Construction of analytically tractable mean-field theories for quantum models, II: susceptibilities and energy bounds for the Hubbard model

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Construction of analytically tractable mean-field theories for quantum models

II. Susceptibilities and energy bounds for the Hubbard model

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Abstract. The mean-field theory for the Hubbard model constructed in the preceding paper is worked out in detail. The ferro- and antiferromagnetic susceptibilities are calculated explicitly. It is shown that the singularities suggested by the Stoner theory are spurious since two-particle correlation effects are neglected. At $T=0$, $n=1$ and large U the correct Curie-Weiss behavior is recovered. For $U=\infty$ the antiferromagnetic susceptibility is found to vanish logarithmically at a generic density $n=2/3$, corresponding to a half-filled lower Hubbard band. The magnetic $U-n$ phase diagram is determined for $T=0$; below a critical density $n_c=0.77$ the antiferromagnetic phase is found to be unstable for all U. Rigorous lower and upper bounds on the ground state energy of the Hubbard model in $d=\infty$ are calculated; they almost coincide for $n=1$ and thus determine the exact result very accurately. An investigation of the ground state spectral properties in the ordered phase at fixed density $n_c<n<1$ reveals an interesting transition scenario for increasing U, namely transitions from a paramagnetic metal to an antiferromagnetic metal and then to an antiferromagnetic insulator; further increase of U leads to a reversal of this sequence back to the paramagnetic metal. The theory described here generalizes the well-known, but ad hoc, alloy-analogy approximation and puts it on a firm, thermodynamically consistent basis.

1. Introduction

In the preceding paper [1], referred to in the following as *I*, a general theoretical formalism for the construction of maximally complex, yet analytically tractable mean-field theories (MFTs) for quantum-mechanical models was presented. The need for such MFTs is felt particularly strongly in the case of Hubbard-type models where the existence of a site-diagonal interaction term prohibits an exact *analytic* solution of the model even in the limit of $d=\infty$ dimensions [2]. The mean-field construction developed in *I* is based on a decomposition of a given Hamiltonian into a set of simplified sub-Hamiltonians whose dynamics can be calculated analytically within a self-consistent single-site ("mean-field") approximation. The dynamical *exchange* between the subsystems is then approximated on a mean-field level, too, in terms of a few variational ("mean-field") energy parameters. These parameters are determined by optimizing the resulting mean-field energy. In *I* we applied this construction scheme to the Hubbard model by decomposing the latter into two Falicov-Kimball models for mobile up and down spins, respectively, which are known to be exactly solvable in $d=\infty$ [3, 4]. Thus we derived a MFT valid in the *strong*-coupling regime which, in contrast to Hartree-Fock theory, contains the important atomic solution. This MFT provides a *lower* bound on the exact ground state energy of the Hubbard model and hence complements the Hartree-Fock theory which is valid at weak coupling and provides an *upper* bound. The MFT is conceptually similar to the well-known Hubbard-III solution [5], but – in contrast to the latter – is a thermodynamically consistent, diagrammatically controlled theory with exact limits. There have been numerous attempts in the past based on the so-called "alloy analogy" to extend the Hubbard-III approximation [5] in such a way that it includes solutions with long-range magnetic order [6]. These theories made rather ad hoc assumptions about the form of the fluctuations of magnetic moments and were not able to remove the thermodynamic inconsistencies of the Hubbard-III solution. Indeed, only the exact solution of the Falicov-Kimball model in $d=\infty$ [3, 4] and the MFT construction scheme presented in *I* make it possible to develop the Hubbard-III solution into a controlled, thermodynamically consistent theory.

The aim of this paper is to study the zero-temperature properties of the Hubbard model within the MFT formulated in [7] and rederived in a more general context in *I*, in particular the ground-state phase diagram, spectral properties and the total energy. We restrict ourselves to pure phases and will assume either ferromagnetic or antiferromagnetic instabilities. The paper is organized as follows: in Sect. 2 a mean-field free energy for a general

solution with $A-B$ sublattice structure is presented. The mean-field susceptibilities are derived and discussed in Sect. 3. In Sect. 4 a mean-field phase diagram is constructed. Variational lower and upper bounds on the ground-state energy of the Hubbard model in $d=\infty$ are calculated and compared in Sect. 5. In Sect. 6 the spectral properties of the antiferromagnetic phase are investigated and a sequence of phase transitions is observed. The results are discussed in Sect. 7.

2. Mean-field free energy for the ferromagnetic and antiferromagnetic solutions

One of the main goals of a MFT is to describe, on a simplified "mean-field" level, the thermodynamics of a given model. Thus the phase diagram, i.e. possible instabilities of thermodynamic phases with a given symmetry, may be calculated. Due to the variational character of the MFTs constructed in *I* it is clear how to search for the instabilities of a mean-field solution. The instabilities of a phase with a given global symmetry are signalled by the violation of the stability condition $\bar{V}^2\Omega_{\mathrm{MF}}\leqq 0$, where the nabla operator denotes the total differential with respect to the variational parameters in the mean-field grand potential Ω_{MF}. Although the instabilities can, in principle, be investigated within an even more general context, we restrict our investigation here to ferromagnetic and antiferrogmagnetic instabilities only. For this it is necessary to write down the explicit expressions for the corresponding free energies with broken symmetries. Based on the arguments given in *I* we choose $\lambda_\sigma=1$ and $\lambda_{\mathrm{at}}=-1$ in the general expression for the mean-field free energy (see (22) of *I*). We can further replace the variables E_σ^L by their conjugate variables n_σ (particle density of σ-electrons) via a Legendre transformation. We then obtain the following result for the grand potential per lattice site, valid for a *homogeneous*, spin-polarized ($n_\uparrow \neq n_\downarrow$), i.e. ferromagnetic, solution [7]:

$$\begin{aligned}
&\frac{1}{L}\,\Omega_{\mathrm{MF}}^F(U,T,\mu_\sigma,E_\sigma^I)\\
&=\frac{1}{\pi}\sum_\sigma\int_{-\infty}^{\infty}\mathrm{d}\omega\, f(\omega)\left[\int_{-\infty}^{\infty}\mathrm{d}E\,\rho_\sigma(E)\right.\\
&\quad\times\operatorname{Im}\ln(\omega+\mu_\sigma-E_\sigma^I-\Sigma_\sigma(\omega)-E+i0^+)\\
&\quad\left.+\operatorname{Im}\ln(1+G_\sigma(\omega)\Sigma_\sigma(\omega))\right]+\beta^{-1}\sum_\sigma\ln(1-n_\sigma)\\
&\quad+\beta^{-1}\ln\left[1+\sum_\sigma\kappa_\sigma\exp\{\beta(\mathscr{E}_{-\sigma}-E_\sigma^I)\}\right.\\
&\quad\left.+\kappa_\uparrow\kappa_\downarrow\exp\{\beta(\mathscr{E}_\uparrow+\mathscr{E}_\downarrow-E_\uparrow^I-E_\downarrow^I-U)\}\right],
\end{aligned}\tag{1a}$$

where

$$f(\omega)=[\exp(\beta\omega)+1]^{-1},\quad \beta=1/T,\quad \kappa_\sigma=n_\sigma/(1-n_\sigma)$$

and

$$\begin{aligned}
\mathscr{E}_\sigma&=\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\, f(\omega)\\
&\quad\times\operatorname{Im}\ln\left(1-\frac{UG_\sigma(\omega)}{1+G_\sigma(\omega)\Sigma_\sigma(\omega)}\right).
\end{aligned}\tag{1b}$$

Apart from the ferromagnetic solution we expect, for a bipartite lattice, an antiferromagnetic solution, too. The corresponding grand potential can be constructed in the same way as for the Falicov-Kimball model [4, 7] by generalizing the first term on the r.h.s. of (1a), i.e. by labelling the lattice sites by the additional sublattice index $\alpha=A,B$. We then obtain the following thermodynamic potential, valid also in the antiferromagnetic phase

$$\begin{aligned}
&\frac{2}{L}\,\Omega_{\mathrm{MF}}^{\mathrm{AF}}(U,T,\mu_\sigma,E_\sigma^{I\alpha})\\
&=\frac{1}{\pi}\sum_\sigma\int_{-\infty}^{\infty}\mathrm{d}\omega\, f(\omega)\left[\int_{-\infty}^{\infty}\mathrm{d}E\,\rho_\sigma(E)\right.\\
&\quad\times\operatorname{Im}\ln[(\omega+\mu_\sigma-E_\sigma^{IA}-\Sigma_\sigma^A(\omega)+i0^+)\\
&\quad\times(\omega+\mu_\sigma-E_\sigma^{IB}-\Sigma_\sigma^B(\omega)+i0^+)-E^2]\\
&\quad\left.+\sum_\sigma\operatorname{Im}\ln(1+G_\sigma^\alpha(\omega)\Sigma_\sigma^\alpha(\omega))\right]\\
&\quad+\beta^{-1}\sum_{\alpha,\sigma}\ln(1-n_{\alpha\sigma})\\
&\quad+\beta^{-1}\sum_\alpha\ln\left[1+\sum_\sigma\kappa_\sigma^\alpha\exp\{\beta(\mathscr{E}_{-\sigma}^\alpha-E_\sigma^{I\alpha})\}\right.\\
&\quad\left.+\kappa_\uparrow^\alpha\kappa_\downarrow^\alpha\exp\{\beta(\mathscr{E}_\uparrow^\alpha+\mathscr{E}_\downarrow^\alpha-E_\uparrow^{I\alpha}-E_\downarrow^{I\alpha}-U)\}\right].
\end{aligned}\tag{2}$$

