Density of States near the Mott-Hubbard Transition in the Limit of Large Dimensions

Stefan Kehrein

Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

(Received 6 March 1998)

The zero temperature Mott-Hubbard transition as a function of the Coulomb repulsion U is investigated in the limit of large dimensions. The behavior of the density of states near the transition at $U = U_c$ is analyzed in all orders of the skeleton expansion. It is shown that only two transition scenarios are consistent with the skeleton expansion for $U < U_c$: (i) The Mott-Hubbard transition is "discontinuous" in the sense that in the density of states finite spectral weight is redistributed at U_c. (ii) The transition occurs via a point at $U = U_c$ where the system is neither a Fermi liquid nor an insulator. [S0031-9007(98)07525-5]

PACS numbers: 71.30.+h, 71.27.+a, 71.28.+d

The correlation-induced metal-insulator transition [1] is a fundamental and challenging problem in condensed matter physics. Theoretical work has centered around the Hubbard model, where a metal-insulator transition is expected at half filling for some critical on-site Coulomb repulsion U_c. A new line of approach for studying the metal-insulator transition has recently been opened by the limit of high dimensions [2]. At present this *dynamical mean field theory* seems the only tractable method to obtain exact statements concerning the Mott-Hubbard transition. Such results should be of considerable interest also for the physically relevant three dimensional case.

In the dynamical mean field approach the behavior of the density of states $\rho(\epsilon)$ near the Mott-Hubbard transition at half filling and zero temperature is of particular interest. Georges *et al.* [3] have described in detail a transition scenario where the spectral weight in the vicinity of the Fermi surface vanishes continuously as $U \uparrow U_c$ (compare Fig. 1): In some finite interval $[\epsilon_F - \Delta, \epsilon_F + \Delta]$ around the Fermi surface one finds

$$\int_{\epsilon_F-\Delta}^{\epsilon_F+\Delta} \rho(\epsilon) \to 0 \quad \text{as } U \uparrow U_c\,. \tag{1}$$

This implies that at U_c a finite excitation gap of size 2Δ opens in the density of states turning the Fermi liquid at once into an insulator. However, the analytical solution of the $d \to \infty$ Hubbard model is unfortunately still out of reach and the above transition scenario has been discussed controversially in the literature (see, e.g., Refs. [4,5]).

The purpose of this Letter is to establish constraints regarding possible transition scenarios based on an analysis of the dynamical mean field equations in all orders of the skeleton expansion. Conceptually the arguments are similar to the reasoning used by Luttinger [6] and Langer [7] in order to derive the $(\epsilon - \epsilon_F)^2$ behavior of the imaginary part of the self-energy in the vicinity of the Fermi surface. An asymptotic sum rule for the imaginary part of the self-energy can be established that implies the following constraint for the transition scenario: For all intervals with $\Delta > 0$ around the Fermi surface the limit in Eq. (1) has to be nonzero as $U \uparrow U_c$. Therefore the Mott-Hubbard transition investigated here is either (i) discontinuous in the sense that finite spectral weight is redistributed at U_c, or (ii) there is nonzero spectral weight in any neighborhood of the Fermi surface for $U = U_c$.

Possibility (ii) implies that the density of states is still gapless at the transition, i.e., pseudogaplike with $\rho(\epsilon_F) = 0$ but $\rho(\epsilon) \propto |\epsilon - \epsilon_F|^\alpha$, $\alpha > 0$ in the vicinity of ϵ_F. This would signal the existence of a non-Fermi liquid point separating metallic and insulating regimes. The analysis in this Letter will also provide insights in various analytical approximation schemes devised to solve the dynamical mean field equations.

