Mott-Hubbard Transition in Infinite Dimensions

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We present a solution of the Hubbard model at half filling in the limit of infinite dimensions which corresponds to the Mott-Hubbard insulating phase. We describe the metal-insulator transition between this regime and the Fermi-liquid regime. Our analysis is based on an analytic consideration and exact Monte Carlo simulations at low but finite temperatures.

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Strongly correlated Fermi systems in infinite dimensions were introduced by Metzner and Vollhardt [1]. They have received intensive recent attention because they are simple enough that they are amenable to exact treatment and at the same time retain some of the essential features of finite-dimensional models [2]. In this paper we will focus on the Hubbard model:

$$H=-\sum_{ij\sigma}t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{i}Un_{i\uparrow}n_{i\downarrow}-\mu\sum_{i\sigma}n_{i\sigma}. \quad (1)$$

$-\sum_{ij}t_{ij}e^{ik(i-j)}-\mu=\epsilon_k$ is the unperturbed one-particle energy and μ is the chemical potential which at half filling equals $\frac{1}{2}U$.

In a previous publication Georges and Kotliar [3] constructed a mean-field theory of the Hubbard model *which becomes exact in the limit of infinite dimensionality*. Independently Janis and Vollhardt [4] arrived at the same mean-field equations using a very different approach. Georges and Kotliar also analyzed qualitatively a class of solutions of these equations which describe the Fermi-liquid regime of this model using a mapping onto the single-impurity Anderson model. These ideas have been extended to other strongly correlated electron systems [5].

In this paper we introduce a different class of solutions which describe a Mott insulating phase. We then discuss how the transition between the Fermi-liquid and the Mott insulating phase takes place within the mean-field theory. We will show that one can obtain substantial analytic insights from the mean-field equations. In addition we have obtained an exact, numerical solution of these equations, which we use to check our considerations.

A basic observation in Ref. [3] is that for the purpose of calculating *local* quantities the information about all intersite processes is contained in a single function of frequency, $G_0(i\omega_n)$, which plays the role of the Weiss field in conventional mean-field theories. Given the Weiss field, the local Green's function $G_L(i\omega_n)=-\langle C_\sigma(i\omega_n)\times C_\sigma^{\dagger}(i\omega_n)\rangle_{S[G_0]}$ is calculated from the single-site action

$$S[G_0]=-\int_0^\beta\int_0^\beta C_\sigma^{\dagger}G_0^{-1}C_\sigma d\tau\,d\tau'+U\int_0^\beta C_\uparrow^{\dagger}C_\uparrow C_\downarrow^{\dagger}C_\downarrow d\tau. \quad (2)$$

G_L is related to the Green's function of the Hubbard model in infinite dimension via $-\langle C_K(i\omega_n)C_K^{\dagger}(i\omega_n)\rangle=1/[i\omega_n-\epsilon_K-\Sigma(i\omega_n)]$, so that $G_L(i\omega_n)=\sum_K\{1/[i\omega_n-\epsilon_K-\Sigma(i\omega_n)]\}$. To solve the model we have to compute the Weiss field $G_0(i\omega_n)$ from the self-consistency-condition equation

$$[G_0^{-1}(i\omega_n)-\Sigma(G_0,i\omega_n)]^{-1}=\int\frac{\rho(\epsilon)d\epsilon}{[i\omega_n-\epsilon-\Sigma(G_0,i\omega_n)]}, \quad (3)$$

where $\Sigma(G_0,i\omega_n)\equiv G_0^{-1}-\langle C^{\dagger}C\rangle_{S[G_0]}^{-1}$ is the self-energy of the impurity model (2). After solving for G_0, the self-energy of the Hubbard model is obtained by evaluating Σ at the self-consistent G_0.