When there is no dependence on the sublattice index α, the r.h.s. of (2) reduces the (1). The Eqs. for the functions $\Sigma_\sigma^\alpha(\omega)$, $G_\sigma^\alpha(\omega)$ and the parameters $n_{\alpha,\sigma}$ and $E_\sigma^{I\alpha}$ are obtained from the stationarity of (2) with respect to variations of these veriables. They are explicitly given by

$$\begin{aligned}
G_\sigma^\alpha(\omega)&=\int_{-\infty}^{\infty}\mathrm{d}E\,\rho_\sigma(E)\\
&\quad\times\frac{1}{\omega+\mu_\sigma-E_\sigma^{I\alpha}-\Sigma_\sigma^\alpha(\omega)+i0^+-\dfrac{E^2}{\omega+\mu_\sigma-E_\sigma^{I-\alpha}-\Sigma_\sigma^{-\alpha}(\omega)+i0^+}}
\end{aligned}\tag{3a}$$

$$\Sigma_\sigma^\alpha(\omega)=\frac{Un_{\alpha-\sigma}}{1+G_\sigma^\alpha(\omega)(\Sigma_\sigma^\alpha(\omega)-U)},\tag{3b}$$

$$n_{\alpha\sigma}=-\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\, f(\omega)\operatorname{Im}G_\sigma^\alpha(\omega)\tag{3c}$$

$$\begin{aligned}
&=1-\frac{\exp\{\beta(\mathscr{E}_{-\sigma}^\alpha-E_\sigma^{I\alpha})\}}{Q_\alpha}\\
&\quad\times[1+\kappa_{-\sigma}^\alpha\exp\{\beta(\mathscr{E}_\sigma^\alpha-E_{-\sigma}^{I\alpha}-U)\}]
\end{aligned}\tag{3d}$$

where

$$Q_\alpha = 1 + \sum_\sigma \kappa_\sigma^\alpha \exp\{\beta(\mathscr{E}_{-\sigma}^\alpha - E_\sigma^{I\alpha})\}$$
$$+ \kappa_\uparrow^\alpha \kappa_\downarrow^\alpha \exp\{\beta(\mathscr{E}_\uparrow^\alpha + \mathscr{E}_\downarrow^\alpha - E_\uparrow^{I\alpha} - E_\downarrow^{I\alpha} - U)\}. \quad (3e)$$

The grand potential (2) with Eqs. (3) is able to describe any solution exhibiting spin or charge density wave order. We will investigate only the occurance of second-order phase transitions due to instabilities of the paramagnetic phase with respect to purely ferromagnetic and antiferromagnetic states. These can be found by projecting the general instability condition $\nabla^2 \Omega_{\mathrm{MF}} \geqq 0$ onto directions in the parameter space which correspond to changes in homogeneous and staggered magnetic fields for ferromagnetic and antiferromagnetic instabilities, respectively. They explicitly read

$$\left.\frac{d^2\Omega_{\mathrm{MF}}^F}{dh^2}\right|_{h=0} \geqq 0 \quad (4a)$$

$$\left.\frac{d^2\Omega_{\mathrm{MF}}^{\mathrm{AF}}}{dh_s^2}\right|_{h_s=0} \geqq 0, \quad (4b)$$

where $h_s = h$ on the sublattice A and $h_s = -h$ on the sublattice B. Of course, all the parameters appearing in Ω_{MF} are functions of h and h_s, respectively.

3. Mean-field susceptibilities

The instability criteria of the paramagnetic phase, (4), are closely related to the homogeneous and staggered susceptibilities. The stationarity of Ω_{MF} with respect to all intrinsic parameters (which is a requirement for thermodynamic consistency of the theory) implies

$$\frac{d\Omega_{\mathrm{MF}}^F}{dh} = -\langle m \rangle$$
$$\equiv \frac{1}{2\pi} \sum_{\alpha,\sigma} \sigma \int_{-\infty}^{\infty} d\omega f(\omega) \operatorname{Im} G_\sigma^\alpha(\omega), \quad (5a)$$

and

$$\frac{d\Omega_{\mathrm{MF}}^{\mathrm{AF}}}{dh_s} = -\langle \tilde{m} \rangle$$
$$\equiv \frac{1}{2\pi} \sum_{\alpha,\sigma} \alpha \int_{-\infty}^{\infty} d\omega f(\omega) \operatorname{Im} G_\sigma^\alpha(\omega), \quad (5b)$$

and hence

$$\frac{d^2\Omega_{\mathrm{MF}}^F}{dh^2} = -\chi_F, \quad \frac{d^2\Omega_{\mathrm{MF}}^{\mathrm{AF}}}{dh_s^2} = -\chi_{\mathrm{AF}}. \quad (6)$$

We evaluate the susceptibilities χ_F and χ_{AF} only in the paramagentic phase with $h=0$ and $h_s=0$. The expressions for these susceptibilities are very similar; we derive the homogeneous (ferromagnetic) susceptibility first and then introduce the necessary changes into the final expression to obtain the staggered (antiferromagnetic) susceptibility.

The calculation of the susceptibilities is simplified by using the electron-hole symmetry of the grand potential Ω_{MF}. It follows from the form of (3) that the exchange of electrons and holes, i.e. $\omega \to -\omega$, $E \to -E$, $\mu \to U - \mu$, leads to the following changes of the intrinsic parameters and functions

$$\Sigma_\sigma(\omega) \to U - \Sigma_{-\sigma}^*(-\omega), \quad \mathscr{E}_\sigma \to U - \mathscr{E}_{-\sigma},$$
$$E_\sigma^I \to -E_{-\sigma}^I, \quad n_\sigma \to 1 - n_{-\sigma}. \quad (7)$$

As a consequence we have $\chi = dn_\uparrow/dh$ in the paramagnetic phase, i.e.

$$\chi_F = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega f(\omega)$$
$$\times \operatorname{Im}\left\{\langle G(\omega)^2 \rangle \left(\frac{1}{2} - \frac{dE^I}{dh} - \frac{d\Sigma(\omega)}{dh}\right)\right\}, \quad (8a)$$

where

$$\langle G(\omega)^2 \rangle \equiv \int_{-\infty}^{\infty} dE \rho(E)$$
$$\times [\omega + \mu - E^I - \Sigma(\omega) - E + i0^+]^{-2}, \quad (8b)$$

and $h=0$. The derivatives needed in (8) are obtained from (3). After some manipulations one finds

$$(2\chi_F)^{-1} = T \frac{n^2 - \bar{d}}{n(1-n)(n-\bar{d})}$$
$$+ \frac{(1 - U\mathscr{J}(U))^2}{\mathscr{J}(U)} - U^2 \mathscr{K}(U), \quad (9)$$

where $\bar{d}$ denotes the density of double occupancy

$$\bar{d} = \frac{n^2}{(1-n)^2} \frac{\exp[\beta(2\mathscr{E} - 2E^I - U)}{Q}, \quad (10a)$$

and $\mathscr{I}(U)$, $\mathscr{J}(U)$ and $\mathscr{K}(U)$ are frequency integrals defined by

$$\mathscr{I}(U) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega f(\omega) \operatorname{Im} \frac{\langle G(\omega)^2 \rangle}{\Gamma(\omega)}, \quad (10b)$$

$$\mathscr{J}(U) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega f(\omega)$$
$$\times \operatorname{Im} \frac{\langle G(\omega)^2 \rangle (1 + 2G(\omega)\Sigma(\omega) - UG(\omega))}{\Gamma(\omega)}, \quad (10c)$$

$$\mathscr{K}(U) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega f(\omega)$$
$$\times \operatorname{Im} \frac{(\langle G(\omega)^2 \rangle - G(\omega)^2)}{(1 + G(\omega)\Sigma(\omega))(1 + G(\omega)(\Sigma(\omega) - U))\Gamma(\omega)}, \quad (10d)$$

with

$$\Gamma(\omega) \equiv 1 + 2G(\omega)\Sigma(\omega)$$
$$- UG(\omega) + \Sigma(\omega)(\Sigma(\omega) - U)\langle G(\omega)^2 \rangle. \quad (10e)$$

The three contributions to the inverse susceptibility in (9) have a clear physical interpretation. The first term is a net contribution from the local moments. The second one is a contribution due to the effective interaction between itinerant electrons, and the last one has its origin in the direct interaction between itinerant and local electrons. The form of the susceptibility (9) is generic for the MFT provided by (1), (2). Namely, the *staggered* susceptibility (in the absence of a charge density wave) has the same form as that given by (9) and (10), only the quantity $\langle G(\omega)^2\rangle$ is replaced by

$$\langle G(\omega)^2\rangle \to \frac{G(\omega)}{\omega+\mu-E^I-\Sigma(\omega)+i0^+}. \tag{11}$$

We can hence discuss both the homogeneous *and* the staggered susceptibilities in terms of (9) and (10).

