Zero Temperature Metal-Insulator Transition in the Infinite-Dimensional Hubbard Model

R. Bulla
Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Germany
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The zero-temperature transition from a paramagnetic metal to a paramagnetic insulator is investigated in the dynamical mean field theory for the Hubbard model. The self-energy of the effective impurity Anderson model (on which the Hubbard model is mapped) is calculated using Wilson’s numerical renormalization group method. Results for the quasiparticle weight, the spectral function, and the self-energy are discussed for the Bethe and the hypercubic lattice. In both cases, the metal-insulator transition is found to occur via the vanishing of a quasiparticle resonance that appears to be isolated from the Hubbard bands.

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The Mott-Hubbard metal-insulator transition [1,2] is one of the most fascinating phenomena of strongly correlated electron systems. This transition from a paramagnetic metal to a paramagnetic insulator is found in various transition metal oxides, such as V$_2$O$_3$ doped with Cr [3]. The mechanism driving the Mott-Hubbard transition is believed to be the local Coulomb repulsion $U$ between electrons on a same lattice site, although the details of the transition should also be influenced by lattice degrees of freedom. Therefore, the simplest model to investigate the correlation driven metal-insulator transition is the Hubbard model [4–6]

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i \sigma}^\dagger c_{j \sigma} + c_{j \sigma}^\dagger c_{i \sigma}) + U \sum_i c_{i \sigma}^\dagger c_{i \sigma}^\dagger c_{i \sigma} c_{i \sigma},$$

(1)

where $c_{i \sigma}^\dagger$ ($c_{i \sigma}$) denote creation (annihilation) operators for a fermion on site $i$, $t$ is the hopping matrix element, and the sum $\sum_{\langle ij \rangle}$ is restricted to nearest neighbors. Despite its simple structure, the solution of this model turns out to be an extremely difficult many-body problem. The situation is particularly complicated near the metal-insulator transition, where $U$ and the bandwidth are roughly of the same order and perturbative schemes (in $U$ or $t$) are not applicable.

With the recent development of the dynamical mean field theory (DMFT) [7–9] a very detailed analysis of the phase diagram of the infinite-dimensional Hubbard model became possible. The iterative perturbation theory (IPT) results of [9] gave a first order metal-insulator transition at finite temperatures. The transition occurs within a coexistence region of metallic and insulating solutions extending from $T = 0$ up to $T^* \approx 0.02W$ (where $W$ is the bandwidth). On approaching the metal-insulator transition from the metallic side (i.e., by increasing $U$), the authors of [9] found a quasiparticle peak with vanishing spectral weight which becomes isolated from the upper and lower Hubbard bands. A consequence of this result is that the opening of the gap and the vanishing of the quasiparticle peak do not happen at the same critical $U$. The possibility of this scenario was questioned by various authors [2,10–12]. The criticism is partly based on the fact that the IPT is essentially a second order perturbation theory in $U$ (although iterated due to the self-consistency appearing in the DMFT), whereas the metal-insulator transition happens at $U$ values of the order of the bandwidth.

Nonperturbative methods are clearly needed to clarify the situation. At finite temperatures, the quantum Monte Carlo method (QMC) should give reliable results, and recent QMC calculations by Schlipf et al. [13] gave no indication of a first order transition at finite $T$. The experimentally found first order transition in certain transition metal oxides therefore cannot be due to electronic correlations as modeled in (1), and lattice degrees of freedom will certainly play a role at the transition.

At zero temperature, the isolation of the quasiparticle peak and the appearance of a “preformed gap” were shown by Kehrein [11] to be in contradiction to a skeleton diagram expansion. Also, no preformed gap has been seen in calculations based on the random dispersion approximation (RDA) [12], where the opening of the gap and the vanishing of the quasiparticle peak were found to happen at the same critical $U$. The results for the gap and the quasiparticle weight are obtained in the RDA from finite size scaling of exact diagonalization results of clusters with up to 14 sites.

Both QMC and RDA are nonperturbative approaches which can, in principle, be applied for arbitrary low temperatures (the resolution of the low-frequency behavior in QMC and RDA is limited by the number of time slices or number of sites, respectively). The only nonperturbative approach which is presently able to cover the very low-temperature regime directly in the thermodynamic limit is the numerical renormalization group method (NRG). This method was introduced by Wilson for the Kondo problem [14] and was applied by Krishna-murthy et al. to the impurity Anderson model [15]. It was later shown that the NRG allows for a very accurate calculation of dynamical properties of various impurity models [16,17]. This is important because in the DMFT the self-energy (or equivalently the single-particle spectral function) of an effective
impurity model has to be calculated in the full frequency regime (for first applications to the Hubbard model, see Refs. [18,19]). One therefore expects that the NRG gives equally accurate results for the effective bandwidth Anderson model appearing in the DMFT. However, due to the lack of exact results for, e.g., the metal-insulator transition in the Hubbard model, this cannot be proven thus far.

