sigma(\omega)$. It should be noted, however, that the coherent potential in the Hubbard model is more complicated due to the interaction between particles.

We now want to construct the exact grand potential Ω of the Hubbard model in $d = \infty$. Within the general approach of Baym[15] Ω has the form ($\beta = T^{-1}$, $k_B = 1$)

$$\beta\Omega\{\Sigma\} = \Phi\{G\} - tr(\Sigma G) - tr \ln \left((G^0)^{-1} - \Sigma\right) , \tag{4}$$

where

$$G^0_\sigma(\mathbf{k}, z) = \frac{1}{z + \mu_\sigma - \epsilon(\mathbf{k})} \tag{5}$$

is the free propagator and G is the full Green function which is determined by

$$\frac{\delta\Omega}{\delta\Sigma} = 0 . \tag{6}$$

The quantity Φ is a functional of G and is obtained from a self-consistent perturbation expansion in G for the self-energy Σ ,[15] the latter being defined by

$$\frac{\delta\Phi}{\delta G} = \Sigma . \tag{7}$$

Hence Ω is a functional of Σ only. To define Ω unambiguously, i.e. to reproduce the grand potential for the non-interacting case, one has to impose a boundary condi-

tion on (7), namely $\Phi = 0$ for $\Sigma = 0$. The construction of $\Omega\{\Sigma\}$ amounts to the construction of the functional

$$\Lambda\{\Sigma, G\} = \Phi\{G\} - tr(\Sigma G) \,. \tag{8}$$

For the Hubbard model in $d = \infty$ the self-energy Σ was found to be purely local. Consequently the Λ-functional is fully determined by the local part of Σ and the local part of the full Green function G . So the problem reduces to an *effective single-site theory.* In particular, this means that $e^{-\beta\Lambda}$ can essentially be constructed from a single-site Hubbard model. Technically this is achieved by making use of a functional integral representation for the partition function of the Hubbard model in the *atomic* limit ($t = 0$), where the atomic $U = 0$ propagator, $G^0_{\sigma,at}(z) = (z + \mu_\sigma)^{-1}$, is replaced by an *effective* propagator $\mathcal{G}$ given by[16,11]

$$\mathcal{G} = (G^{-1} + \Sigma)^{-1} \,. \tag{9}$$

To fulfil (7) with the boundary condition $\Lambda = 0$ for $\Sigma = 0$ we must subtract a term $tr \ln G$ from the corresponding local grand potential. Writing the trace explicitly we obtain the exact grand potential for the Hubbard model in $d = \infty$

$$\begin{aligned} \Omega\{G, \Sigma\} \;=\; & -LT \ln \Bigg[\int D\psi D\psi^* \exp \Bigg\{ \sum_{n=-\infty}^{\infty} \sum_{\sigma} \psi^*_\sigma(n) \mathcal{G}_\sigma(i\omega_n)^{-1} \psi_\sigma(n) \\ & -U \int_0^\beta d\tau \psi^*_\uparrow(\tau)\psi_\uparrow(\tau)\psi^*_\downarrow(\tau)\psi_\downarrow(\tau) \Bigg\} \Bigg] \;-\; LT \sum_{n=-\infty}^{\infty} \sum_{\sigma} \ln G_\sigma(i\omega_n) \\ & -T \sum_{n=-\infty}^{\infty} \sum_{\mathbf{k},\sigma} \ln[i\omega_n + \mu_\sigma - \Sigma_\sigma(i\omega_n) - \epsilon(\mathbf{k})] \,, \end{aligned} \tag{10}$$

where $\omega_n = (2n + 1)\pi T$ are Matsubara fermion frequencies, and $\psi_\sigma, \psi^*_\sigma$ are Grassmann variables. Note that the potential Ω can be viewed as a functional of Σ only, as described above, or equivalently as a functional of both Σ *and* G with the supplementary condition (7). In (10) we used the latter approach. The condition (7) can then be expressed as

$$\frac{\delta\Omega}{\delta G} = 0 \,. \tag{11}$$

It should be pointed out that, in contrast to the approach of Baym,[15] we did not attempt to calculate $\Phi\{G\}$, but rather $\Lambda\{\Sigma, G\}$. Indeed, $\Phi\{G\}$ is *not* the suitable quantity to determine because of the dependence of the effective propagator $\mathcal{G}$, (9), on both G and Σ. At least for the problem under investigation, where only the local parts of G and Σ enter, it is Λ, not Φ , which can be found in closed form. Of course, Φ can be obtained from Λ by the Legendre transformation (8).