The only place where the precise nature of the lattice enters the mean-field equations is in the density of states $\rho(\epsilon)\equiv\sum_K\delta(\epsilon-\epsilon_K)$. We view $\rho(\epsilon)$ as a parameter in the mean-field equations. The hypercubic lattice in infinite dimensions gives a Gaussian density of states [6]. We use a bounded density of states, which captures essential features of the band structures in *finite* dimensions. At half filling the model is particle-hole symmetric and it is convenient to define quantities which are odd functions of Matsubara frequency: $\tilde{G}_0^{-1}=G_0^{-1}-\frac{1}{2}U$ and $\tilde{\Sigma}(G_0)=\Sigma(G_0)-\frac{1}{2}U$.

In Ref. [3] Georges and Kotliar analyzed the qualitative behavior of the solutions of (2) under the assumption that G_0 is finite at zero frequency and $\mathrm{Im}G_0(i\omega_n=\Omega+i\delta)\neq 0$, which they showed implies Fermi-liquid behavior. Here we would like to point out that the system of Eqs. (2),(3) can have a different class of solutions which describe a Mott-Hubbard insulator. They are characterized by a G_0 which *diverges* at zero Matsubara frequency. This behavior is very natural if we think in terms of the mapping onto the Anderson model proposed in Ref. [3]. In that picture the original electron is split into a local degree of freedom which captures the localized aspect and a conduction band which reflects the itinerant aspect of the strong-correlation problem. The local degree of freedom hybridizes with the conduction band. $\tilde{G}_0$ is parametrized by the hybridization function $\Delta(\epsilon)$ of the Anderson model [3], $\tilde{G}_0^{-1}=i\omega_n+(\mu-\frac{1}{2}U)-\pi^{-1}\int\Delta(\epsilon)d\epsilon/(i\omega_n-\epsilon)$. The Fermi-liquid regime has $\Delta(0)\neq 0$ which binds the conduction electrons and the local moment to form quasiparticles. The insulating behavior that we find at half filling, $\mu=\frac{1}{2}U$, corresponds to a hybridization function which *vanishes* as we approach

zero energy, i.e., $\Delta(0)=0$.

When the hybridization function vanishes at zero frequency the Kondo model obtained from the Anderson model by eliminating the charge degree of freedom scales to weak coupling as shown by Whittoff and Fradkin [7]. We then have a realization of the paramagnetic insulating solution; the charge degrees of freedom are frozen while the spin degrees of freedom are free to fluctuate.

To exhibit our new type of solution analytically we take a semicircular density of states $\rho(\epsilon)=(2/\pi D^2)(D^2-\epsilon^2)^{1/2}$. We work in the limit $U\gg D$, and start with the assumption (which we will show is self-consistent) that $\tilde{G}_0^{-1}(i\omega_n)\sim i\omega_n$ that is $\Delta(i\omega_n)\to 0$ as $i\omega_n\to 0$. Substituting this into (2), one finds that the action becomes almost local (in imaginary time) at low energies, or in the language of the Anderson model, it reaches the atomic limit. The local Green's function and $\Sigma(G_0,i\omega_n)$ are then evaluated by taking an average of the two magnetic Hartree-Fock (HF) solutions,

$$G_L(i\omega)=\frac{1/2}{G_0^{-1}(i\omega_n)-U}+\frac{1/2}{G_0^{-1}(i\omega_n)} \tag{4}$$

which gives $\tilde{\Sigma}=(\frac{1}{2}U)^2\tilde{G}_0(i\omega_n)$.

Once more we emphasize that while the magnetic HF solution of the Anderson model is invalid when $\Delta(0)\neq 0$, the results of Ref. [7] imply that the magnetic Hartree-Fock solution is qualitatively correct for large U, since $\Delta(0)=0$, and in this case the Kondo coupling renormalizes to zero at low energies.