We first reveal the asymptotics of the susceptibilities in two limiting cases: $U\to 0$ and $U=\infty$, $n=1$, $T\to 0$. In the former case we obtain, to leading order in U, $(n^2-\bar{d})/[n(1-n)(n-d)]\approx \beta U$ and

$$(2\chi_F)^{-1}\approx\left[\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\, f(\omega)\,\mathrm{Im}\langle G(\omega)^2\rangle\right]^{-1}-U. \tag{12}$$

This is precisely the Hartree-Fock (Stoner) susceptibility which formally diverges at a critical interaction strength U_c given by the first term on the r.h.s. of (12) [8]. However, this divergence must not be taken seriously since Hartree-Fock is a *weak*-coupling theory which is no longer applicable at values of the order of $U\simeq U_c$. Indeed, from (9) we see that the Stoner-instability at U_c does not occur at all since there exist quadratic (and higher order) terms in U which originate from genuine two-particle correlations and which tend to suppress this instability or, at least, shift it to higher U-values [9]. On the other hand, in the Heisenberg limit $n=1$, $U\to\infty$ and $T\to 0$, the mean-field susceptibility (9) correctly reproduces the Curie law, since only the first term of (9) survives in leading order. This means that in this limit the MFT (2) not only reproduces the ground (Néel) state, but also the relevant excitations.

From (9) we can learn about the differences between the thermodynamically consistent MFT defined by (2) and the Hubbard-III solution [5]. The latter approximation has no free energy, but its self-energy can be obtained from (3) if we put $E_\sigma^I=0$ and *drop* Eq. (3d). It was already shown earlier [10] that this approximation does not reproduce the Curie law in the Heisenberg limit. Actually, if we calculate the susceptibility with $E_\sigma^I=0$ we obtain the Hubbard-III result

$$(2\chi_{\mathrm{III}})^{-1}=\frac{1}{\mathscr{J}(U)}(1-U\mathscr{J}(U)), \tag{13}$$

which contains only the linearized term due to the effective interaction of itinerant electrons. It thus reproduces the Stoner susceptibility in the weak-coupling limit correctly, but fails to reproduce the Curie law in the Heisenberg limit because there is no net contribution of the *local* moments. Moreover, the susceptibility remains finite even at $T=0$, $n=1$, $U=\infty$, where all spin states have the same energy $E=0$ and thus all susceptibilities *must diverge*. To understand this we note that in (9) the *square* of the numerator of (13) appears which has the correct asymptotics. The origin of the square lies in the parameters E_σ^I which mediate the effective interaction between the itinerant electrons. There is no direct interaction between the itinerant electrons in the two theories, since only local electrons interact directly with the itinerant ones. Hence the difference between our MFT, (2), and the Hubbard-III solution is that the former theory treats the auxiliary local electrons consistently while the latter one removes them from the theory in an uncontrolled way. The importance of the energy parameters E_σ^I in the MFT defined by (2) can also be seen from a comparison of the susceptibility (9) and that for the Falicov-Kimball model [3], where the corresponding density-density correlation function for the static electrons is given by [11]

$$(2\chi_{\mathrm{FK}})^{-1}=\frac{T}{n(1-n)}-U^2\mathscr{K}(U), \tag{14}$$

i.e. where the second term of (9) is missing. We can see that the mean-field parameters E_σ^I mediate a genuine dynamical energy exchange between itinerant ↑- and ↓-electrons and thus also change significantly the dynamics of the Falicov-Kimball model on which the MFT is based. We will see later that (9) and (14) actually predict different phases for the ground state in some limits.

4. Mean-field phase diagram

Using (9) we may construct the phase boundaries between the (anti-)ferromagnetic and the paramagnetic phase. We confine our investigation to $T=0$. By that we reduce the number of relevant parameters but do not change the essential features of the phase diagram. We will investigate separately the case $U=\infty$ and that of finite U. For $U=\infty$ the only relevant parameter is the particle density (band filling) and we do not expect the existence of an antiferromagnetic solution for $n<1$. For $U<\infty$ the phase space is more complex (n and U are relevant) and we expect an antiferromagnetic ground state close to half filling. For all explicit numerical evaluations the density of states (DOS) of the non-interacting electrons is chosen to be a half-ellipse, corresponding to a Bethe lattice with coordination number $Z=\infty$. This DOS closely resembles that of lattices in $d=3$ and its simple form allows one to gain valuable analytic insight into the results.

4.1. $U=\infty$

In the mean-field grand potential (2) with Eqs. (3) we may directly put $U=\infty$. The same is true for the susceptibilities (9)-(11). From (3c) we obtain $\Sigma(\omega)=-\nu G(\omega)^{-1}$ for the paramagnetic solution, where $\nu=n/2$ describes the band filling, e.g. $n=1$ implies a half filled band ($\nu=\frac{1}{2}$), etc.. Furthermore, at $U=\infty$ we have $\bar{d}=0$ and

$$\lim_{U\to\infty}[U^2\mathscr{K}(U)]=g_0(\nu,T) \tag{15a}$$

$$\lim_{U\to\infty}[-U\mathscr{J}(U)]=g_1(\nu,T) \tag{15b}$$

$$\mathscr{J}(U=\infty)=g_2(\nu,T) \tag{15c}$$

where

$$g_l(\nu,T)=\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\, f(\omega)\,\mathrm{Im}\,\frac{(G(\omega))^l\langle G(\omega)^2\rangle}{G(\omega)^2-\nu\langle G(\omega)^2\rangle}. \tag{15d}$$

In the case of a Bethe lattice, where $G(z)=1/(z-G(z))$ for non-interacting electrons, we find explicit expressions for the inverse susceptibilities at $T=0$:

$$\chi_F^{-1}=-\frac{2}{\pi\sqrt{1-\nu}}\left[-\sqrt{1-x^2}+\frac{(\cos^{-1}x)^2}{\sqrt{1-x^2}}\right], \tag{16a}$$

$$\chi_{\mathrm{AF}}^{-1}=-\frac{2(1-\theta(\bar{\mu}))^2}{S(\bar{\mu})}+\frac{2}{1-\nu}S(\bar{\mu}), \tag{16b}$$

where

$$S(\bar{\mu})=\frac{1}{4\pi\sqrt{1-\nu}}P\int_{-1/x}^{1}\frac{\mathrm{d}z}{z}\sqrt{1-z^2x^2}. \tag{16c}$$

Here $x=\bar{\mu}/2\sqrt{1-\nu}$ with $\bar{\mu}=\mu-E^I$ as the renormalized chemical potential, θ is the step function and P stands for the principal value. We note that $\bar{\mu}$ is connected with the band filling via (3d) which at $U=\infty$ is given by

$$\nu=\frac{1+Y}{3+Y}, \tag{17a}$$

with

$$Y=\frac{2}{\pi}(\sin^{-1}x+x\sqrt{1-x^2}). \tag{17b}$$

Equations (16)–(17) enable one to evaluate the susceptibilities as functions of the particle density n or the hole density $\delta=1-n$. Note that it is not necessary to know the bare value of the chemical potential μ (i.e. the shift E^I). Both inverse susceptibilities are plotted in Fig. 1. They reproduce two exact properties of the model, namely $\chi\to 0$ for $n\to 0$ and $\chi^{-1}\to 0$ for $n\to 1$. The latter property is a consequence of the degeneracy of the Hubbard model at $U=\infty$, $T=0$, and $n=1$. This asymptotic behavior thus serves as an important test of the reliability of any approximate theory in the strong-coupling regime. Neither of the susceptibilities shows an instability, i.e. $\chi^{-1}>0$ for $n<1$. Although the ferromagnetic correlations are stronger than the antiferromagnetic ones, they are not sufficient to create long-range order. This means that, within our MFT, neither a saturated ("Nagaoka") nor a non-saturated ferromagnetic state is stable in the thermodynamic limit. An interesting feature is seen in the staggered susceptibility for one-third filling ($\nu=\frac{1}{3}$). This value of ν corresponds to a *half-filled* lower Hubbard band ($\mu=E^I$), i.e. $\bar{\mu}=0$ in (17). Note that the band remains symmetric about its center in this case and carries a weight 2/3 compared to the upper (empty) band. For $\nu\to\frac{1}{3}$ the quantity $S(\bar{\mu})$, (16c), diverges and hence the staggered susceptibility itself vanishes logarithmically. In this situation the magnetization is no longer a linear function of the field; this indicates the breakdown of linear-response theory. The logarithmic divergence of the *inverse* staggered susceptibility at $\nu=\frac{1}{3}$ and $U=\infty$ is caused by the perfect-nesting of particles in the lower Hubbard band and, hence, is analogous to the logarithmic divergence of χ^{stag} itself at half-filling ($\nu=\frac{1}{2}$ and $U>0$).