The expression for Ω in (10) may be interpreted as the thermodynamic potential of L *separate* lattice sites where electrons can interact (first two terms on the r. h. s.), which are immersed in a fermionic bath made of non-interacting, itinerant electrons moving in a homogeneous, complex field Σ (last term). There is no direct coupling between the electrons on different lattice sites; rather, they communicate only with the effective medium through their propagator $\mathcal{G}$. Generally $\Sigma_\sigma(z)$ are arbitrary complex functions with the Herglotz property (i.e. $\Sigma_\sigma(z^*) = \Sigma_\sigma(z)^*$ and $Im\Sigma_\sigma(z) \propto \pm Imz$). Only when the system of the interacting electrons is in equilibrium with the surrounding bath, i.e. when (6) and (11) are fulfilled, do the complex functions $\Sigma_\sigma(z)$ and $G_\sigma(z)$ become the self-energy and and the diagonal element of the Green function of the Hubbard model in $d = \infty$, respectively.— A different construction of the local equation for the self-energy of the Hubbard model in $d = \infty$ was recently presented by Georges and Kotliar,[17] who mapped the lattice model onto a single-impurity Anderson model supplemented by a self-consistency condition. Their equation for Σ corresponds to (11).

We can rewrite the formal Grassmann functional integral using the Hubbard-Stratonovich transformation

$$\exp\Big\{ -U\int_0^\beta d\tau \psi_\uparrow^*(\tau)\psi_\uparrow(\tau)\psi_\downarrow^*(\tau)\psi_\downarrow(\tau)\Big\} \;=$$

$$\int D\eta D\xi \exp\Big\{ -\frac{1}{2}\int_0^\beta d\tau \Big[\eta^2(\tau)+\xi^2(\tau)$$

$$+\sqrt{2U}\big\{\eta(\tau)[\psi_\uparrow^*(\tau)\psi_\uparrow(\tau)-\psi_\downarrow^*(\tau)\psi_\downarrow(\tau)]+i\xi(\tau)[\psi_\uparrow^*(\tau)\psi_\uparrow(\tau)+\psi_\downarrow^*(\tau)\psi_\downarrow(\tau)\big\}\Big]\Big\}. \qquad (12)$$

Eq. (12) is equivalent to the standard operator identity

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \equiv \frac{1}{4}\left[(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})^2-(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})^2\right] \tag{13}$$

for the Hubbard interaction, where the two terms on the r.h.s. correspond to charge and spin fluctuations, respectively. In (12) these fluctuations are described by real fluctuating fields $\xi(\tau)$ and $\eta(\tau)$, respectively. Note that the square of the integrand on the l.h.s. of (12) is not zero because the fields $\psi_\sigma(\tau)$ are distributions! The grand potential (10) can then be represented as

$$\begin{aligned}\Omega\{G,\Sigma\} \;=\; & \\ -LT\sum_\sigma \sum_{n=-\infty}^{\infty}\left[\int_{-\infty}^{\infty} dE\,\rho_\sigma(E)\ln[i\omega_n+\mu_\sigma-\Sigma_\sigma(i\omega_n)-E]+\ln\left(1+G_\sigma(i\omega_n)\Sigma_\sigma(i\omega_n)\right)\right] & \\ -\; LT\ln\left[\int D\eta D\xi\exp\left\{-\frac{1}{2}\sum_{\nu=-\infty}^{\infty}(\xi_\nu^2+\eta_\nu^2)\right.\right. & \\ \left.\left.+\sum_\sigma\sum_{n=-\infty}^{\infty}\left[\ln(1+\sigma\sqrt{\tfrac{U}{2}}\hat{\eta}\hat{\mathcal{G}}_\sigma+i\sqrt{\tfrac{U}{2}}\hat{\xi}\hat{\mathcal{G}}_\sigma)\right]_{n,n}\right\}\right], & \end{aligned} \tag{14}$$

where $(\hat{\xi})_{m,n}=\xi_{m-n}$, $(\hat{\eta})_{m,n}=\eta_{m-n}$, $(\hat{\mathcal{G}}_\sigma)_{m,n}=\delta_{m,n}\mathcal{G}_\sigma(i\omega_n)$. Expression (14) determines the *exact* grand potential of the $d=\infty$ Hubbard model.

