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Analytically Tractable Mean-Field Theory for Interacting Electrons at Strong Coupling

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A mean-field theory for the Hubbard model at strong-coupling is presented. It extends the well-known, but ad hoc, alloy-analogy approximation and puts it on a firm, thermodynamically consistent basis. The magnetic ordering is studied and the mean-field phase diagram in the $U-n$ plane is determined for $T=0$. The investigation of the spectral properties away from half filling reveals a sequence of magnetic and metal-insulator transitions for increasing U.

The Hubbard model is the generic model for strongly correlated electrons. The first step towards a *dynamical* mean-field theory (MFT) for the Hubbard model was due to Hubbard himself [1]. The socalled "Hubbard-III solution" is a self-consistent single-site approximation that reproduces the weak-coupling limit (on-site interaction $U \to 0$) and the atomic limit (hopping constant $t=0$) correctly. This approximation corresponds to the coherent potential approximation for static disorder. Unfortunately it has serious deficiencies; in particular, it is not a thermodynamic theory, i.e. there exists no generating functional and thus it is diagrammatically uncontrolled. Moreover, the Hubbard-III solution does not allow for any magnetic order and does not describe the Heisenberg limit ($n=1$, $T \to 0$, $U \gg t$). Instead it yields a paramagnetic phase without low-lying quasiparticle states. There have been numerous attempts in the past to remove the deficiencies of this approximation [2]. However, none of these attempts resulted in a thermodynamically consistent approximation scheme. Only recently, by using the limit of high dimension for fermionic lattice systems [3], has it become possible to put the Hubbard-III solution on a firm, thermodynamically consistent and diagrammatically controlled basis [4]. This seems worthwhile since even for $d=\infty$ the solution of the Hubbard model is not analytically tractable. Sofar only a simplified model, where one of the spin species remains static ("spinless Falicov-Kimball model") is analytically solvable in $d=\infty$ [5-7]. In this case the self-energy of the itinerant electrons in the homogeneous phase coincides with that in the Hubbard-III solution. Thus one may utilize the exact (i.e. thermodynamically consistent) solution of the Falicov-Kimball model in $d=\infty$ to construct an *analytically tractable* MFT for the Hubbard model at strong coupling [4,8]. In the paramagnetic phase of this MFT the frequency-dependent self-energy $\Sigma_\sigma(\omega)$ for σ-electrons is determined by the single-site equation

$$G_\sigma(\omega) = \mathcal{G}_\sigma(\omega)[1-n_{-\sigma}+n_{-\sigma}/(1-U\mathcal{G}_\sigma(\omega))] \quad \text{(1a)}$$

$$\equiv G^0_\sigma(\omega-\Sigma_\sigma(\omega)-E^I_\sigma) \quad \text{(1b)}$$

where $\mathcal{G}_\sigma(\omega)=[(G_\sigma(\omega))^{-1}+\Sigma_\sigma(\omega)]^{-1}$ and $G^0_\sigma(\omega)$ is the local (i. e. diagonal) element of the Green function of non-interacting electrons with spin σ and density n_σ. The energy E^I_σ describes the effective ("mean-field") energy of the localized σ-electrons and enters as a dynamical quantity. It has to be determined so that the corresponding free energy functional is maximal w.r.t. variations of E^I_σ. Hence E^I_σ is determined by [8]

$$n_\sigma = 1-\frac{1}{Q}e^{\beta(\mathcal{E}_{-\sigma}-E^I_\sigma)}[1+\kappa_{-\sigma}e^{\beta(\mathcal{E}_\sigma-E^I_{-\sigma}-U)}] \quad (2)$$

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

$$\begin{aligned} Q &= 1+\sum_\sigma \kappa_\sigma e^{\beta(\mathcal{E}_{-\sigma}-E^I_\sigma)} \\ &+ \kappa_\uparrow\kappa_\downarrow e^{\beta(\mathcal{E}_\uparrow+\mathcal{E}_\downarrow-E^I_\uparrow-E^I_\downarrow-U)} \end{aligned} \quad (3)$$

is the partition function of a renormalized atomic problem with

$$\mathcal{E}_\sigma = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega f(\omega) Im \ln[1-U\mathcal{G}_\sigma(\omega)] \quad (4)$$

as the energy shift of the static electrons in the Falicov-Kimball model due to the interaction with the itinerant electrons, where $f(\omega) = [\exp(\beta\omega) + 1]^{-1}$. Eqs. (1–4) contain the essence of our MFT for strongly interacting electrons. They differ from the Hubbard-III solution due to the existence of the dynamical variables E_σ^I which are thus seen to play a key rôle: they introduce the energy exchange between up and down-electrons which is missing in the Hubbard-III solution and make the theory thermodynamically consistent. The MFT defined by (1) –(4) has the following properties [4,8]: (i) it is based on an explicit free-energy functional Ω_{MF}, (ii) the ground state energy is a rigorous *lower* bound on the exact ground state energy of the Hubbard model in $d = \infty$, (iii) magnetic long-range order is possible, (iv) at $T = 0$, $n = 1$ and $U \gg t$ the Heisenberg limit comes out correctly.

Eqs. (1) – (4) may be used to construct a magnetic phase diagram for the Hubbard model. Here we restrict ourselves to ferromagnetic and antiferromagnetic (AF) phases in the ground state. The phase boundary of the paramagnetic phase is determined from the divergence of the corresponding susceptibility. We found an AF but no ferromagnetic instability. The $U - n$ phase diagram at $T = 0$ is shown in Fig. 1 (U is measured in units of $t^* = t\sqrt{2d}$). It confirmes the expectations concerning AF ordering at strong coupling. The absence of AF order for $n = 1$ at weak coupling is a deficiency whose origin is the same as in the Hubbard-III solution, i. e. is due to the separation of the dynamics of up and down spins [9]. Only at large U does the scattering of mobile σ-electrons by static $(-\sigma)$-electrons give an essentially correct description of the physical mechanism responsible for AF ordering. Hence, due to its very construction, our MFT is expected to be reliable in the intermediate and strong-coupling regime, but not at weak coupling and small doping (shaded region in Fig. 1).

The ordered phase can be further investigated with respect to its spectral properties. Depending on whether the DOS is finite or zero at $\omega = 0$, the phase is a metal or an insulator, respectively. One finds that the AF phase remains metallic even across the magnetic transition. However, as U is increased at fixed density the order parameter increases and the DOS decreases until, at a critical value of U, a metal-insulator transition occurs. The estimated phase boundary within the AF regime is plotted in Fig. 1. It shows that, away from half-filling, the Hubbard model displays a rather subtle sequence of magnetic and metal-insulator transitions for increasing U.

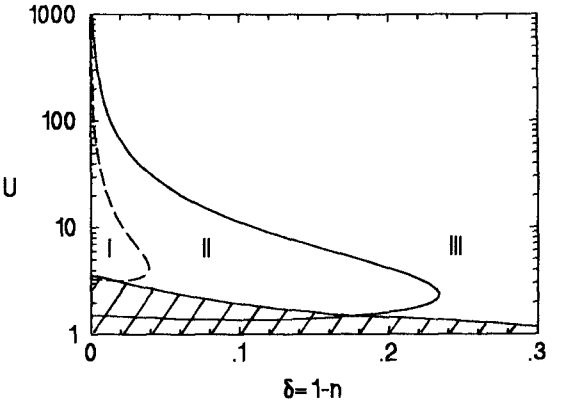

Fig.1 : Mean-field phase diagram for the Hubbard model at $T = 0$. I: AF insulator, II: AF metal, III: paramagnetic metal.

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