Numerical Solution of the $d=\infty$ Hubbard Model: Evidence for a Mott Transition

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We present a numerical solution of the infinite-dimensional Hubbard model at finite temperature in the paramagnetic phase. The problem reduces to a single-impurity Anderson model supplemented by a self-consistency condition. Using Monte Carlo methods and complete enumeration we determine the imaginary-time Green's function, the density of doubly occupied sites, and the compressibility close to half filling. All three quantities present direct evidence for a Mott insulating phase above a critical value of U.

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Strongly correlated Fermi systems have been the subject of intense research in the last few years. Recently, the limit of large dimensionality [1,2] has been shown [3,4] to provide a natural mean-field picture of these systems. Exact mean-field equations have been established for the one-particle Green's function in this limit [3,5,6], which map a lattice problem in dimension $d=\infty$ (e.g., the Hubbard model or the Kondo lattice) onto a single-impurity model supplemented by a self-consistency condition [3]. This is still quite a difficult problem, however, and no full solution has been found until now [6]. The present paper discusses a numerical method to solve this problem. We apply it to the paramagnetic phase of the Hubbard model and present numerical results which provide direct evidence for a metal-insulator transition at half filling.

Consider the Hubbard model,

$$H=-\sum_{\langle ij\rangle\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.}+U\sum_i n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

in which the hopping t_{ij} is scaled in such a way that the kinetic and interaction energies remain of the same order of magnitude as $d\to\infty$ [7]. For a d-dimensional hypercubic lattice with nearest-neighbor hopping, t_{ij} must be scaled as $t_{ij}=1/2\sqrt{d}$ and the free ($U=0$) density of states (DOS) $D(\epsilon)$ acquires a Gaussian form in the $d\to\infty$ limit [7]: $D(\epsilon)=(1/\sqrt{\pi})\exp(-\epsilon^2)$. In this case $D(\epsilon)$ is unbounded, while for the Bethe lattice with connectivity $Z=2d\to\infty$ and $t_{ij}=1/\sqrt{Z}$, the DOS takes a semicircular form $D(\epsilon)=\theta(2|\epsilon|)\sqrt{1-\epsilon^2}/2\pi$ [1].

Mean-field equations.—One-particle properties for the $d=\infty$ Hubbard model can be obtained from the study of an auxiliary impurity problem defined by the following single-site action [3,5]:

$$S_{\text{imp}}=U\int_0^\beta d\tau\, n_\uparrow(\tau)n_\downarrow(\tau)-\int_0^\beta d\tau\int_0^\beta d\tau'\sum_\sigma c_\sigma^{\dagger}(\tau)G_0^{-1}(\tau-\tau')c_\sigma(\tau')\,. \tag{2}$$

Here, G_0 has to be determined *self-consistently* from the requirement that the interacting Green's function $G(\tau-\tau')=-\langle Tc(\tau)c^{\dagger}(\tau')\rangle_{S_{\text{imp}}}$ of S_{imp} coincides with the site-diagonal Green's function of the lattice problem. This condition reads

$$G(i\omega_n)=\tilde{D}(i\omega_n+\mu-G_0(i\omega_n)^{-1}+G(i\omega_n)^{-1}) \tag{3}$$

in which $\tilde{D}$ is the Hilbert transform of $D(\epsilon)$: $\tilde{D}(z)=\int_{-\infty}^{+\infty}d\epsilon\, D(\epsilon)/(z-\epsilon)$ and the Matsubara frequencies are given by $\omega_n=(2n+1)\pi/\beta$. G_0 and G are fully determined by the solution of the impurity model supplemented by the constraint (3). The self-energy $\Sigma(i\omega_n)=G_0(i\omega_n)^{-1}-G(i\omega_n)^{-1}$ associated with the solution of Eqs. (2),(3) coincides with the self-energy of the lattice model, which becomes $\mathbf{k}$ independent in the $d\to\infty$ limit [1]. The one-particle Green's function of the lattice model thus reads $G(\mathbf{k},i\omega_n)=[i\omega_n+\mu-\epsilon_{\mathbf{k}}-\Sigma(i\omega_n)]^{-1}$. These equations, which have the physical content of a *mean-field theory,* are valid in the *paramagnetic* phase of the model, on which we will concentrate exclusively in this paper. Similar equations can be derived in phases with long-range magnetic order [2,6].