Now we show that the ansatz $\Delta(i\omega_n)\to 0$ as $i\omega_n\to 0$ is indeed self-consistent. The Hilbert transform of the semicircular density of states, $\int\rho(\epsilon)d\epsilon/(z-\epsilon)$, is given by $2/[z+(z^2-D^2)^{1/2}]$ and the self-consistency equation becomes

$$[\tilde{G}_0^{-1}-\tilde{\Sigma}(G_0)]^{-1}=\frac{2}{i\omega_n-\tilde{\Sigma}(G_0)+i\,\mathrm{sgn}(\omega_n)\{D^2+[\omega_n+i\tilde{\Sigma}(G_0)]^2\}^{1/2}}, \tag{5}$$

which leads to

$$4g_0^{-2}-U^2g_0x-4g_0^{-1}x+(U^2-D^2)=0, \tag{6}$$

where for convenience, we define $x=\omega_n$ and $\tilde{G}_0=-ig_0$, $\tilde{\Sigma}=-i\sigma$ so that g_0 and σ are positive when $\omega_n>0$. This is a cubic equation in g_0^{-1} which can be solved in closed form. Only one of the three roots corresponds to the physical solution. For small frequencies, the solution has a simple form $g_0^{-1}=U^2x/(U^2-D^2)$ (which requires $U>D$) for large frequencies $g_0^{-1}=x$. When $U\gg D$, which is the region where the expansion around the atomic limit is valid, it is possible to approximate the solution of the equation (analytically continued to real frequencies) as

$$\tilde{G}_0^{-1}=\omega-\omega\frac{4\omega^2-U^2-[(4\omega^2-U^2)^2-4(4\omega^2+U^2)D^2]^{1/2}}{2(4\omega^2+U^2)}. \tag{7}$$

The spectral function consists of two features centered around $\omega=\pm U/2$ with width $2D$, arising from the finite imaginary part of the square root. The hybridization function can be estimated, $\Delta(i\omega_n)=\tilde{G}_0^{-1}(i\omega_n)-i\omega_n\simeq i\omega_nD^2/(U^2-D^2)$, as $\omega_n\to 0$.

Thus we have shown that $\tilde{G}\to i\omega$, $\tilde{G}_0\to(i\omega)^{-1}$, and $\tilde{\Sigma}\to(i\omega)^{-1}$ in the low-frequency limit is a solution of the infinite-dimensional Hubbard model. This solution describes a Mott-Hubbard insulator characterized by a divergent self-energy and a gap in the single-particle spectrum of order $U-2D$.

A crucial question is how one goes from the Fermi-liquid solutions characterized by Fermi-liquid low-frequency behavior, $\tilde{\Sigma}(i\omega_n)\sim -i\omega_n$, to the Mott-Hubbard insulator regime described in this paper. To answer this question, we go back to the metallic solution and gradually increase the interaction U. As described in Ref. [5], the Fermi-liquid regime at half filling corresponds to the formation of the Abrikosov-Suhl Kondo resonance in the Anderson model. Equation (3) constitutes a functional equation for the Weiss field $G_0^{-1}(i\omega_n)$ which cannot be solved analytically (we will turn to its numerical solution below). To gain insight into the mechanism that destroys the Fermi-liquid resonance peak one would like to project the functional equation on a small space of "relevant variables."

Since $\Delta(0)$ is unrenormalized in the Fermi-liquid regime, we focus on a variable W, which describes the region over which the effective hybridization is nonzero at low energies. In the Anderson-model analogy it is the effective bandwidth of the conduction electrons. We envision an approximate parametrization of the exact solution of the system, at low frequencies, of the form $\tilde{G}_0^{-1}=-i\,\mathrm{sgn}(\omega_n)D/2+O(i\omega_n)$ for $|\omega_n|<W$, and $G_0^{-1}\approx i\omega_n$ for $|\omega_n|>W$. Imagine solving the system (2)–(5) by iteration. At the nth step we have some finite value of $W=W^{(n)}$, and obtain from the impurity model a self-energy $\tilde{\Sigma}=[1-1/Z(G_0)]\omega+O(\omega^2)$. For a large U/D, Z is just the inverse of the Kondo temperature, $Z(G_0)=4(W^{(n)}/D)\exp(-\pi U/4D)$. The next step in the iteration, is to solve Eq. (5), which gives, $W^{(n+1)}=4W^{(n)}\exp(-\pi U/4D)$.