Although the self-energies $\Sigma_\sigma(i\omega_n)$ are local, different frequencies are non-trivially coupled through the infinitely many fields η and ξ. In other words, although the interaction between electrons on different lattice sites has been reduced to an interaction of electrons with a mean field, the dynamics of the latter interaction is still non-trivial. Hence the many-body nature of the Hubbard model is seen to survive even in $d=\infty$. Thereby the explicit evaluation of the exact self-energy from (14) is made impossible.

In the following we want to find the minimal, controllable approximation to (14) that leads to solvable equations. As a first step one might try to solve (14) in the

static limit ($\eta_\nu = \xi_\nu = 0$ for $\nu \neq 0$), although there is no physical justification for that. It seems that even this restricted problem cannot be solved explicitly, since the coupling between frequencies is still present. Indeed, the evaluation of Ω appears to be possible only if the coupling is removed, e.g. by decoupling one species of particles from the surrounding medium. This is achieved by restricting the dynamics of the Hubbard model (1) to that of the simplified Hubbard model.

3 The simplified Hubbard model

In the simplified Hubbard model[6–8] one of the spin species, say $\uparrow$, is mobile while the other one ($\downarrow$) is fixed, i.e. $t_\uparrow = -t$, $t_\downarrow = 0$. In the limit $d \to \infty$ it can be solved exactly by various techniques.[9–11] In this case one has $\mathcal{G}_\downarrow(i\omega_n) = (i\omega_n + \mu_\downarrow)^{-1}$ and the static approximation becomes exact. This fact can be understood both in the time and in the frequency representation. The time dependent atomic propagator has the Markov property, i. e.

$$G_\downarrow(\tau - \tau'')G_\downarrow(\tau'' - \tau') = G_\downarrow(\tau - \tau') \tag{15}$$

for any $0 < \tau' < \tau'' < \tau \leq \beta$. This is equivalent to a separation of the dynamics of the two spin populations, as can be demonstrated in a diagrammatic perturbation expansion in frequency space (see Fig.1). There is no energy transfer at vertices between up and down spins due to the δ-function dispersion of fixed electrons . Effectively this means that closed loops factorize and thus contribute only globally. This decoupling of the dynamics of opposite spins was first utilized in the solution of the deep impurity X-ray scattering problem.[18]

Let us denote the grand potential of the simplified model, where σ-spins are mobile and $(-\sigma)$-spins are fixed, by Ω_σ . Say the $\uparrow$-spins were mobile. Introducing $n_\downarrow$, the density of static electrons, into the grand potential $\Omega_\uparrow$ and performing the analytic continuation to real frequencies we finally get[11]

$$\Omega_\uparrow(T, \mu_\uparrow, \mu_\downarrow, n_\downarrow; \{G_\uparrow\}, \{\Sigma_\uparrow\}) \;=$$

$$\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f_T(\omega)\Big\{\int_{-\infty}^{\infty} dE\rho_\infty(E) Im\ln(\omega+\mu_\uparrow-\Sigma_\uparrow(\omega)-E+i0^+)$$

$$+ Im\ln\left(1+G_\uparrow(\omega)\Sigma_\uparrow(\omega)\right)\Big\} + T[(1-n_\downarrow)\ln(1-n_\downarrow)+n_\downarrow\ln n_\downarrow] + (\epsilon_\uparrow-\mu_\downarrow)n_\downarrow\,, \quad (16)$$

where $f_T(\omega)$ is the Fermi function and

$$\epsilon_\uparrow = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f_T(\omega)\, Im\ln\left(1-\frac{UG_\uparrow(\omega)}{1+G_\uparrow(\omega)\Sigma_\uparrow(\omega)}\right) \quad (17)$$

is an energy shift of the atomic level of static electrons due to the closed loops of mobile electrons. Note that only $G_\uparrow(\omega)$ and $\Sigma_\uparrow(\omega)$, describing the mobile electrons, remain frequency-dependent variational parameters in (16), while the down spins enter only through *one* frequency independent (global) parameter, namely $n_\downarrow$. According to (6) and (11) $\Omega_\uparrow$ is stationary with respect to variations of $G_\uparrow(\omega)$, $\Sigma_\uparrow(\omega)$ for arbitrary ω and $n_\downarrow$.