Equations (2),(3) are *exact* for the hypercubic and Bethe lattice in the limit $d\to\infty$ only, in which case $D(\epsilon)$ takes the Gaussian and semicircular form, respectively. They can, however, be considered as a mean-field description in more general instances, with an arbitrary DOS $D(\epsilon)$: This local approximation amounts to ignoring momentum conservation in all *skeleton* diagrams for the self-energy, while frequency conservation is retained.

Numerical method.—Our numerical solution of the self-consistent problem consists in the iteration of two steps: (1) The calculation of the imaginary-time Green's function $G(\tau)$ for a given $G_0(\tau)$. This requires solving the impurity problem (2), and is of course the most difficult step of the procedure. (2) The calculation of an updated function $G_{0,\text{new}}$ from the above solution. This is achieved by first Fourier transforming G_0 and G and then using the self-consistent Eq. (3) in the form

$$G_{0,\text{new}}(i\omega_n)=\Sigma(i\omega_n)+1/\tilde{D}(i\omega_n+\mu-\Sigma(i\omega_n))\,,$$

where $\Sigma(i\omega_n)=G_0(i\omega_n)^{-1}-G(i\omega_n)^{-1}$.

This procedure is iterated at a fixed value of the chemical potential μ until convergence is reached, starting from an arbitrary G_0.

$S_{\rm imp}$ can be viewed [3] as the effective dynamics governing the impurity orbital c_σ in the Anderson model of a magnetic impurity hybridized with a conduction band [8]. To solve it, we have used the algorithm of Hirsch and Fye [9] for the Anderson model which works directly with the imaginary-time Green's functions $G_0(\tau),G(\tau)$. The interval $[0,\beta]$ is discretized in L slices of size $\Delta\tau$ ($\beta=L\Delta\tau$). A decoupling of the interaction term in $S_{\rm imp}$ is performed through L auxiliary Ising variables. For a given spin configuration, the trace over fermions can then be taken. For large grids ($L\geq 18$) we have used a single-spin flip Monte Carlo method to sample spin configurations, as in Ref. [9]. For $L\leq 16$, we have been able to sum over all 2^L spin configurations by a single-spin flip complete enumeration based on Gray's code [10]: As evidenced below, this increases the accuracy dramatically.

Remarkably, this iterative algorithm is found to converge rapidly to a solution (G_0,G) of Eqs. (2),(3). Typical examples are displayed in Fig. 1, for which a convergence up to 10^{-6} was obtained for $L=16$ in 4 iterations when using Gray's code [11].

Numerical results.—We concentrate in this paper on the half-filled case (setting $\mu=U/2$) and study the paramagnetic solution as a function of temperature and U. Of course, on a bipartite lattice and at very low temperature $T<T_{\rm Neel}$, the solution with lowest free energy is antiferromagnetic. In this paper, however, we are only interested in describing the interplay between Fermi-liquid behavior and localization within the paramagnetic solution, as is, e.g., commonly done in the theoretical descriptions of ^{3}He [12]. We have investigated both a Gaussian DOS and square DOS $D(\epsilon)=\frac{1}{2}$ for $-1<\epsilon<1$ without finding qualitative differences in the results of our simulations (cf. however [13]).