The Hamiltonian of the Hubbard model is

$$H = -\frac{t}{\sqrt{d}} \sum_{(ij),\alpha} c_{i\alpha}^\dagger c_{j\alpha} + U \sum_i \left(c_{i\uparrow}^\dagger c_{i\uparrow} - \frac{1}{2}\right)\left(c_{i\downarrow}^\dagger c_{i\downarrow} - \frac{1}{2}\right),$$

where the hopping matrix elements are scaled as $t_{ij} \to t/\sqrt{d}$ to obtain a physically meaningful limit of large

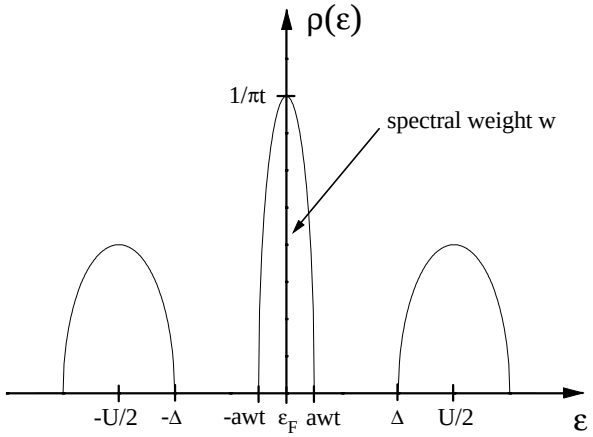

FIG. 1. Hypothetical density of states near a metal-insulator transition with vanishing spectral weight in the vicinity of the Fermi surface.

 0031-9007/98/81(18)/3912(4)$15.00

dimensions [2]. In the sequel t sets the energy scale and half filling corresponds to $\epsilon_F = 0$. For $d \to \infty$ an effective action describing the single-site dynamics of one fermionic degree of freedom $(c_{0\alpha}, c_{0\alpha}^\dagger)$ can be written as (for details, see Ref. [3])

$$S_{\text{eff}} = -\int_0^\beta d\tau\, d\tau' \sum_\alpha c_{0\alpha}^\dagger(\tau)\mathcal{G}^{-1}(\tau - \tau')c_{0\alpha}(\tau') + U\int_0^\beta d\tau\left(c_{0\uparrow}^\dagger(\tau)c_{0\uparrow}(\tau) - \frac{1}{2}\right) \times \left(c_{0\downarrow}^\dagger(\tau)c_{0\downarrow}(\tau) - \frac{1}{2}\right). \quad (2)$$

All local correlation functions of the original Hubbard model can be derived from (2). The effective action is supplemented by a self-consistency condition relating the Weiss local field $\mathcal{G}(\tau - \tau')$ and the local propagator $G(\tau - \tau') = -\langle T c_0(\tau) c_0^\dagger(\tau')\rangle$.

We will investigate the self-consistency problem by using a Bethe lattice with a large coordination number. On a Bethe lattice the self-consistency condition takes a particularly simple form [3],

$$\mathcal{G}^{-1}(i\omega_n) = i\omega_n - t^2 G(i\omega_n). \quad (3)$$

The discussion will be restricted to zero temperature, half filling, and the *paramagnetic phase*. Solutions with magnetic ordering are therefore excluded [8].

The k-independent self-energy of the Hubbard model is given by $\Sigma(\epsilon^+) = \mathcal{G}^{-1}(\epsilon^+) - G^{-1}(\epsilon^+)$ or

$$\Sigma(\epsilon^+) = \epsilon^+ - t^2\int_{-\infty}^{\infty} d\omega\, \frac{\rho(\omega)}{\epsilon^+ - \omega} - \left(\int_{-\infty}^{\infty} d\omega\, \frac{\rho(\omega)}{\epsilon^+ - \omega}\right)^{-1},$$

where $\rho(\epsilon) = -\frac{1}{\pi}\,\mathrm{Im}\,G(\epsilon^+)$ is the local density of states and $\epsilon^+ = \epsilon + i0^+$. By introducing the principal value integral $\Lambda(\epsilon) = \mathrm{P}\int_{-\infty}^{\infty} d\omega\, \frac{\rho(\omega)}{\epsilon - \omega}$ one can split the self-energy into its real and imaginary parts $\Sigma(\epsilon^+) = K(\epsilon) - iJ(\epsilon)$ leading to

$$K(\epsilon) = \epsilon - t^2\Lambda(\epsilon) - \frac{\Lambda(\epsilon)}{\Lambda(\epsilon)^2 + \pi^2\rho(\epsilon)^2}, \quad (4)$$

$$J(\epsilon) = -\pi t^2\rho(\epsilon) + \frac{\pi\rho(\epsilon)}{\Lambda(\epsilon)^2 + \pi^2\rho(\epsilon)^2}. \quad (5)$$

Notice that $\rho(\epsilon)$ is symmetric and therefore $\Lambda(\epsilon)$ is antisymmetric at half filling.