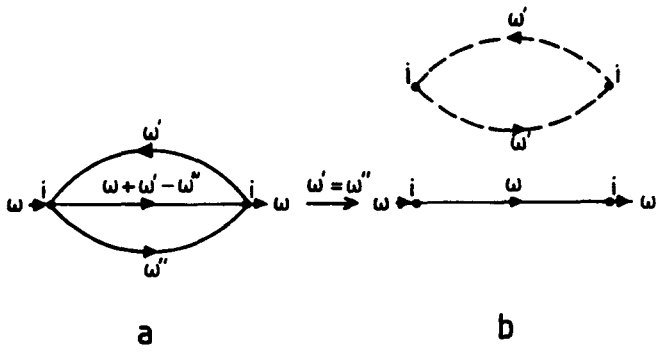

Fig. 1. Diagrammatic demonstration of the simplifications arising from a restriction of the dynamics of the electrons. The second order contribution to the local self-energy $\Sigma_{\uparrow,ii}(\omega)$ in $d=\infty$ is shown: (a) Hubbard model, full lines correspond to $\mathcal{G}_\uparrow$, $\mathcal{G}_\downarrow$; (b) simplified model with $\downarrow$-spins static; full line: $\mathcal{G}_\uparrow$, broken line: $\mathcal{G}_\uparrow^{at}$, i. e. $\mathcal{G}_\downarrow$ with $t_\downarrow = 0$.

4 Mean field expression for the grand potential of the Hubbard model

The exact grand potential for the simplified Hubbard model in $d = \infty$, Ω_σ, will now be used to construct an approximate grand potential Ω_{MF} for the Hubbard model. This is achieved as follows. Let the density of σ-particles be given by n_σ. We first restrict the dynamics of the Hubbard model, where both spin species are dynamical, to that of two simplified models where only one spin species is dynamical ($\uparrow$ and $\downarrow$, respectively) and the other is static. There is then no energy exchange between the two spin populations. In the second step the missing exchange is introduced on a *mean field* level by parametrizing it in terms of a few mean-field energy parameters.

To construct a grand potential Ω_{MF} for the Hubard model out of the potentials Ω_σ, we note that Ω_{MF} should (i) depend linearly on Ω_σ and $\Omega_{-\sigma}$, (ii) be symmetric in the spin index and, (iii) reproduce the atomic limit correctly. For the theory to be self-consistent we require that the particle densities $n_\uparrow$ and $n_\downarrow$ determined from $\Omega_\uparrow, \Omega_\downarrow$ and Ω_{MF} be the same, i. e. $n_\sigma = -\partial\Omega_x/\partial\mu_\sigma$ with $\Omega_x = \Omega_\uparrow, \Omega_\downarrow, \Omega_{MF}$, since all these potentials describe systems with the same particle densities n_σ. The simplest possible choice for Ω_{MF} is

$$\Omega_{MF} = \Omega_\uparrow + \Omega_\downarrow - \Omega_{at} \,, \tag{18}$$

where $\Omega_{at} = -T\ln(1+e^{\mu_\uparrow/T}+e^{\mu_\downarrow/T}+e^{(\mu_\uparrow+\mu_\downarrow-U)/T})$ is the grand potential of the atomic problem. The above self-consistency conditions require the chemical potentials μ_σ to be adjustable. This may be taken into account by introducing two pairs of energies E^L_σ, E^I_σ, where E^L_σ describes the effective mean field energy of fixed σ-spins, and E^I_σ parametrizes the mean energy *transfer* between mobile and fixed spins. E^I_σ shifts the center of the band of mobile electrons relative to the free case. This dynamical simplification is illustrated in Fig.2.