One of the simplest indicators of the degree of correlations is the fraction of doubly occupied sites $\langle D\rangle=\langle n_\uparrow n_\downarrow\rangle$. A plot of $\langle D\rangle$ as a function of temperature for various values of U is given in Fig. 2 for the square DOS (the results for the Gaussian DOS are qualitatively very similar). At very high temperature ($T\gg U$), $\langle D\rangle$ approaches the atomic value $\langle D\rangle_{\rm at}=1/[2+2\exp(U/2T)]$. The data display a characteristic low-temperature behavior: For U not too large, $\langle D\rangle$ initially *decreases* with temperature, reaches a minimum, and increases again. This feature is characteristic of incipient localization effects in a strongly correlated Fermi liquid in a regime dominated by spin fluctuations [14]. Starting from the low-temperature Fermi-liquid regime with an entropy γT per particle, the system can gain free energy upon heating by increasingly localizing the particles (i.e., decreasing $\langle D\rangle$) in order to take advantage of a larger spin entropy (which would be of order ln2 in a solid phase) [15]. The inset of Fig. 2 shows the temperature T_m at which this minimum is found as a function of U. Above $U=U_c\simeq 3$ ($U_c\simeq 3.7$ for the Gaussian DOS), we have been unable to locate a minimum of $\langle D\rangle$ vs T above $T=\frac{1}{32}$. We interpret this as the signature of a localized Mott phase for $U>U_c\simeq 3$ at $T=0$. Indeed, a localized phase has a finite spin entropy already at $T\simeq 0$ and cannot gain free energy by decreasing $\langle D\rangle$ upon heating.

In order to confirm the existence of a Mott transition we have performed simulations away from half filling to

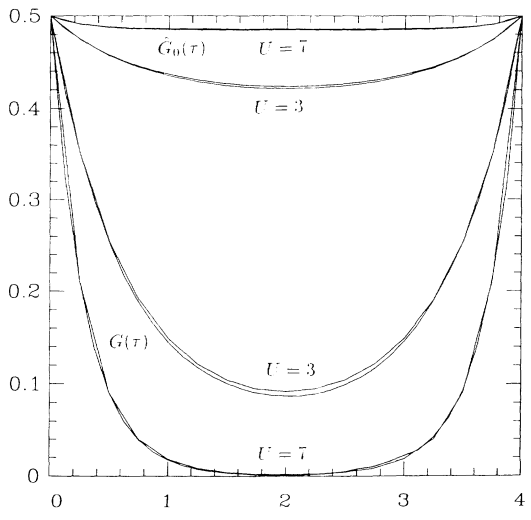

FIG. 1. Green's functions $G(\tau)$ and $\hat{G}_0(\tau)$ [defined by $\hat{G}_0(i\omega_n)^{-1}=G_0(i\omega_n)^{-1}-U/2$] at half filling and $\beta=4$ for $U=3$ (itinerant phase) and $U=7$ (localized phase), obtained by Monte Carlo simulations for $L=32$ and by exact enumeration for $L=16$ (square DOS).

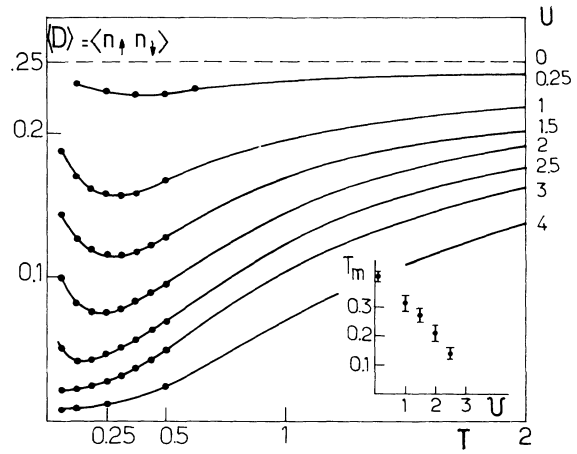

FIG. 2. Density of doubly occupied sites vs temperature at half filling for various values of U (square DOS). Very similar results are obtained for the Gaussian DOS. Inset: Temperature at which $\langle D\rangle$ is minimum vs U.

obtain the chemical potential μ as a function of density n, and we compute the compressibility $\kappa=\partial n/\partial\mu$. The latter requires an extremely good accuracy on μ vs n: Exact enumeration is the key point here. Figure 3 displays plots of $\hat{\mu}=\mu-U/2$ versus density at $\beta=1/T=4$. For $U=3$ and $U=7$, we display the three curves obtained for $L=4,8,12$ ($\Delta\tau=1,0.5,0.33$). All these data are obtained at constant μ and a relative precision of 10^{-6} is reached on the computed density. These curves clearly extrapolate (as $L\to\infty$) to $\hat{\mu}=0$ for $U=3$, and apparently to a *nonzero* value of $\hat{\mu}\simeq 1.7$ for $U=7$. We consider this as the signature of the Mott phase, with a discontinuity of μ vs n at $T=0$. Indeed $T=1/\beta=0.25$ is small compared to the Mott gap that we find at $U=7$, and our simulation cannot really exclude that the discontinuity is not actually smoothed out by an exponentially small amount $\exp(-\beta\Delta_{\mathrm{Mott}})$. This change of regime at finite T can be very abrupt, as evidenced by the inset of Fig. 3, displaying the inverse compressibility κ^{-1}. We estimate $U^*(\beta=1/T=4)\simeq 4.7$, $U^*(\beta=1/T=2)\simeq 7.5$.