The vanishing of χ_{AF} for $\nu=\frac{1}{3}$ at $U=\infty$ is an exact property of the Falicov-Kimball model and sofar went unnoticed in the investigation of this model. The appearance of such a singularity in χ_{AF}^{-1} suggests the existence of an interesting, new coupling of the electrons in the case when the lattice is occupied by an equal number of single up-spins, down-spins and empty sites (i.e. $n_\uparrow=n_\downarrow=\frac{1}{3}$). It might even be the precursor of the formation of a new phase with lower symmetry. This point demands a more detailed investigation. We note that, *if* a genuine band splitting occured even in the exact solution of the Hubbard model, some kind of non-analyticity should exist in this solution, too, at the generic band-filling of $\nu=1/3$ i.e. $n=2/3$.

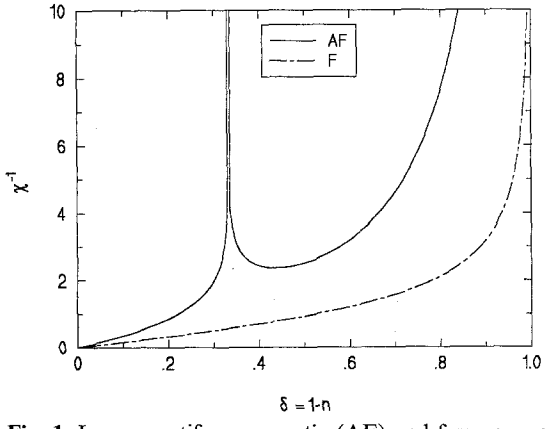

Fig. 1. Inverse antiferromagnetic (AF) and ferromagnetic (F) susceptibility of the $U=\infty$ Hubbard model vs. hole concentration $\delta=1-n$. The inverse AF susceptibility diverges logarithmically at $\delta=1/3$

4.2. $U<\infty$

For finite interaction U the susceptibilities have to be evaluated numerically. At half filling, $\nu=\frac{1}{2}$ (i.e. $n=1$), the ground state is expected to be antiferromagnetic. In the Heisenberg limit, $U\gg t$, and in dimensions $d\gg 1$ it will correspond to a Néel-state with local moments. By contrast, in the weak-coupling limit an itinerant antiferromagnetic state is expected to be formed where the imaginary part of the self-energy of the electrons is zero at the Fermi level, without quasiparticle-behavior being exhibited away from the Fermi level. We thus expect $\chi_{\mathrm{AF}}<0$ for all $U>0$. In Fig. 2 a plot of $U\chi_{\mathrm{AF}}^{-1}$ vs. U is shown. Obviously there is *no* antiferromagnetic phase for $U\lesssim 1.5$ in units of the hopping constant, in spite of the fact that the susceptibility (9) reduces to the Stoner result which

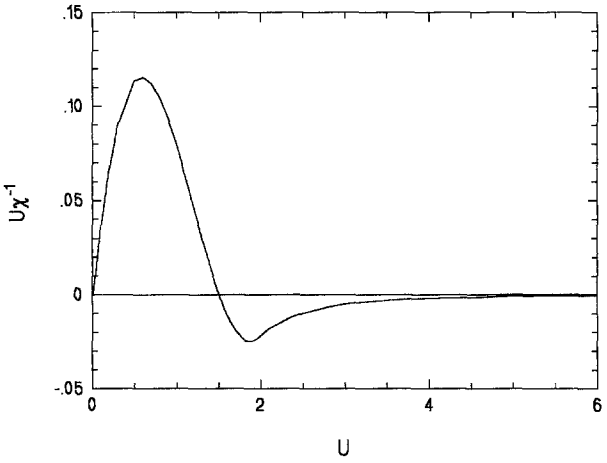

Fig. 2. Inverse antiferromagnetic susceptibility times U, $U\chi_{\mathrm{AF}}^{-1}$, vs. interaction U for $n=1$. Long-range order occurs only above $U_c \cong 1.5$

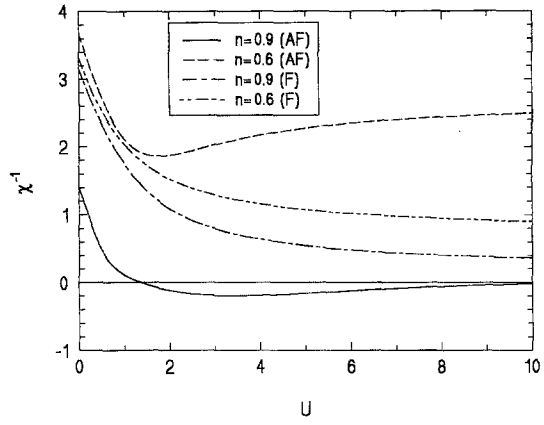

Fig. 3. Inverse antiferromagnetic (AF) and ferromagnetic (F) susceptibility vs. U for various fillings n

suggests antiferromagnetism for arbitrarily small U. To explain this apparent contradiction we have to extend the asymptotic result in (12) beyond leading order. For $\nu = \frac{1}{2}$ and small U we find

$$\chi_{\mathrm{AF}}^{-1} = -2U + \left[\frac{1}{\pi}\int_{-\infty}^{\tilde{\mu}} \mathrm{d}\omega\, \mathrm{Im}\, \frac{G(\omega)}{\omega - \frac{U}{2} - i\,\mathrm{Im}\,\Delta\Sigma(\omega)}\right]^{-1}, \quad (18)$$

where $\Delta\Sigma(\omega)$ is the correction to the Hartree-Fock self-energy. The r.h.s. of (18) becomes negative (thus indicating the antiferromagnetic instability) in the limit $U \to 0$ if and only if the integral in the denominator diverges. This is only the case if $\mathrm{Im}\,\Delta\Sigma(\tilde{\mu} = U/2) = 0$, i.e. if the imaginary part of the self-energy vanishes at the Fermi level. The MFT defined by (2) violates this property in the U^2 contribution to the self-energy. The reason why the MFT fails to produce an antiferromagnetic ground state in the weak-coupling regime lies in its very construction, i.e. in the decomposition of the Hubbard Hamiltonian into two Falicov-Kimball models which are coupled on an approximate level via the mean-field energy parameters $E_\sigma^{I,L}$. As discussed in *I* this MFT may be viewed as an improvement of the Hubbard-III approximation [5] which is now thermodynamically consistent and diagrammatically controlled due to the existence of the additional energy parameters $E_\sigma^{I,L}$. In spite of these improvements the MFT still exhibits, at small U, a well-known deficiency of the Hubbard-III approximation, namely a non-vanishing self-energy at the Fermi level for *all* $n > 0$ [12, 13]. As first pointed out by Kawabata [14] this is due to the dynamical separation of up and down-spins in the Hubbard-III approximation, where mobile σ-electrons are scattered by static $(-\sigma)$-electrons. Such a separation is also intrinsically present in our improved approximation where an antiferromagnetic ground state is made possible precisely by the existence of the additional energy parameters $E_\sigma^{L,I}$. At *large* U this type of scattering gives an essentially correct description of the

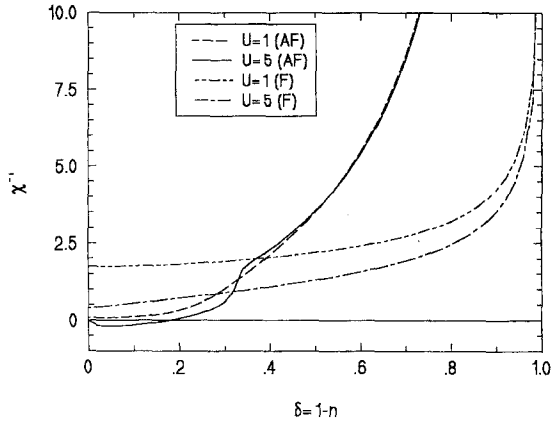

Fig. 4. Inverse antiferromagnetic (AF) and ferromagnetic (F) susceptibility vs. δ for various values of U

physical mechanism responsible for the antiferromagnetic ordering. At *small* U, however, the antiferromagnetic instability has a different origin, namely is due to a combination of the quasiparticle structure of the low-lying excitations and the perfect-nesting property of the lattice. The above MFT is hence unable to describe the crossover to the correct small-U behavior and produces a transition to a paramagnet at $U_c \cong 1.5$. From Fig. 2 we see that, for large U, χ_{AF}^{-1} quickly approaches zero (from the negative side!). It suggests an approximate degeneracy between the antiferromagnetic and paramagnetic mean-field solutions in the strong coupling regime; this is also clearly borne out by the respective energies (see below).