The chemical potentials entering $\Omega_\uparrow, \Omega_\downarrow$ and Ω_{at} must then be changed as

$$\mu_\uparrow \rightarrow \begin{cases} \mu_{\uparrow,at} \equiv \mu_\uparrow - E^L_\uparrow, & \text{in } \Omega_{at} \\ \mu_{\uparrow,\uparrow} \equiv \mu_\uparrow - E^I_\uparrow, & \text{in } \Omega_\uparrow \\ \mu_{\uparrow,\downarrow} \equiv \mu_\uparrow - E^L_\uparrow + E^I_\uparrow, & \text{in } \Omega_\downarrow \,. \end{cases} \tag{19}$$

In the case of $\mu_\downarrow$ all spins on the r.h.s. of (19) must be reversed.

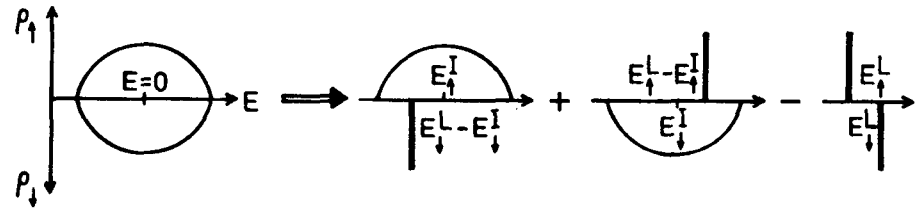

Fig. 2. Restriction of the dynamical exchange between opposite spins is illustrated in terms of the densities of state of ↑ and ↓ spins.

The mean field energies $E^{L,I}_\sigma$ have been introduced in such a way that they enter as variational parameters in Ω_{MF} and are thus determined from $\partial\Omega_{MF}/\partial E^{L,I}_\sigma = 0$; this condition is identical with our self-consistency condition $n_\sigma = -\partial\Omega_x/\partial\mu_\sigma$. Eliminating E^L_σ from Ω_{MF} we arrive at an explicit expression for Ω_{MF}:

$$\begin{aligned} &\Omega_{MF}(T, \mu_\sigma, n_\sigma, E^I_\sigma; \{\Sigma_\sigma\}, \{G_\sigma\}) \;= \\ &\frac{1}{\pi}\sum_\sigma \int_{-\infty}^{\infty} d\omega f_T(\omega)\Big[\int_{-\infty}^{\infty} dE \rho_\sigma(E)\, Im\, \ln(\omega + \mu_\sigma - E^I_\sigma - \Sigma_\sigma(\omega) - E + i0^+) \\ &\qquad + \; Im\, \ln(1 + G_\sigma(\omega)\Sigma_\sigma(\omega))\Big] \; + \; T\sum_\sigma \ln(1 - n_\sigma) \\ &+ T \ln\Big[1 + \sum_\sigma \kappa_\sigma exp[(\epsilon_{-\sigma} - E^I_\sigma)/T] + \kappa_\uparrow\kappa_\downarrow exp[(\epsilon_\uparrow + \epsilon_\downarrow - E^I_\uparrow - E^I_\downarrow - U)/T]\Big] \,, \end{aligned} \tag{20}$$

where $\kappa_\sigma = n_\sigma/(1-n_\sigma)$ and

$$\epsilon_\sigma = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f_T(\omega) Im \ln\left[1 - \frac{UG_\sigma(\omega)}{1+G_\sigma(\omega)\Sigma_\sigma(\omega)}\right] \tag{21}$$

is a shift of the atomic $(-\sigma)$-energy level as in (17). In Ω_{MF} the functions $\Sigma_\sigma(\omega), G_\sigma(\omega)$ and the parameters E^I_σ, n_σ appear as conjugate variables and are now determined by $\delta\Omega_{MF}/\delta G_\sigma = \delta\Omega_{MF}/\delta\Sigma_\sigma = 0$ and $\partial\Omega_{MF}/\partial n_\sigma = \partial\Omega_{MF}/\partial E^I_\sigma = 0$, respectively. The corresponding equations are:

$$G_\sigma(\omega) = \int_{-\infty}^{\infty} dE \rho_\sigma(E) \frac{1}{\omega + \mu_\sigma - E^I_\sigma - \Sigma_\sigma(\omega) - E + i0^+} \tag{22a}$$

$$\Sigma_\sigma(\omega) = \frac{Un_{-\sigma}}{1+G_\sigma(\omega)(\Sigma_\sigma(\omega)-U)} \tag{22b}$$