We investigate solutions near the metal-insulator transition coming from the metallic side $U \uparrow U_c$ [9]. A key role in this transition in the limit of large dimensions is played by the fixed value of the density of states at the Fermi surface $\rho(\epsilon_F) = 1/\pi t$ for the half filled case for $U < U_c$ [10]. This is due to the Fermi liquid property $J(\epsilon_F) = 0$. In the zero temperature metal-insulator transition scenario described by Georges *et al.* [3] the spectral weight w in the vicinity of the Fermi surface vanishes continuously while still $\rho(\epsilon_F) = 1/\pi t$ for $U < U_c$. Rephrased mathematically, the local density of states separates in a low- and a high-energy part for $U \uparrow U_c$,

$$\rho(\epsilon) = \rho_l(\epsilon) + \rho_h(\epsilon), \quad (6)$$

where $\rho_h(\epsilon)$ vanishes in some finite interval $[-\Delta, \Delta]$ around the Fermi surface. The low-energy part $\rho_l(\epsilon)$ describes a quasiparticle resonance at the Fermi surface with a continuously vanishing spectral weight w as $U \uparrow U_c$. Equation (6) is identical to the ansatz of Moeller *et al.* [11]; see also Fig. 1.

Because of the pinning $\rho_l(\epsilon_F) = 1/\pi t$ the quasiparticle resonance at the Fermi surface has a width of order wt. The existence of one single low-energy scale wt in this transition scenario implies that the following scaling ansatz becomes possible in the limit $w \to 0$ [11],

$$\rho_l(\epsilon) = \frac{1}{t} f\left(\frac{\epsilon}{wt}\right). \quad (7)$$

The dimensionless function $f(x)$ is normalized, $\int_{-\infty}^{\infty} dx\, f(x) = 1$, and fulfills $f(0) = 1/\pi$. This implies

$$\int_{-\Delta}^{\Delta} d\epsilon\, \rho(\epsilon) = w \to 0 \quad \text{for } U \uparrow U_c. \quad (8)$$

$\rho_h(\epsilon)$ also has some w dependence since it contains the remaining spectral weight $1 - w$. This weak dependence will be of no importance in the following discussion.

We now show that the above transition scenario cannot be realized within the skeleton expansion. It is taken for granted here that the transition occurs at a finite critical $U_c < \infty$ as supported by numerical calculations for nonzero temperature (see Ref. [3]).

Before proceeding with actual calculations we present an intuitive argument why the scenario (6) is not consistent with the skeleton expansion. Consider a (hypothetical) density of states near a metal-insulator transition as sketched in Fig. 1. For simplicity we assume that $f(x)$ has compact support in $[-a, a]$. Then for sufficiently small w the principal value integral $\Lambda(\epsilon)$ develops zeros for $\epsilon = \pm\epsilon_0$ with ϵ_0 of order $\sqrt{w}\,t$. Obviously $awt \ll \epsilon_0 \ll \Delta$ and therefore ϵ_0 lies in the gap $\rho(\pm\epsilon_0) = 0$ in the limit $w \to 0$. In this case $\Lambda(\epsilon_0) = 0$ leads to a δ-function-like contribution in $J(\epsilon)$ according to Eqs. (4) and (5). Hence a density of states as depicted in Fig. 1 enforces an imaginary part of the self-energy that vanishes everywhere in the gap *except* for δ functions at $\pm\epsilon_0$ [12] [notice that according to Eq. (5) $J(\epsilon)$ is well behaved for all other energies including the band edges]. In the skeleton expansion the imaginary part of the self-energy is related to the available phase space for scattering processes. With the above ansatz for $\rho(\epsilon)$, however, this phase space does not increase when passing from the small energy interval $[-awt, awt]$ to $[-\Delta, \Delta]$. Therefore the resonance of $J(\epsilon)$ in the gap cannot be explained in any order of the skeleton expansion. This argument can be generalized also to situations without a true gap.