To construct the $U-n$ phase diagram the susceptibilities have to be calculated away from half filling. The result for the inverse susceptibilities as functions of U are shown in Fig. 3. We see that the antiferromagnetic correlations quickly become weaker for decreasing n. Figure 4 displays the inverse susceptibilities as functions of hole concentration. Again the antiferromagnetic correlations become weaker more rapidly than the ferromagnetic ones. Note that at large interaction values, i.e. above the Mott-Hubbard ("split-band") value U_c^{MH} (where

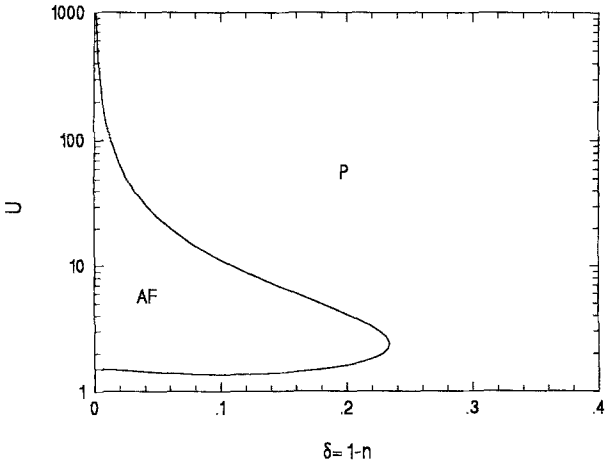

Fig. 5. Mean-field phase diagram for the Hubbard model at $T=0$. *P:* paramagnetic phase, AF: antiferromagnetic phase

$U_c^{\mathrm{MH}}=2$ for the Bethe-lattice with $n=1$), a non-analyticity at $n=2/3$ develops in the staggered susceptibility; this is a precursor of the logarithmic singularity at $U=\infty$. We did not find any numerical evidence for a ferromagnetic instability and thus the MFT, (2), either yields an antiferromagnetic or a paramagnetic ground state. The mean-field phase diagram is plotted in Fig. 5. For $n<n_c\simeq 0.77$ only a paramagnetic phase exists. On the basis of our results and the above discussion we may expect that the thermodynamics obtained with our MFT is reliable in the strong-coupling regime. It should be noted, however, that the energies of different phases obtained within our MFT are very close for large U. Hence we cannot definitely exclude the existence of some mixed phases with more complicated symmetry-breaking order parameters.

5. Lower and upper bounds on the ground-state energy

MFTs constructed within the general scheme of I have the advantage of providing exact bounds (either lower or upper) on the ground state energy of the model under investigation. In the case of the Hubbard model the dynamics, and hence the solution itself, remains non-trivial even in $d=\infty$ [2]. In this situation the calculation of narrow bounds is of considerable interest.

We will now show that the MFT defined by (2) provides the best *lower* bound on the Hubbard model known sofar. In addition, as already discussed in I, the best self-consistent [15] *upper* bound obtained from the general partition scheme of I is the Hartree-Fock energy. This approximation can be further improved by means of the Gutzwiller projection [16, 17], the results of which in $d=\infty$ reduce to that of the Gutzwiller approximation [18, 2]. We thus take the Gutzwiller energy based on the projected (anti-)ferromagnetic/paramagnetic Hartree-Fock wave function as the upper bound on the ground-state energy of the Hubbard model in $d=\infty$. We first construct the general expressions for the mean-field ground-state energies from (2) and for the Gutzwiller approximation, respectively. Then we investigate the cases $U=\infty$ and $n=1$ explicitly.

The total energy per lattice site of the mean-field solution (2) is given by $(\Omega_{\mathrm{MF}}+\mu N)/L$, where N is the number of electrons. We know already (see Fig. 5) that the ground state of the Hubbard model within this MFT is either a paramagnet or a pure antiferromagnet. In these cases the total energy can be written as

$$E_{\mathrm{TOT}}^{\mathrm{MF}}(U,n)=-\frac{1}{\pi}\int_{-\infty}^{\mu}\mathrm{d}\omega\,\omega\,\mathrm{Im}\,\frac{z_A+z_B}{\sqrt{z_A z_B}}\times G(\sqrt{z_A z_B})-\sum_{\alpha}E_\alpha n_\alpha, \tag{19}$$

where $z_\alpha=\omega-E_\alpha-\Sigma_\alpha(\omega)$, and $G(z)=\int \mathrm{d}E\rho(E)\,[z-E]^{-1}$ is the diagonal element of the paramagnetic Green function. In (19) we assumed that $n_{A,\sigma}=n_{B,-\sigma}$ and $E_\alpha\equiv E_\uparrow^{I\alpha}=E_\downarrow^{I-\alpha}$. The effective chemical potential $\bar{\mu}=\mu-E$, $E=(E_A+E_B)/2$, is determined by fixing the total particle density $n=n_A+n_B$. We are then left with two thermodynamic order parameters, $m=(n_A-n_B)$ and $\Delta E=(E_A-E_B)/2$, which are to be determined self-consistently together with the self-energies $\Sigma_{A,B}(\omega)$. If $\alpha=\pm 1$ for A, B, respectively, then

$$\Sigma_\pm(\omega)=\frac{U_\mp}{1-U_\pm\zeta_\pm(\omega)}, \tag{20a}$$

$$\zeta_\pm(\omega)=[G_\pm(\omega)^{-1}+\Sigma_\pm(\omega)]^{-1}, \tag{20b}$$

with

$$U_\pm=\frac{U}{2}(n\pm m), \tag{20c}$$

$$G_\pm(\omega)=\frac{z_\mp}{\sqrt{z_+ z_-}}\,G(\sqrt{z_+ z_-}). \tag{20d}$$

The equations for ΔE and m, respectively, are

$$m=-\frac{1}{\pi}\int_{-\infty}^{\bar{\mu}}\mathrm{d}\omega\,\mathrm{Im}[G_+(\omega)-G_-(\omega)], \tag{21a}$$

$$\Delta E=\frac{1}{2\pi}\int_{-\infty}^{\bar{\mu}}\mathrm{d}\omega\,\mathrm{Im}[\ln(1-U\zeta_+(\omega))-\ln(1-U\zeta_-(\omega))]. \tag{21b}$$

The total energy can be rewritten in terms of the parameters m and ΔE as

$$E_{TOT}^{\mathrm{MF}}(m,\Delta E)=-\Delta E m-\frac{1}{\pi}\int_{-\infty}^{\bar{\mu}}\mathrm{d}\omega\,\omega\int_{-\infty}^{\infty}\mathrm{d}E\rho(E)\times\mathrm{Im}\,\frac{2\omega-\Sigma_+(\omega)-\Sigma_-(\omega)}{(\omega+\Delta E-\Sigma_+(\omega))(\omega-\Delta E-\Sigma_-(\omega))-E^2}. \tag{22}$$

Note that, for fixed m, $\partial E_{\mathrm{TOT}}^{\mathrm{MF}}/\partial(\Delta E)=0$ corresponds to (21a), which establishes a relation $\Delta E=\Delta E(m)$, while the *total* derivative $dE_{\mathrm{TOT}}^{\mathrm{MF}}/dm=0$ corresponds to (21b). Equations (21)–(22) must be complemented by an equa-

tion for the chemical potential $\bar{\mu}$ in terms of n

$$n=-\frac{1}{\pi}\int_{-\infty}^{\bar{\mu}} d\omega \int_{-\infty}^{\infty} dE\rho(E) \times \mathrm{Im}\frac{2\omega-\Sigma_+(\omega)-\Sigma_-(\omega)}{(\omega+\Delta E-\Sigma_+(\omega))(\omega-\Delta E-\Sigma_-(\omega))-E^2}. \quad (23)$$

For given m and ΔE the Eqs. (20) and (23) form a closed set of equations for $\Sigma_\pm$ and $\bar{\mu}$ and thus determine the ground state properties of the MFT defined in (2), the ground state energy of which yields a rigorous lower bound on the exact ground state energy (see Eq. (30) of *I*). The state giving an optimal lower bound $E_{\mathrm{TOT}}^{\mathrm{MF}}$, is then found as follows: first we fix the magnetization m and *maximize* $E_{\mathrm{TOT}}^{\mathrm{MF}}$ w.r.t. ΔE, i.e. solve (21a), and then we *minimize* $E_{\mathrm{TOT}}^{\mathrm{MF}}$ w.r.t. m, with $\Delta E=\Delta E(m)$, i.e. solve (21b), since, just as in the exact solution, the free energy must always be a minimum in m. The importance of the mean-field parameters $E^{I\alpha}$ was already stressed in Sect. 3, where we discussed their influence on the susceptibilities and the thermodynamics. We can now also demonstrate their *quantitative* influence on the energy of the ground state. If we put $\Delta E=0$ we obtain the following (non-self-consistent [15, 19]) lower and upper bounds (cf. *I*) for the ground state energy of the Hubbard model $E_{\mathrm{TOT}}(U,n)$:

$$2E_{\mathrm{TOT}}^{\mathrm{FK}}\left(\frac{U}{2},n\right)\leqq E_{\mathrm{TOT}}(U,n)\leqq E_{\mathrm{TOT}}^{\mathrm{FK}}(U,n), \quad (24a)$$

where

$$E_{\mathrm{TOT}}^{\mathrm{FK}}=-\frac{1}{2\pi}\int_{-\infty}^{\mu} d\omega\omega \int_{-\infty}^{\infty} dE\rho(E) \times \mathrm{Im}\frac{2\omega-\Sigma_+(\omega)-\Sigma_-(\omega)}{(\omega-\Sigma_+(\omega))(\omega-\Sigma_-(\omega))-E^2}, \quad (24b)$$

is the total energy of the Falicov-Kimball [3, 4] model. The l.h.s. of (24a) is the lower bound proposed by Langer and Mattis [20] which has recently been shown [21] to yield good quantitative results for $d=1$, 2 in spite of its non-self-consistency.