$$n_\sigma = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f_T(\omega) Im G_\sigma(\omega) \tag{22c}$$

$$= 1 - \frac{\exp[(\epsilon_{-\sigma} - E^I_\sigma)/T]}{Q}\left[1 + \kappa_{-\sigma}\exp[(\epsilon_\sigma - E^I_{-\sigma} - U)/T]\right] \tag{22d}$$

where

$$Q = 1 + \sum_\sigma \kappa_\sigma \exp[(\epsilon_{-\sigma} - E^I_\sigma)/T] + \kappa_\uparrow\kappa_\downarrow \exp[(\epsilon_\uparrow + \epsilon_\downarrow - E^I_\uparrow - E^I_\downarrow - U)/T]\,. \tag{23}$$

Setting $\rho_\uparrow(E) = \rho_\infty(E)$ and $\rho_\downarrow(E) = \delta(E)$, this set of equations coincides with the exact solution of the simplified model in $d = \infty$. The grand potential (20) constructed above defines a thermodynamically consistent, conserving approximation for the Hubbard model in the entire range of input parameters t, U, T and μ_σ (or n_σ). The solution (22) is particle-hole symmetric. The self-energies $\Sigma_\sigma(\omega)$ are determined from CPA-like algebraic equations and possess the necessary Herglotz property assuring uniqueness of the solution for fixed n_σ and E^I_σ. The self-energy does not, however, fulfil the Luttinger theorem,[19] i. e. $Im\Sigma_\sigma(0) \neq 0$ unless there is a band gap. This is a consequence of the simplified energy transfer between up and down spins taken over from the simplified Hubbard model where $Im\Sigma_\sigma(0) \neq 0$ is an exact property.

Luttinger's theorem does not hold when there is a degeneracy in momentum space at $T = 0$. Such a degeneracy is present in the case of fixed spins. Note, however, that the subtle question of possible degeneracy in the exact solution for the Hubbard model has not been answered yet in generality. Our mean field theory is therefore applicable either to the calculation of spectral properties away from the Fermi-level discontinuity or to global, e. g. thermodynamic, features of the model. In this respect it is complementary to Fermi liquid theory and the approach of Ref. 17.

In analogy to Ω_σ the grand potential Ω_{MF} can also be obtained diagrammatically. Let $\Omega_{(n)} = U^n \int d\nu \; D_\uparrow^{(n)} D_\downarrow^{(n)}$ be a diagrammatic contribution to Ω_{MF} with n vertices, where $D_\sigma^{(n)}$ is the part of the diagram due to σ-spins and $\int d\nu$ is the integral over all intermediate states. In our MFT $\Omega_{(n)}$ is evaluated by use of the spin-symmetric replacement (cf. Fig.1)

$$\int d\nu \; D_\uparrow(\mu_\uparrow) D_\downarrow(\mu_\downarrow) \rightarrow \int d\nu \left[\sum_\sigma D_{-\sigma}^{at}(\mu_{-\sigma,\sigma}) D_\sigma(\mu_{\sigma,\sigma}) - D_\uparrow^{at}(\mu_{\uparrow,at}) D_\downarrow^{at}(\mu_{\uparrow,at}) \right] . \quad (24)$$

Here the superscript *at* means that the propagators are made static (atomic limit, $t = 0$). The construction of Ω_{MF} is conceptually similar to that of the Hubbard-III solution;[6] actually the self-energy $\Sigma(\omega)$ derived from Ω_{MF} coincides with the Hubbard-III solution in the paramagnetic phase ($h = 0$) either at $T = 0$ or $n = 1$. Note, however, that the latter approximation has a number of serious deficiencies (it does not allow for any magnetic order and does not reproduce the Heisenberg limit at $n = 1$ and $U \rightarrow \infty, T \rightarrow 0$). Moreover, there is no generating functional for the Hubbard-III solution, and thus it is diagrammatically uncontrolled. For example, the contribution from closed loops of mobile electrons that leads to the shift ϵ_σ in (20),(22) is neglected. By contrast, the mean-field solution (22) correctly reproduces the Heisenberg model with the Curie susceptibility and allows for antiferromagnetic ordering, at least at large U. The fact that this limit is described correctly in our theory is due to the existence of the mean field energies $E_\sigma^{L,I}$, which simulate the effect of magnetic fluctuations. These parameters are missing in the Hubbard-III solution.