Let us formalize this reasoning. The method used is a demonstration by contradiction, i.e., we first assume that solutions of the $d \to \infty$ self-consistency conditions with the property (8) exist. In the sequel $f(x)$ need not have compact support. Consider the value of $\Lambda(\Delta)$ in the limit $w \to 0$. The contribution from the states $|\epsilon| < \Delta$ in the principal value integral for $\Lambda(\Delta)$ behaves as

$$\int_{-\Delta}^{\Delta} d\epsilon \, \frac{\rho(\epsilon)}{\Delta - \epsilon} \approx \frac{1}{\Delta} \int_{-\Delta}^{\Delta} d\epsilon \, \rho(\epsilon) = w/\Delta \,,$$

whereas the remaining spectral weight of order w^0 for $|\epsilon| > \Delta$ contributes an essentially w-independent negative term. Therefore eventually $\Lambda(\Delta) < 0$, and thereby, according to (4)

$$K(\Delta) > \Delta \quad \text{for } w \to 0 \,. \tag{9}$$

It will be demonstrated below that the skeleton expansion implies $K(\Delta) \le 0$, yielding a contradiction. In order to show this we derive a sum rule for the imaginary part of the self-energy. The self-energy can be expressed in the following manner in a skeleton expansion [13]:

$$\Sigma(z) = [\text{all possible skeleton diagrams with the unperturbed propagator } \mathcal{G}(z) \text{ replaced by the true propagator } G(z)] \,. \tag{10}$$

The diagrams in this series can be analyzed in an elegant way introduced by Langer [7]: The imaginary part of a skeleton diagram is given by all possible Cutkosky cuts across the internal lines. Diagrams with cuts across n internal hole and $n + 1$ internal particle lines contribute

$$\int_0^{\infty} d\omega_1 \cdots d\omega_{n+1} \, \delta\Big(\sum_{i=1}^{n+1} \omega_i - \epsilon\Big) \times \prod_{i=1}^{n} \Big[\int_0^{\omega_i} d\xi_i \, \rho(\xi_i)\rho(\xi_i - \omega_i) \Big] \times \rho(\omega_{n+1})\Gamma^{(n)}(\xi_1, \xi_1 - \omega_1, \xi_2, \xi_2 - \omega_2, \ldots, \omega_{n+1}) \tag{11}$$

to $J(\epsilon)$, where $\Gamma^{(n)}$ describes generalized vertex functions [7]. In the vicinity of the Fermi surface this expansion gives the well-known behavior of the imaginary part of the self-energy for $\epsilon \to \epsilon_F$ [6]

$$J(\epsilon) = \sum_{n=1}^{\infty} \frac{\Gamma_n \, \rho(\epsilon_F)^{2n+1}}{(2n)!} (\epsilon - \epsilon_F)^{2n},$$

where the coefficients Γ_n are given by the above vertex functions and their derivatives in the infrared limit. The reason behind the increasing powers of ϵ is the restriction of the available phase space for scattering processes in (11) in the limit $\epsilon \to 0$.

Next we investigate the behavior of $\int_{-\Delta}^{\Delta} d\epsilon \, J(\epsilon)$ in the limit $w \to 0$. The key observation is that the ansatz (8) *automatically* leads to a restriction of the available phase space for scattering processes on an energy scale smaller than Δ: We can consider the limit $w \to 0$ in (11) and this leads to an expression for the integrated $J(\epsilon)$,

$$\int_{-\Delta}^{\Delta} d\epsilon \, J(\epsilon) = \sum_{n=1}^{\infty} \tilde{\Gamma}_n \Big(\frac{w}{2}\Big)^{2n+1} . \tag{12}$$