We now turn to the upper bounds. The r.h.s. of (24a) is the best non-self-consistent upper bound on the ground state energy of the Hubbard model obtained by partitioning the Hubbard Hamiltonian into subsystems with static and dynamic electrons. *Self-consistent* upper bounds are provided by Hartree-Fock and Gutzwiller-projected Hartree-Fock wave functions, respectively. The total energy for a Gutzwiller-projected spin density wave (i.e. with $A-B$ sublattice structure) with $n_\uparrow \neq n_\downarrow$ in $d=\infty$ is given by

$$E_{\mathrm{TOT}}^{G}(U,n)=\tfrac{1}{2}\sum_\alpha\left\{Ud_\alpha+\sum_\sigma\left[E_{\alpha\sigma}n_{\alpha\sigma}-q_\sigma^{-1}\int_{-\infty}^{0} d\omega\omega\rho\left(\frac{z_\sigma(\omega)}{q_\sigma}\right)\frac{z_{\alpha\sigma}(\omega)}{z_\sigma(\omega)}\right]\right\}+\mu n, \quad (25)$$

where $q_\sigma=\sqrt{q_{A\sigma}q_{B\sigma}}$, $z_{\alpha\sigma}(\omega)=\omega+\mu-E_{\alpha\sigma}$, $z_\sigma(\omega)=\sqrt{z_{A\sigma}(\omega)z_{B\sigma}(\omega)}$ and

$$q_{\alpha\sigma}=\frac{1}{n_{\alpha\sigma}(1-n_{\alpha\sigma})}\left[\sqrt{(1-n_\alpha+d_\alpha)(n_{\alpha\sigma}-d_\alpha)}+\sqrt{d_\alpha(n_{\alpha-\sigma}-d_\alpha)}\right]^2. \quad (26)$$

with $n_\alpha=n_{\alpha\uparrow}+n_{\alpha\downarrow}$ and $n_\sigma\equiv h_{A\alpha}+n_{B\sigma}$. For $n_\uparrow=n_\downarrow$ this reduces to the results obtained earlier [22, 23]. Equation (25) contains μ, $E_{\alpha\sigma}$, $n_{\alpha\sigma}$ as variational parameters which may be used to minimize the total energy E_{TOT}^{G} for fixed n. The Hartree-Fock ground-state energy is obtained from (25) if we put $q_{A\sigma}=q_{B\sigma}=1$ and $d_\alpha=n_{\alpha\uparrow}n_{\alpha\downarrow}$. In this case the energies $E_{\alpha\sigma}$ are the Hartree potentials.

5.1. $n=1$

In Fig. 6 the three upper bounds obtained from *(i)* the Falicov-Kimball model, *(ii)* the Hartree-Fock, and *(iii)* the Gutzwiller-projected Hartree-Fock wave function are shown for half-filling. (Note that the upper bound obtained from the Falicov-Kimball model, (24b), is never a good one since only one half of the electrons are mobile, whereby the ground state energy at $U=0$ is only half that of the exact result for the Hubbard model). All three approximations yield an antiferromagnetically ordered state for arbitrarily small U, in contrast to the MFT defined in (2). In Fig. 7 the lower bound on the ground state energy of the Hubbard model in $d=\infty$ obtained with $E_{\mathrm{TOT}}^{\mathrm{MF}}$, (22), is shown in comparison with the non-self-consistent one of Langer and Mattis [20, 21], (24a). The self-consistency of the mean-field bound, i.e. the existence of the dynamical mean-field energies $E_\sigma^{I\alpha}$, is seen to improve the latter bound substantially. In Fig. 8 the best lower bound, $E_{\mathrm{TOT}}^{\mathrm{MF}}$, and the best upper bound, E_{TOT}^{G}, are combined. Obviously they are very close and

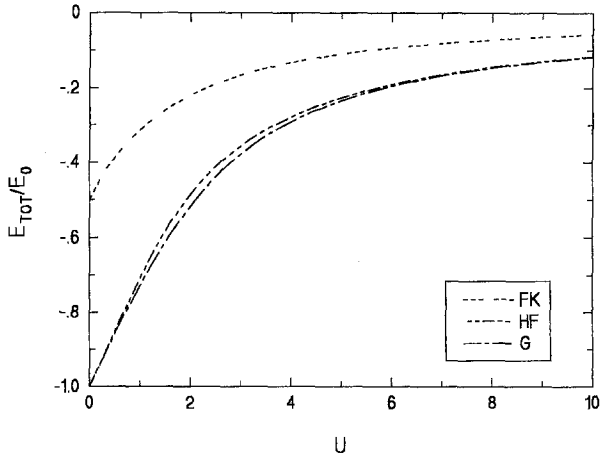

Fig. 6. Three upper bounds on the ground-state energy of the Hubbard model in $d=\infty$ at $n=1$ as functions of U; the energy is normalized to E_0, the absolute value of the energy of non-interacting particles: *(i)* Gutzwiller-projected, antiferromagnetic Hartree-Fock wave function (G), *(ii)* antiferromagnetic Hartree-Fock wave function (HF), *(iii)* Falicov-Kimball model (FK)

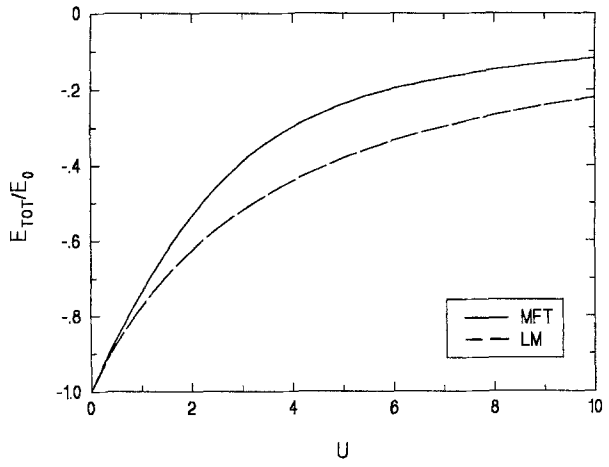

Fig. 7. Two lower bounds on the ground-state energy of the Hubbard model in $d=\infty$ for $n=1$ as functions of U: *(i)* mean-field theory defined in (2) (MFT), *(ii)* non-self-consistent bound by Langer and Mattis [20] (LM)

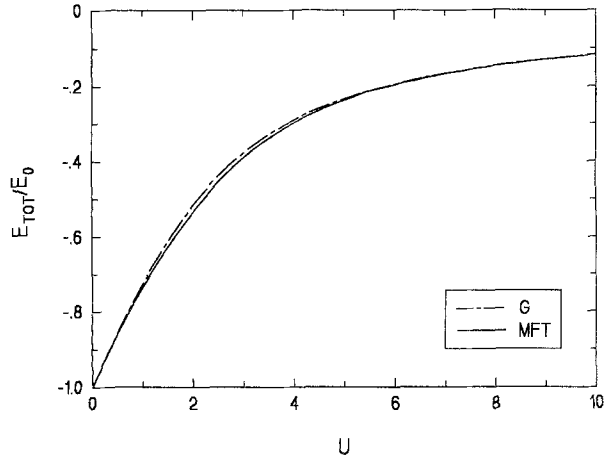

Fig. 8. Combination of the best lower (MFT) and upper (G, AF) bounds on the ground state energy of the Hubbard model in $d=\infty$ for $n=1$ as taken from Figs. 7, 6

hence do not leave much space for improvements. These bounds therefore provide an excellent numerical approximation to the unknown exact result. The quantitative accuracy is quite surprising in view of the rather different *physical* properties of the approximations. (Indeed, even the paramagnetic solution of (20)-(21), i.e. the Hubbard-III solution, fits the ground-state energy of the Hubbard model very well). This shows once more that the ground-state energy is a rather insensitive quantity. It also illustrates that, to obtain a reasonable quantitative agreement with exact results, approximate theories should contain a set of variational parameters which can be used to optimize the energy functional.