The localized phase is also directly apparent on the Green's functions $G_0(\tau)$,$G(\tau)$ themselves. These are displayed in Fig. 1 at $\beta=4$ for $U=3$ and $U=7$. It is striking that the decay of $G(\tau)$ with τ is much more rapid in the localized phase. Indeed extrapolation to large β in the Fermi-liquid phase reveals a decay as $1/\tau$ for large τ, as expected, and an exponential decay in the localized phase, as expected when the spectral density has a gap at $T=0$.

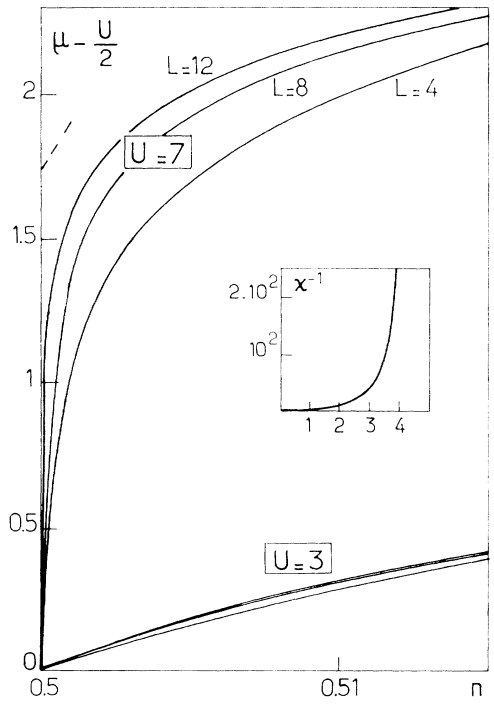

FIG. 3. Shifted chemical potential vs density at $\beta=4$ for $U=3$ and $U=7$ and for three values of $L=4,8,12$, as obtained by exact enumeration for the square DOS. The dashed line is a linear extrapolation to $1/L=0$. Inset: Inverse compressibility κ^{-1} vs U.

Discussion.—Using three different and largely independent quantities, we have found consistent evidence for a localized regime, for large enough U ($U_c\simeq 3$ for the square DOS, $\simeq 3.7$ for the Gaussian DOS). In the itinerant phase for $U\le U_c$ we have noticed an increasing tendency to localize below a temperature scale T_m (that we associate with spin fluctuations), and a second temperature scale ($\simeq U$) associated with the crossover to the atomic regime. Above U_c the first temperature scale disappears.

It is instructive to compare these findings to the Gutzwiller approximation (GA) scheme on which most theoretical descriptions of the Mott transition have relied up to now [14,16]. The $T=0$ phase diagram is in qualitative agreement with this approximation, which yields $U_c^{\mathrm{GA}}=4$ for the square DOS and $U_c^{\mathrm{GA}}=8/\sqrt{\pi}\simeq 4.5$ for the Gaussian DOS. Of course, in contrast to the GA, $\langle D\rangle$ is nonzero at $T=0$ even in the localized phase and cannot serve as an order parameter. This is because the GA misses completely the higher energy scale associated with charge fluctuations.

At finite temperatures, however, we find a phase diagram markedly different from the results of various attempts to extend the GA to $T>0$ [14,17]. A localized phase is *not* entered upon heating for $U\le U_c$ even though an increasing degree of correlation is observed below T_m (Fig. 2). Rather, we find that $U^*(T)$ *increases* rapidly with T. In our opinion the first-order Mott transition at $T\neq 0$ for $U\le U_c$ found within GA schemes is to be interpreted as the crossover associated with T_m (cf. inset of Fig. 2).