It is clear that for large U the effective bandwidth iterates to zero, reaching the insulating regime. For small U/D, solving the impurity model gives a Z of order unity. The iteration step then gives $W\cong D$. This is the Fermi-liquid regime. Separating these two regimes is the critical U_c. In this scenario the Mott transition is driven by the shrinking of the dynamical range of the Fermi-

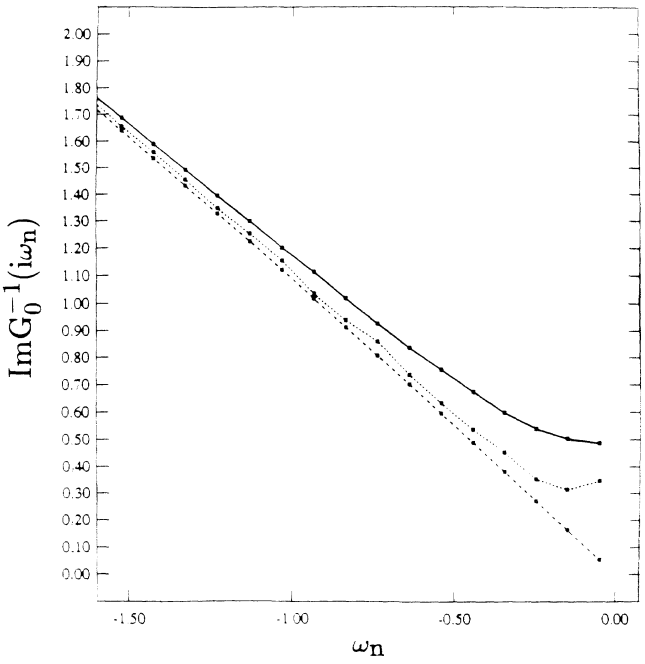

FIG. 1. The imaginary part of the Weiss field $\tilde{G}_0^{-1}$ as a function of Matsubara frequency for $U=2$ (solid line), $U=3$ (dotted line), and $U=3.6$ (dashed line), at $\beta=64$. All energy scales are renormalized by the half bandwidth $D=1$. For $U<U_c$ the Weiss field approaches its unrenormalized zero-frequency value $D/2$. For $U>U_c$ it matches the analytical solution of Eq. (6) in the text, $\mathrm{Im}(\tilde{G}_0^{-1})=-\omega_n$, $\omega_n\to\infty$, and $\mathrm{Im}(\tilde{G}_0^{-1})=-U^2\omega_n/(U^2-D^2)$, $\omega_n\to 0$.

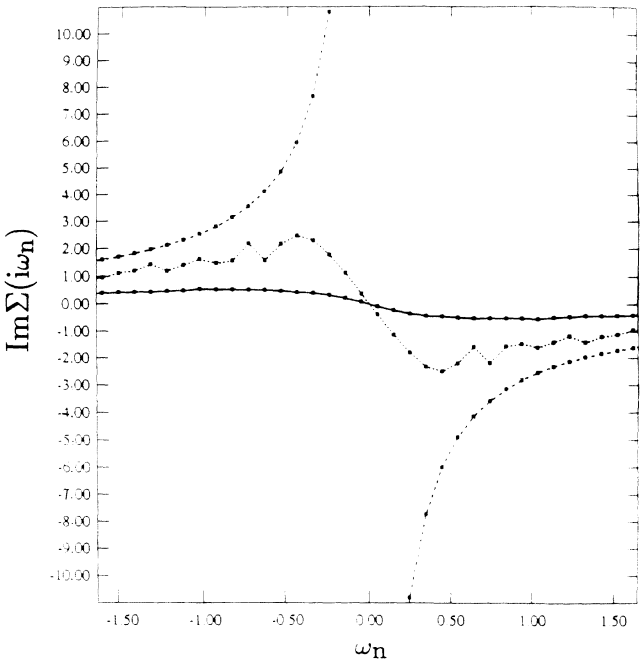

FIG. 2. The self-energy $\tilde{\Sigma}$ as a function of Matsubara frequency for $U=2$ (solid line), $U=3$ (dotted line), and $U=3.6$ (dashed line), at $\beta=64$. For $U<U_c$ the self-energy is linear at low frequencies with a slope increasing with U. The noise of the plot at $U=3$ is due to the proximity to the critical U.