5.2. $U=\infty$

Another interesting limit is that of very strong interaction, $U=\infty$. In this case the ground-state energy is only a function of the particle density $0\leqq n\leqq 1$. The MFT defined by (2) greatly simplifies in this limit since, according to Fig. 1, the ground state is always paramagnetic. The MFT yields a lower bound on the ground state energy of the $U=\infty$ Hubbard model which reads

$$E_{\mathrm{TOT}}^{\mathrm{MF}}(n)=-\frac{8}{3\pi}(1-\nu)^{3/2}(1-x^2)^{3/2}, \tag{27}$$

where $x(\nu)$, (16d), is determined by (17). A good upper bound is not easily constructed in the limit $U=\infty$: the Hartree-Fock approximation becomes meaningless and we have to resort to ground state energies obtained with Gutzwiller-projected ferromagnetic or antiferromagnetic wave functions. To simplify the matter we restrict our discussion to pure phases. For a hypercubic lattice it was shown by Fazekas et al. [24] that for $\delta_F\leqq\delta\leqq 1$, $\delta_F\simeq 0.42$, a paramagnetic phase has the lowest energy, while for $0\leqq\delta\leqq\delta_F$ a ferromagnetic phase is favored. The energy of these homogeneous phases is given by

$$E_{\mathrm{TOT}}^{G}=\sum_{\sigma}\frac{1}{q_\sigma}\int_{-\infty}^{0}\mathrm{d}\varepsilon\,\rho\left(\frac{\varepsilon+\mu+\sigma\Delta E}{q_\sigma}\right)\varepsilon$$
$$+\mu n+\Delta E m, \tag{28}$$

where $q_\sigma=2(1-n)/(2-n-\sigma m)$ and $\mu,\Delta E$ and m are independent variational parameters. The above upper and lower bounds are plotted in Fig. 9 as functions of the hole concentration $\delta=1-n$. Which one of these bounds is closer to the actual energy of the Hubbard model cannot be answered unambiguously. At least we know that the MFT defined by (2) is a thermodynamically consistent theory which gives a correct description of the ground-state (Curie-Weiss) susceptibility at large U; hence we expect it to provide an adequate description of the ground state itself, too. In other words, we expect the lower bound to be much better than the upper one. Note that at small δ a *saturated* ferromagnet ($n_\uparrow=n$, $n_\downarrow=0$; "Nagaoka state") is found to be unstable since the *unsaturated* ferromagnet described by the Gutzwiller wave function

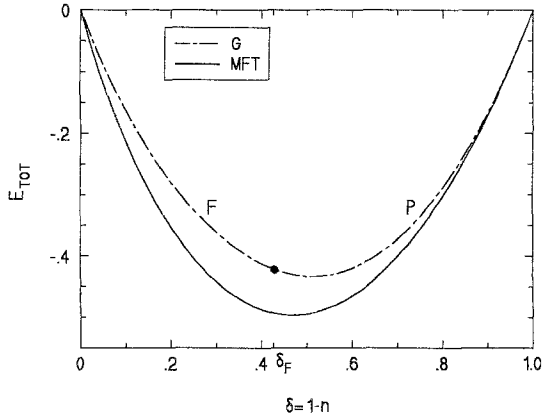

Fig. 9. Bounds on the ground-state energy of the $U=\infty$ Hubbard model in $d=\infty$ as functions of δ; lower bound: mean-field theory defined in (2) (MFT), upper bound: Gutzwiller-projected paramagnetic (G, P) and ferromagnetic (G, F) Hartree-Fock wave function for $\delta>\delta_F=0.42$ and $\delta<\delta_F$, respectively

(providing an upper bound) has a lower energy. This result which was here derived for a Bethe lattice (having a bounded density of states) agrees with that for a hypercubic lattice in $d=\infty$ [24, 25]. On the other hand the bounds in Fig. 9 shed no light on the stability of the *non*-saturated ferromagnetic state. Such a state would be ruled out if a paramagnetic upper bound could be found that lies below a lower bound for the ferromagnetic solution. This shows that we must improve the upper bound to disprove ferromagnetism. A comparison of Figs. 8 and 9 indicates that the dynamics of the Hubbard model for $n<1$ is indeed much more complex than for $n=1$ and that it is more difficult to estimate the reliability of different approximation schemes in this case.

6. Spectral properties of the antiferromagnetic phase

In the paramagnetic phase the one-electron Green function of the MFT investigated here is identical to that obtained within the Hubbard-III approximation. This is so in spite of the existence of an additional variational energy parameter $E^I \equiv E^I_\uparrow = E^I_\downarrow$, and is due to the fact that E^I only renormalizes the chemical potential if the symmetry is unbroken. Indeed, in the paramagnetic phase the one-electron DOS or the self-energy give no indication at all of any thermodynamic instability of the system towards an antiferromagnetic phase – this information is provided by the *susceptibility* (a two-particle quantity). It is therefore of interest to investigate the one-particle spectral function in the ordered phase and to find out how it differs from that in the paramagnetic phase. To this end Eqs. (20)–(21) must be solved for the thermodynamic parameters m and ΔE, as well as for the self-energy $\Sigma_\alpha(\omega)$ and the DOS $(-1/\pi)\,\mathrm{Im}\,G_\alpha(\omega)$, $\alpha = A, B$, for $n=1$ (note that $n_{\uparrow\alpha} = n_{\downarrow -\alpha}$). For $U > U_c \cong 1.5$ a solution with $m>0$ and $\Delta E > 0$ is found. It should be emphasized that the magnetization m and the energy difference ΔE are conjugate variables and that m is non-zero *if and only if* ΔE is non-zero. This clearly shows that in the absence of the energy parameters E^I_σ (as in the case of the Hubbard-III approximation) an antiferromagnetic phase cannot exist. Due to electron-hole symmetry, (7), at $n=1$ the renormalized chemical potential is fixed at $\bar{\mu} = U/2 + \Delta E$.

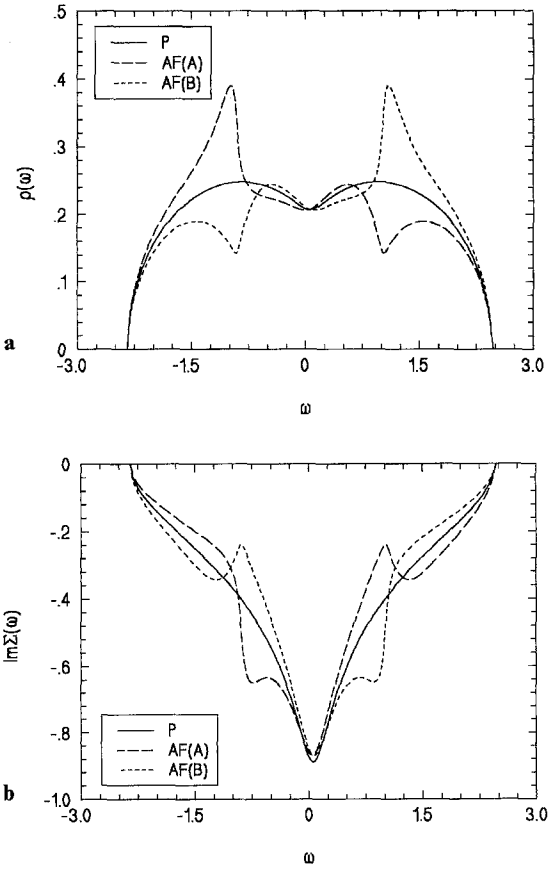

Fig. 10. **a** Single-particle density of states (DOS) $\rho(\omega)$, and **b** imaginary part of the self-energy $\mathrm{Im}\,\Sigma(\omega)$ vs. frequency ω for $U=1.52$ (with optimized parameters $m=0.127$, $\Delta E=0.077$) in the antiferromagnetic phase for A- and B-sublattices (AF (A), AF (B)) in comparison with the paramagnetic (P) Hubbard-III solution

The DOS and the imaginary part of the self-energy for $U=1.52$, i.e. in the antiferromagnetic phase just above the transition point, are shown in Fig. 10 in comparison with the paramagnetic solution. While the DOS remains almost unchanged at the renormalized Fermi level, $\omega=0$, the broken symmetry leads to considerable modifications at $\omega \simeq \pm\bar{\mu}$, where the integral $\mathscr{K}(U)$, (10d), is maximal (but still finite). A qualitatively similar behavior of the DOS has been obtained within a cluster generalization of the alloy analogy solution which introduces short-range antiferromagnetic correlations [26]. Increasing the interaction (and hence m and ΔE) to $U=1.6$ has a strong effect (see Fig. 11): a central band around $\omega=0$ splits off from the upper and lower ("satellite") bands. While the DOS at $\omega=0$ still essentially retains its value of the paramagnetic state, the DOS of the majority electrons is strongly peaked around the maximum of $\mathscr{K}(U)$. However, in contrast to the Hartree-Fock solution or the exact solution of the Falicov-Kimball model in $d=\infty$ [3, 4] the DOS does not exhibit an actual divergence and, most importantly, is still finite at $\omega=0$. A decisive difference between the DOS of the paramagnetic and antiferromagnetic solutions first appears at $U \simeq U_c^{\mathrm{MH}} = 2$. While the (spurious!) paramagentic Hubbard-III solution becomes insulating at $U = U_c^{\mathrm{MH}}$, the antiferromagnetic solution in our MFT remains metallic, since the DOS is still finite at $\omega=0$. In the antiferromagnetic phase the metal-insulator transition does not occur until a considerably larger value $U_{\mathrm{MIT}}^{\mathrm{AF}} \simeq 3.3$ is reached. The DOS of the antiferromagnetic state for $U=3.5 > U_{\mathrm{MIT}}^{\mathrm{AF}}$ is shown in Fig. 12. At this U-value the self-energy has a very intricate structure which is not shown here. These results indicate that the antiferromagnetic long-range order is not only described by two-particle quantities (susceptibilities) but also leads to significant changes on the one-particle level.