5 States with broken symmetry

Besides the paramagnetic state discussed so far, our theory can also describe states with broken symmetry. For example, to discuss a solution with finite magnetization $m = n_\uparrow - n_\downarrow \neq 0$ the spin dependence of the parameters E_σ^I and n_σ in (20) has to be kept, even in the case $h = 0$. The instability of the paramagnetic state towards such a ferromagnetic state is found as usual from the divergence of the susceptibility χ, equal to the negative second derivative of Ω_{MF} with respect to h. Alternatively, one may calculate the inverse of χ by taking the second derivative of Ω_{MF} with respect to the order parameter m. An instability is then signalled by $\chi^{-1} \leq 0$. Numerical investigations of (22) in the limit $U = \infty$, $T = 0$ show that $\chi > 0$ for all n. The paramagnetic state is found to have a lower energy than *any* spin polarized solution. This is in contrast to an analytic result obtained by us at an earlier stage of this work, where we *assumed* that for $T = 0, U = \infty$ and $\delta = 1 - n \ll 1$ there exists a strongly polarized ferromagnetic state ($n_\uparrow < 1, n_\downarrow \ll 1$) in the thermodynamic limit. We then found the Nagaoka state to decay into an unsaturated ferromagnet with a band of minority spins. In fact the current numerical calculations show that the assumption $n_\downarrow \ll 1$ does not lead to the correct ground state.

In the case of an antiferromagnetic state one has the additional complication of a broken translational symmetry. The grand potential Ω_{MF}, (20), then has to be modified by introducing A-B sublattices. In general one has to add one more index to all variables in (20) that refers to their sublattice (e. g. $n_\sigma \to n_{\alpha\sigma}, \alpha = A, B$). In the case of a pure antiferromagnet ($n_{A\sigma} = n_{B-\sigma}$) only those terms in Ω_{MF} have to be modified which depend on the density of states, i. e. one has to replace the first term in (20) by

$$\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega f_T(\omega) \int_{-\infty}^{\infty} dE \rho_\sigma(E)$$

$$\times Im \ln \left[\Big(\omega + \mu_\sigma - E_\sigma^I - \Sigma_\sigma(\omega)\Big)\Big(\omega + \mu_{-\sigma} - E_{-\sigma}^I - \Sigma_{-\sigma}(\omega)\Big) - E^2 \right] \quad (25)$$

as in the case of the simplified Hubbard model.[11] The spin index is then uniquely coupled with the sublattice index and the magnetic field, which enters Ω_{MF} via μ_σ,

coincides with the *staggered* field. The instability of the paramagnetic state with respect to antiferromagnetic fluctuations is again signalled by the divergence of the second derivative of Ω_{MF} (with the substitution (25)) with respect to h. For $U \ll t$ we obtain Hartree-Fock theory. However, the terms beyond Hartree-Fock lead to $Im\Sigma \neq 0$ (see the discussion in Sec.4). This implies that in our theory at $n = 1$ the Hubbard model has no antiferromagnetic state at very low U even for lattices with perfect nesting. On the other hand in the Heisenberg limit ($U \gg t, n = 1, T \to 0$) one finds for the inverse staggered susceptibility

$$\chi^{-1} = 2[T + \theta(U,T)]\,, \tag{26}$$

where θ is still a function of U and T, with $\theta = 0$ for $U = \infty, T = 0$. For fixed U the T-dependence of θ is only exponentially small. For fixed T the leading U-dependence is $\theta \propto -1/U$. This indicates that there exists a finite critical temperature $T_N \propto 1/U$, the Néel temperature, at which the transition to the antiferromagnetic state occurs.

6 Discussion

We derived in this paper an exact expression for the grand potential of the Hubbard model in $d = \infty$ in closed form. From this we constructed a comprehensive, thermodynamically consistent, conserving mean field theory for the Hubbard model. It is applicable in the entire range of input parameters and is exact in the following limits: (i) free case (for $U \to 0$ Hartree-Fock is reproduced), (ii) atomic limit ($t = 0$), (iii) simplified Hubbard model ($t_\sigma = -t, t_{-\sigma} = 0$) in $d = \infty$, (iv) Heisenberg antiferromagnet ($U \gg t, n = 1$). This is the first approximate theory which correctly reproduces these non-trivial opposite limits. In particular, no other mean-field-type theory has so far been able to yield the Curie susceptibility in the Heisenberg limit.[20] That means that our theory not only describes the ground state correctly in this limit, but even the excited states.