The coefficients $\tilde{\Gamma}_n$ are averages of the functions $\Gamma^{(n)}(\xi_1, \xi_1 - \omega_1, \xi_2, \xi_2 - \omega_2, \ldots, \omega_{n+1})$ over the Fermi liquid region: In (11) the vertex functions are probed only on the Fermi liquid energy scale of order wt in the integral $\int_{-\Delta}^{\Delta} d\epsilon \, J(\epsilon)$. Therefore one can infer the scaling behavior of $\tilde{\Gamma}_n$ with w from the behavior in the infrared limit: $\tilde{\Gamma}_n \propto \Gamma_n$ for $w \to 0$ [14]. On the other hand, from the scaling ansatz (7) one deduces $\Gamma_n \propto w^{-2n}$ with a w-independent proportionality constant depending on the function $f(x)$. Therefore the terms in the series (12) are of order w leading to

$$\int_{-\Delta}^{\Delta} d\epsilon \, J(\epsilon) = \alpha w t^2 + O(w^2) \tag{13}$$

with some dimensionless constant α that is finite for an integrable function $f(x)$. Since $K(\epsilon)$ and $J(\epsilon)$ are connected by a Kramers-Kronig relation [6],

$$K(\epsilon) = \frac{1}{\pi} \, \mathrm{P} \int_{-\infty}^{\infty} d\omega \, \frac{J(\omega)}{\epsilon - \omega} \,, \tag{14}$$

Eq. (13) implies that the positive contributions to $K(\Delta)$ in (14) vanish for $w \to 0$, leading to

$$K(\Delta) \le 0 \quad \text{for } w \to 0 \,. \tag{15}$$

Equations (9) and (15) are in obvious contradiction in the limit $w \to 0$: For sufficiently small but *nonzero* w, depending on the detailed structure of the upper and lower Hubbard bands and the function $f(x)$, these two relations exclude each other. Therefore we obtain a contradiction already for some $U < U_c$ *in* the metallic regime. This excludes solutions of the dynamical mean field equations describing the transition scenario (1) within the skeleton expansion.

In this context a comment on the frequently used "iterated perturbation theory" (IPT) approach [15] to $d \to \infty$ problems seems in order. IPT is second order perturbation theory for the self-energy in U where the Weiss propagator $\mathcal{G}(\epsilon^+)$ is used for the internal lines,

$$J^{(\mathrm{IPT})}(\epsilon) = \pi U^2 \int_0^{\epsilon} d\mu \, \rho_0(\epsilon - \mu) \times \int_0^{\mu} d\nu \, \rho_0(-\nu)\rho_0(\mu - \nu) \tag{16}$$

with $\rho_0(\epsilon) = -\frac{1}{\pi} \, \mathrm{Im} \, \mathcal{G}(\epsilon^+)$. This approximation leads to a metal-insulator transition that is *not seen* when the full propagator is used for the internal lines in similar schemes [10]. Since the noninteracting density of states $\rho_0(\epsilon)$ develops resonances on the energy scale $\sqrt{w}\, t$ close to a hypothetical metal-insulator transition like in Fig. 1, similar resonances are found in $J^{(\mathrm{IPT})}(\epsilon)$. This mechanism permits one to fulfill the self-consistency conditions

within the IPT approximation. However, from the results in this Letter it is clear that such resonances in $J^{(\mathrm{IPT})}(\epsilon)$ are an artifact of the non-self-consistent approximation used: If *all* orders of perturbation theory are summed up there is no phase space for scattering states available on the energy scale $\sqrt{w}\,t$. This observation raises serious doubts whether IPT incorporates the correct mechanism that actually drives the transition.

In summary in this Letter we have investigated the zero temperature metal-insulator transition in the half-filled Hubbard model in the paramagnetic phase on a Bethe lattice with large connectivity [8]. The framework used for this investigation was the skeleton expansion to all orders: The pointwise convergence of the skeleton expansion in the metallic phase is the basic *assumption* (but compare [16]) used in this Letter. Therefore our analysis was restricted to the metallic side of the transition since the skeleton expansion is known not to converge for an insulator.