To our knowledge the MFT described in this paper is the first thermodynamically consistent theory that allows for an explicit, analytically tractable description of the transition scenario in the Hubbard model: as U is increased (at fixed density n) there is first a transition at

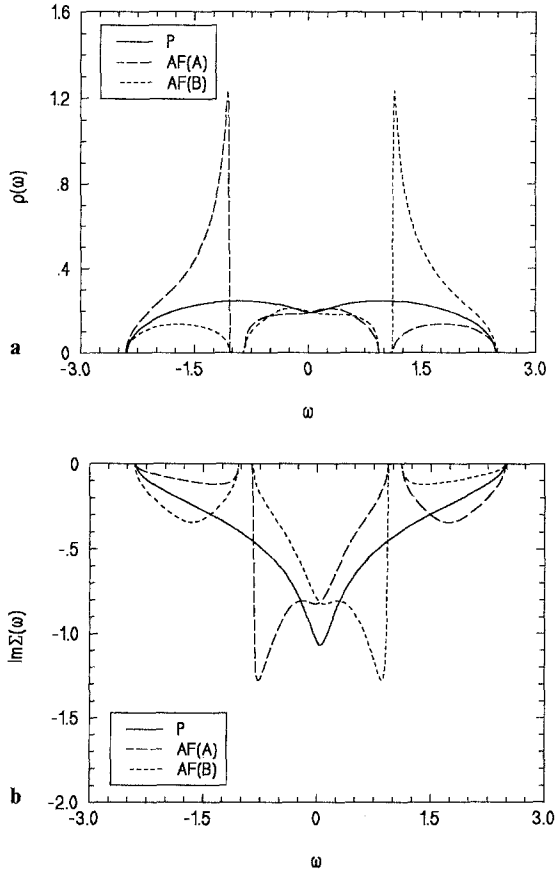

Fig. 11a, b. Same quantities as in Fig. 10 for $U=1.6$ (with $m=0.398$, $\Delta E=0.259$); a central band has split off from the satellites

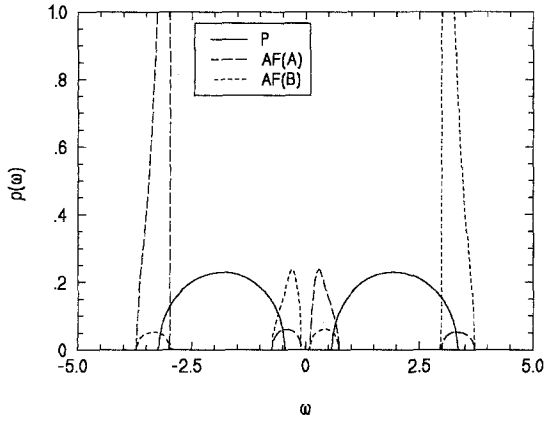

Fig. 12. Single-particle DOS vs. ω for $U=3.5$ (with $m=0.741$, $\Delta E=1.236$); a gap has opened at the renormalized Fermi level

U_c from a paramagnetic metal to an antiferromagnetic metal and then, at $U_{\mathrm{MIT}}^{\mathrm{AF}}$, into an antiferromagnetic insulator. In Figs.- 10–12 this behavior was evaluated for $n=1$ since numerical calculations are particularly simple then. On the other hand for $n=1$ we do not expect our MFT to give an accurate description of spectral properties of the model, at least for $U<U_c\simeq 1.5$, since the perfect nesting property of the lattice is expected to lead to $U_c=0$. Nevertheless the above scenario is also valid

Fig. 13. General phase transition scenario for the Hubbard model at $T=0$ and fixed density n ($0.77<n<1$) as a function of U; the phases correspond to a paramagnetic metal (P, M), antiferromagnetic metal (AF, M), antiferromagnetic insulator (AF, I)

for $n<1$. In Fig. 13 we show the most general transition sequence described by our MFT for $0.77=n_c<n<1$ at $T=0$: apart from the first two transitions at U_c and $U_{\mathrm{MIT}}^{\mathrm{AF}}$ (denoted by $U_{c,1}$ and $U_{\mathrm{MIT},1}^{\mathrm{AF}}$, respectively, in Fig. 13) there are, in general, two more transitions as U is further increased: back into the antiferromagnetic metal at $U_{\mathrm{MIT},2}^{\mathrm{AF}}$ and then back into the paramagnetic metal at $U_{c,2}$. It is quite probable that there exists a density n_c^*, $n_c<n_c^*<1$, such that for $n_c<n<n_c^*$ the transition at $U_{\mathrm{MIT},i}^{\mathrm{AF}}$ ($i=1,2$) to an antiferromagnetic insulator does not occur at all, i.e. the systems remains metallic for all values of U; this question needs further investigation.

7. Discussion

In this paper we presented the results of a detailed study of the ground state properties of an analytically tractable mean-field theory (MFT) for the Hubbard model derived in the preceding paper [1]. The MFT is based on a self-consistent superposition of two Falicov-Kimball models and on the exact analytic solution of the latter model in $d=\infty$ dimension [3, 4]. The corresponding mean-field free energy functional, (2), was used to determine the ferromagnetic and antiferromagnetic susceptibilities (only pure phases were considered). It was found that the inverse susceptibilites are determined by three contributions, namely terms due to the interaction *(i)* between local moments, *(ii)* between local moments and itinerant electrons and *(iii)* between itinerant electrons. In the limit $U\to 0$ the susceptibilities reduce to the Stoner results. However, the singularity suggested by the Stoner theory was shown to be artificial, i.e. based on an invalid approximation where genuine two-particle correlations are completely neglected. The latter correlation effects lead to contributions proportional to U^2 in the inverse susceptibility which suppress the Stoner instability. Indeed, a phase instability can *only* arise due to these very correlation contributions. In the limit $T=0$, $n=1$, $U\to\infty$ the susceptibilities give the correct Curie-Weiss behavior. For $U=\infty$ the staggered susceptibility χ_{AF} was found to *vanish* logarithmically at a filling $n=\frac{2}{3}$ due to perfect nesting in the lower Hubbard band. This singularity separates two regions: one, where the antiferromagnetic correlations are dominated by an interaction between itinerant quasiparticles ($n<2/3$), and one with an enhanced interaction between local magnetic moments ($1\geqq n>2/3$). The band filling $n=2/3$ is generic since it corresponds to a half-filled lower Hubbard band. In the case of finite interactions the ground state was found to be antiferromagnetic even away from half filling, i.e. for $n_c(U)\leqq n\leqq 1$ except for $U<U_c\cong 1.5$ where the ground state is para-

magnetic for all n. The latter feature is artificial and arises because the MFT does not yet provide a proper description of the transition between the strongly-correlated (local-moment) regime in the Heisenberg limit to the weakly-correlated (Fermi-liquid) regime. Indeed, the MFT never leads to a Fermi liquid, since there exist local moments (static electrons) in the theory for all $U > 0$ [14].

The ground-state energy due to the mean-field solution (2) yields a lower bound on the ground-state energy of the Hubbard model in $d = \infty$. Combining this result with the upper bound obtained from the Gutzwiller-projected spin-ordered Hartree-Fock wave function we determined rigorous bounds on the exact energy of the Hubbard model at $T = 0$ in $d = \infty$. In particular, for $n = 1$ these bounds are found to be very close, leaving hardly any room for quantitative improvements. This accuracy is due to the presence of variational mean-field parameters in the energy functional (2) which allow one to optimize the energy.

By studying the spectral properties of the antiferromagnetic phase we found that at $T = 0$ and fixed density ($0.77 \lesssim n < 1$) there exists, in general, a sequence of transitions for increasing interaction U where the system goes from a paramagnetic metal to an antiferromagnetic metal and then to an antiferromagnetic insulator; upon further increase of U these two transitions occur once more in reversed order until the paramagnetic metal is reached again.

In summary, the MFT defined by (2) is a thermodynamically consistent theory applicable in the whole range of input parameters. It is primarily designed to describe the Hubbard model in the intermediate and strong-coupling regime, where the local magnetic moments play a dominant rôle. The MFT may be viewed as an improvement of the Hubbard-III approximation which is thermodynamically consistent and where magnetic excitations are incorporated. As such our MFT puts the alloy analogy (Hubbard-III) solution on a firm basis and thus gives it new significance. It should be stressed that only in the paramagnetic state and only in the case of *single-particle* quantities (e.g. the self-energy) do the results of our MFT coincide with those of the Hubbard-III solution. In fact, *two-particle* quantities (e.g. the susceptibilities) are very different even in the paramagnetic phase. – In the next step the $U - n - T$ phase diagram should be investigated in more detail. Disorder can easily be included; in the presence of disorder the antiferromagnetic phase at $n = 1$ and small U will be suppressed anyway. Furthermore, the MFT described here could be improved so as to recover Fermi liquid behavior at small U [13], at least for non-bipartite lattices. Clearly this improvement must be fitted into the general construction scheme developed in *I* to make the resulting MFT thermodynamically consistent. Such an improved MFT would then provide the first analytic, thermodynamically consistent description of the transition from a Fermi liquid to a local-moment-dominated regime within the Hubbard model.

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