The theory is diagrammatically controlled, i. e. the entire perturbation theory is summed by assuming a simplified energy transfer between up and down spins. How-

ever, as a consequence of the simplified energy transfer the imaginary part of the self-energy does not vanish at the Fermi surface unless there is a gap. Hence Luttinger's theorem is not fulfilled. Our theory can therefore not be used to investigate questions related to Fermi liquid behavior of the Hubbard model. Rather, it may be applied to calculate spectral properties away from the Fermi-level discontinuity, and to construct a global phase diagram for the Hubbard model. It may also be applied to other fermionic models (e. g. $t-J$ model, periodic Anderson model, etc.) and can be extended to include disorder. This allows one to investigate the interplay between interactions and disorder on the same mean field level.

Finally, we would like to comment on the role of the mean field energies $E_\sigma^{L,I}$, whose existence is crucial to obtain a thermodynamically consistent, conserving theory. These energies, which renormalize the spin-dependent chemical potentials μ_σ, enter as variational parameters in our theory. For fixed n_σ they *maximize* the free energy, as do the chemical potentials μ_σ. It can be shown that at $T=0$ the ground state energy obtained from our mean field theory is an *exact lower bound* for the ground state energy of the Hubbard model in $d=\infty$.[21]

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References

[1] M.C.Gutzwiller, Phys.Rev.Lett. **10**, 159 (1963); J.Hubbard, Proc. Roy. Soc. London. **A276**, 238 (1963); J.Kanamori, Prog. Theor. Phys. **30**, 275 (1963)

[2] C.Itzykson and J.M.Drouffe, *Statistical Field Theory*, Vol.I and II (Cambridge University Press, Cambridge, 1989)

[3] W.Metzner and D.Vollhardt, Phys.Rev.Lett. **62**, 324 (1989)

[4] For reviews, see E.Müller-Hartmann, Int.J.Mod.Phys. **B3**, 2169 (1989); D.Vollhardt, Physica **B169**, 277 (1991)

[5] E.Müller-Hartmann, Z.Phys. **B74**, 507 (1989), ibid. **B76**, 211 (1989)

[6] J.Hubbard, Proc.Roy.Soc. London,Ser. **A281**, 401 (1964)

[7] M.C.Gutzwiller, Phys.Rev. **137**, A1726 (1965)

[8] L.M.Falicov and J.C.Kimball, Phys.Rev.Lett. **22**, 997 (1969); T.Kennedy and E.H.Lieb, Physica **A138**, 320 (1986); E.H.Lieb, Physica **A140**, 240 (1986)

[9] U.Brandt and C.Mielsch, Z.Phys.B **75**, 365 (1989), ibid.B **79**, 295 (1990), ibid. **B82**, 37 (1991)

[10] P.van Dongen and D.Vollhardt, Phys.Rev.Lett. **65**, 1663 (1990)

[11] V.Janiš, Z.Phys. **B83**, 227 (1991)

[12] D.Sherrington and S. Kirkpatrick, Phys.Rev.Lett. **32**, 1792 (1975)

[13] R.J.Elliot, J.A.Krumhansl and P.L.Leath, Rev.Mod.Phys. **46**, 465 (1974)

[14] R.Vlaming and D.Vollhardt, Preprint RWTH-ITP-C 6/91, Technische Hochschule Aachen, submitted to Phys.Rev. B

[15] G.Baym, Phys.Rev. **127**, 836 (1962)

[16] V.Janiš, Phys.Rev. **B40**, 11331 (1989)

[17] A.Georges and G.Kotliar, preprint, Rutgers University, June 1991

[18] P.Nozières and C.T.De Dominicis, Phys.Rev. **178**, 1097 (1969)

[19] J.M.Luttinger, Phys.Rev. **121**, 942 (1961)

[20] A.Kawabata, Progr.Theor.Phys. **48**, 1793 (1972)

[21] V.Janiš and D.Vollhardt, to be published