liquid regime, the height of the quasiparticle peak remains unrenormalized. Related ideas have been put forward by Khurana [8].

To confirm these qualitative arguments, we solve Eqs. (2),(3) numerically using quantum Monte Carlo simulations. The procedure to compute $\Sigma(G_0)$ is based on the algorithm of Hirsch and Fye and of Gubernatis, Hirsch, and Scalapino [9] who studied the single-impurity Anderson model. The functional equation is solved using an iterative procedure. The technical details of the simulations will be discussed elsewhere. The Mott-Hubbard transition with the semicircular density of states is found at $U\approx 3.1$ for $D=1$ (all energy scales are renormalized by D), which is slightly lower than the result obtained from the Gutzwiller approximation, where U_c is calculated to be $32D/3\pi$ [10,11]. In Fig. 1 we show plots of $(\mathrm{Im}\tilde{G}_0)^{-1}$ vs ω_n for $U=2$, $U=3$, and $U=3.6$. Figure 2 shows the self-energy for the same values of the interaction. Below U_c we distinguish two Fermi-liquid subregimes characterized by small and large slopes of the self-energies, respectively. The plot for $U=2$ is characteristic of the weakly correlated Fermi-liquid regime where the Weiss field $\tilde{G}_0^{-1}$ decreases monotonically with frequency. The plot for $U=3.0$ is representative of the strongly correlated Fermi-liquid regime characterized by a small dip in $\tilde{G}_0^{-1}$, making it to increase towards its zero-frequency value $\frac{1}{2}D$ as we reduce the frequency. The behavior for $U>U_c$ is completely consistent with our analytic arguments. The numerical results are obtained at an inverse temperature $\beta=64$. The agreement of the numerical data with our analytic arguments gives us confidence that no new features will appear as we take the $\beta\to\infty$ limit. To further confirm the opening of a gap, we also measured the discontinuity in the chemical potential versus occupation number as shown in Fig. 3. At finite temperatures the metal-insulator transition we obtained becomes a crossover. However, this crossover is quite sharp. For example, at finite temperatures for $U>U_c$ the μ vs n curve should be continuous because there is always activation from the lower to the upper Hubbard band. Nevertheless the curves in Fig. 3 obtained at finite temperatures are nearly discontinuous because the temperature is much smaller than the Mott-Hubbard gap.

We also measured the *local* spin-spin autocorrelation function of the Hubbard model, in imaginary time. It is given by the spin-spin correlator of the impurity model. Our measurements are consistent with the following behavior: On the insulating side of the transition there is long-range order in imaginary time $\lim_{\tau\to\infty}\langle m(\tau)m(0)\rangle = m>0$ for $U>U_c$ and it decays to zero on the metallic side. $m=0$ for $U<U_c$.

In this Letter we have focused on the paramagnetic one-particle Green's function of lattice models in infinite dimensions with a bounded density of states. We also