Finally, we show how the transition to a Mott phase for $U>U_c$ (i.e., the breakdown of Fermi-liquid behavior) can be understood theoretically at $T=0$. Let us represent the $T=0$ local Green's function by its spectral density $\rho(\omega)=-(1/\pi)\,\mathrm{Im}G(\omega+i0^+)$. In the picture of Ref. [3], $\rho(\omega)$ has a three-peak structure in the Fermi-liquid regime: a narrow quasiparticle resonance at $\omega=0$, of width $Z\simeq T_K$, and two satellite peaks corresponding to the upper and lower Hubbard bands. The impurity model (2) is in a local-moment regime at half filling, associated with the low-energy scale T_K (Kondo temperature) below which spin fluctuations are quenched. Clearly, the Mott phase must correspond to *a suppression of the Kondo effect in the impurity model,* so that the Kondo resonance (quasiparticle peak) disappears and the $T=0$ spectral density develops a gap (or a pseudogap, see [13]) at zero frequency.

We now imagine solving the impurity model iteratively as in our algorithm, starting from an arbitrary G_0. A convenient parametrization of the latter at half filling is $G_0(i\omega_n)^{-1}-U/2=i\omega_n-\tilde{\Delta}(i\omega_n)$, in which $\tilde{\Delta}$ is the Hilbert transform of an even function $\Delta(\omega)$. In the Anderson model framework [cf. Eq. (2)], $\Delta(\omega)$ is essentially

the density of states of the conduction band. We will show that for large enough U, $\Delta(\omega)$ itself must eventually develop a gap [13]. The Kondo effect no longer takes place in that case since no hybridization with conduction electrons at the Fermi level is possible in the impurity model (the flow is towards weak Kondo coupling). At any given step of the iteration, we can characterize the low-frequency behavior of $\Delta(\omega)$ by its width W_0 and its value at zero energy, $\Delta(0)$. In the first part of the iteration, the impurity model must be solved for G. Decomposing $\rho(\omega)$ into a coherent part $\rho_{\rm coh}$ (the Kondo quasiparticle resonance) and an incoherent part $\rho_{\rm inc}$, and neglecting the latter together with all lifetime effects, we can approximate ρ at low frequencies by $D(\omega/T_K)$ where D is the free DOS. T_K is a nonuniversal quantity, but basically depends on U, $\Delta(0)$, and W_0 only. The self-consistency condition is then used to provide a new G_0 (i.e., a new Δ) from ρ. Within the above approximation, one finds that $\Delta(0)$ is invariant under iteration [and equal to $1/\pi^2 D(0)$], and the new width $W_{0,\rm new}$ is of order $T_K(W_0,U)$ [18]. Hence for large U, W_0 is *decreased upon iteration,* and one quickly reaches a regime in which W_0 is smaller than other energy scales (i.e., U and $\mu=U/2$). Using the relevant expression for $T_K(W_0,U)$ in this regime [19], one gets a recursion relation for the width, valid when U is very large: $W_0^{(n+1)} \simeq W_0^{(n)}[UD(0)]^{-1/2}\exp[-\pi^3 UD(0)/4]$. Hence, for large U, W_0 (and $Z \simeq T_K$) must converge to zero, which shows that the Fermi-liquid fixed point is unstable. $W_0=0$ signals the opening of a gap [13] in both $\Delta(\omega)$ and $\rho(\omega)$.

Even though it has been obtained under rough approximations and for large U, this recursion relation does have an unstable fixed point at a finite value of U. It lacks, however, the nonlinear terms which are crucial to allow a description of the transition (they would be induced by incoherent and lifetime effects).

In conclusion, we have demonstrated the possibility of solving the $d=\infty$ mean-field equations for strongly correlated systems with moderate computational effort. We expect this approach to significantly increase our understanding of these systems in the near future.

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Note added.— We have also learned of work similar to ours by Rozenberg, Zhang, and Kotliar [20].

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[11] The final results are obtained by extrapolating to small $\Delta\tau$ ($L\rightarrow\infty$). For the range of parameters studied, this turned out to be safely possible provided $\Delta\tau$'s of order 0.5 are reached.

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