An important constraint for the transition scenario follows from the asymptotic sum rule (13) for the imaginary part of the self-energy. This sum rule leads to a *competition* between the availability of phase space for scattering states and the suppression of spectral weight in the density of states in the vicinity of the Fermi surface. This competition must be taken into account when investigating the Mott-Hubbard transition in the limit of large dimensions. It eliminates the scenario of a metal-insulator transition with vanishing spectral weight in the vicinity of the Fermi surface; compare Eq. (1). Only two transition scenarios are consistent with the skeleton expansion for $U < U_c$: (i) A "discontinuous" transition occurs at $U = U_c$ in the sense that finite spectral weight is redistributed. (ii) For $U = U_c$ there is nonzero spectral weight in any neighborhood of the Fermi surface (pseudogap behavior), corresponding to some non-Fermi-liquid point separating metallic and insulating regimes. Careful numerical studies are required to establish whether such a pseudogap solution of the self-consistency equations is possible. Finally, the competition effect demonstrated above can be expected to be of importance for nonzero temperature too.

The author is greatly indebted to D. Vollhardt, P. G. J. van Dongen, F. Gebhard, and W. Metzner for valuable discussions and many important remarks. Discussions on related subjects with W. Hofstetter, J. Schlipf, and M. Kollar are acknowledged.

[1] N. F. Mott, Philos. Mag. **6**, 287 (1961).
[2] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[3] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[4] F. Gebhard, *The Mott Metal-Insulator Transition* (Springer-Verlag, Berlin, 1997).
[5] D. E. Logan and P. Nozières, Philos. Trans. R. Soc. London A **356**, 249 (1998).
[6] J. M. Luttinger, Phys. Rev. **121**, 942 (1961).
[7] J. S. Langer, Phys. Rev. **124**, 997 (1961).
[8] This is the usual setting in the literature for investigating the Mott-Hubbard transition also on other lattices. However, it should be kept in mind that the $T = 0$ Mott-Hubbard transition is generically hidden by an antiferromagnetic (AF) phase. For a critical discussion, see, e.g., Ref. [4]. But notice that the self-consistency condition (3) is identically also realized for a fully frustrated lattice with random couplings t_{ij} where there is no such AF phase (for details, see Ref. [3]). Instead of the Bethe lattice we can therefore also use this fully frustrated model as the starting point.
[9] In the literature often two critical points $U_{c1} < U_{c2}$ are discussed [3,5]. This leads to a coexistence region $[U_{c1}, U_{c2}]$ of an insulating and a metallic solution. The idea is that at U_{c1} the insulating gap and at U_{c2} the quasiparticle peak of the corresponding branch of solution vanishes. Notice that the discussion in this Letter always focuses on the metallic branch; therefore U_c as defined in this Letter corresponds to the above U_{c2}.
[10] E. Müller-Hartmann, Z. Phys. B **76**, 211 (1989).
[11] G. Moeller, Q. Si, G. Kotliar, M. Rozenberg, and D. S. Fisher, Phys. Rev. Lett. **74**, 2082 (1995).
[12] The existence of resonances in $J(\epsilon)$ on the energy scale $\pm\sqrt{w}\,t$ in this transition scenario was already observed by X. Y. Zhang, M. J. Rozenberg, and G. Kotliar, Phys. Rev. Lett. **70**, 1666 (1993).
[13] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).
[14] This proportionality holds uniformly in n, i.e., the infrared limit is approached uniformly for all n as $w \to 0$. This is due to the separation of the Hamiltonian in a gapped high-energy part and an effective low-energy Kondo Hamiltonian after a suitable unitary transformation that becomes possible when (1) holds [11]: The low-energy Hamiltonian can be made dimensionless after dividing by wt and its dimensionless couplings remain essentially unchanged as $U \uparrow U_c$. Therefore all $\Gamma^{(n)}$ contain a trivial overall w^{-2n} dependence and remain otherwise form-invariant functions of dimensionless variables ξ_i/wt as $U \uparrow U_c$. This unitary mapping to a well-understood Kondo Hamiltonian also guarantees that all vertex functions in (11) are well behaved in the Fermi liquid region of order wt around ϵ_F. Both these properties need no longer hold for $U \uparrow U_c$ in a pseudogap-transition scenario with a critical point at U_c.
[15] A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992).
[16] Notice, however, that the existence of the skeleton expansion is already needed for the derivation of the local nature of perturbation theory in infinite dimensions along the lines of Metzner and Vollhardt [2].