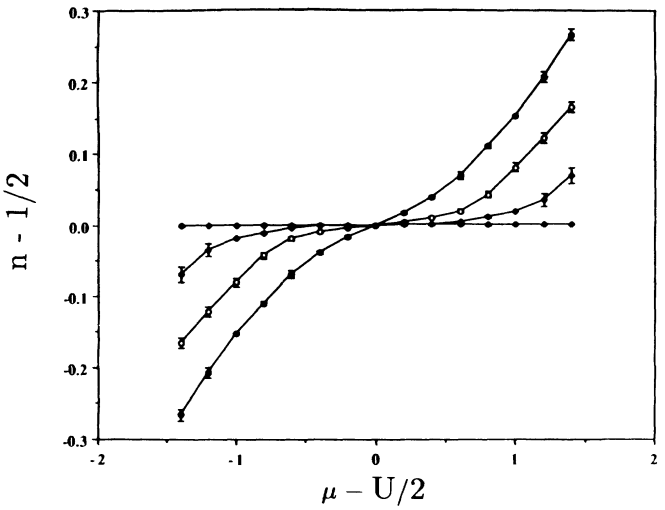

FIG. 3. The particle occupation as a function of the chemical potential $\mu - \frac{1}{2}U$ for $U=2.2$, 3, 4, and 6 (top to bottom as on right-hand side), at $\beta=4$.

studied the unbounded Gaussian density of states. In this case the numerical results for G_0 and the self-energy are very similar to that of unbounded ones. However, analytically can be seen that there is a *qualitative* difference in the spectral function of the local Green's function G: In the unbounded case, above U_c the one-particle spectral function has a *pseudogap* at the Fermi level. The rate at which the density of states decays at zero energy is simply related to the decay of the Hilbert transform of the density of states at infinity. $\mathrm{Im}G(\omega)\sim\rho(\omega-1/\omega)$, $\omega \rightarrow 0$.

In this Letter we concentrated on the paramagnetic solution in order to bring out the physics of the charge degrees of freedom. The physics of this phase depends only on the density of states. Müller-Hartmann [6] has shown that in infinite dimensions several lattice dispersions (some which correspond to non-nested lattices) share the same density of states. The nature of the magnetic order and the magnetic transition temperature requires one to specify more information on the form of the dispersion than just the density of states. Nonfrustrated lattices have antiferromagnetic transition temperatures which are exponentially small for small U, and of order t^2/U for large U, with a maximum transition temperature at U of order t. Frustrated lattices can have much lower transition temperatures. The semicircular density of states used in our calculations can be realized in a Cayley tree with infinite coordination number [12]. This lattice is not frustrated and is bipartite. As a result, at zero temperature it has antiferromagnetic long-range order for an arbitrary value of U. The semicircular density of states is also realized in a lattice where every site is connected to every other site and the hopping matrix elements are independent Gaussian random variables suitably scaled as the inverse square root of the number of lattice sites to have a good thermodynamic limit. While this model has randomness, the one-particle Green's function is nonrandom, i.e., it is self-averaging. This model is very frustrated and it does not order magnetically.

To summarize, we have found a new regime for the infinite-dimensional Hubbard model at half filling. We showed that the large-U narrow quasiparticle feature [3] disappears above a critical value of U. This is due to a divergence in the inverse of the self-consistent Weiss field G_0, which allows our $d=\infty$ model to map onto an Anderson model with *vanishing effective hybridization* at the Fermi level [$\Delta(0)=0$]. The Kondo model obtained from the Anderson model via the Schrieffer-Wolff transformation then flows to zero coupling at low energies. In this case the self-energy Σ has a pole singularity at zero frequency which reflects the opening of a Mott-Hubbard gap in the one-particle spectrum. Our solution for the case of very large U is essentially the same as that in Hubbard III [13]. What has been accomplished in this paper is (1) to show how Hubbard-like physics emerge in the limit of large d and large U, (2) to obtain a true Fermi-liquid solution on the metallic side of the transition, and (3) to show how a transition between the two regimes takes place as we change the value of U.

Upon the completion of this work, we have received a preprint from Mark Jarrel who has used a similar numerical procedure. We also learned that similar work was performed by A. Georges and W. Krauth. We would like to thank C. Castellani, J. Ferrer, F. Gebhard, and Q. Si for useful discussions. This work was supported by the NSF under Grant No. DMR 89-15895. The bulk of the numerical calculations were performed using a Cray-YMP at University of Illinois, Urbana-Champaign supercomputer center.

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