Here we concentrate on the Mott-Hubbard metal-insulator transition at zero temperature and half-filling. At $T = 0$, this transition is usually hidden by the tendency of the model to form an antiferromagnetic ground state (as long as no frustration by, e.g., longer range hopping, is included). The results are discussed for both the Bethe lattice with infinite coordination number and the infinite-dimensional hypercubic lattice. The hopping matrix element in the Hamiltonian (1) is scaled as $t = t' \sqrt{Z}$ with $Z$ the number of nearest neighbors. In the following, we set $t' = 1$ as the unit for the energy scale. The resulting free densities of states for the Bethe and the hypercubic lattice are

$$
\rho_B(\epsilon) = \frac{1}{2\pi} \sqrt{4 - \epsilon^2} : |\epsilon| \leq 2, \\
\rho_{hc}(\epsilon) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\epsilon^2}{2}\right).
$$

The effective bandwidth $W = 4\sqrt{\int d\epsilon \rho(\epsilon)\epsilon^2}$ is $W = 4$ for both $\rho_B$ and $\rho_{hc}$ (the factor 4 is chosen so that the $W$ corresponds to the actual bandwidth of the semielliptic density of states $\rho_B$).

Figure 1a shows the $U$ dependence of the quasiparticle weight

$$
Z = \frac{1}{1 - \frac{\partial \Re\Sigma(\omega)}{\partial \omega}|_{\omega=0}},
$$

for both lattices. Despite the different lattice structure, the critical value of $U$ is approximately the same for both the Bethe and the hypercubic lattice, $U_{c,B} = 5.88 = 1.47W$ and $U_{c,hc} = 5.80 = 1.45W$. The different behavior of the $Z(U)$ curves for small values of $U$ can be understood from the second order perturbation theory which gives $Z(U) = 1.0 - 0.082U^2 + O(U^4)$ for the Bethe lattice [12] and $Z(U) = 1.0 - 0.12U^2 + O(U^4)$ for the hypercubic lattice.

Figure 1b shows the NRG result for the Bethe lattice together with results from calculations using the RDA [12] and the IPT [9]. The NRG and RDA results agree very well up to $U = 2.5$, but the NRG gives a long tail in the $Z(U)$ curve ending at a critical $U_c$ which is considerably larger than the $U_{c,RDA} = W$. In my view, the difference for $U > 2.5$ may be a consequence of the small system sizes presently taken into account in the RDA.

The $Z(U)$ curve from the IPT already starts to deviate from the NRG result for very small values of $U$. It was found earlier that the critical $U$ is overestimated by the IPT ($U_{c,IPT} = 1.65W$ [9]) and that the projective self-consistent method (PSCM) [9,20] gives a lower $U_{c,PS} = 1.46W$ which is in remarkable agreement with the NRG result. The $Z(U)$ curve from the QMC for small finite temperatures and a Bethe lattice density of states (not shown here) agrees well with the NRG result for $T = 0$ up to $U = 4.5$ [13]. The critical values obtained from the QMC (e.g., $U_{c,QMC} = (1.26 \pm 0.01)W$ for $T = 1/30$) are smaller than those from the NRG and the $U_{c,QMC}(T)$ curve shows a negative slope, a consequence of the higher spin entropy of the insulating phase.

The spectral functions $A(\omega)$ for the Bethe and the hypercubic lattice are compared in Fig. 2 for $U = 0.8U_c = 0.99U_c$ and $U = 1.1U_c$ (for details of the numerical calculations, see [19]). Although the semielliptic density of states $\rho_B$ is confined to the interval $[-2, 2]$, whereas the Gaussian density of states $\rho_{hc}$ has no cutoff, the
structures appearing in the spectral functions are very similar. In the metallic phase (for large enough values of $U$) the spectral function shows the typical three-peak structure with upper and lower Hubbard bands centered at $\pm U/2$ and a quasiparticle peak at the Fermi level. For $U = 0.99U_c$, the quasiparticle peak in both Bethe and hypercubic lattice seems to be isolated (within the numerical accuracy) from the upper and lower Hubbard bands, similar to what was observed in the IPT calculations for the Bethe lattice [9]. Consequently, the gap appears to open discontinuously at the critical $U$ (whether the spectral weight between the Hubbard bands and the quasiparticle peak is exactly zero or very small but finite cannot be decided with the numerical approach used here). Note that, due to the broadening of the spectra [19], an accurate resolution of the high-energy features, e.g., the band edges of the Hubbard bands, is not possible.

A few more points should be made concerning the existence of a finite critical $U$. In a single DMFT iteration, a metallic input produces a metallic solution irrespective of the value of $U$—similar to the standard single-impurity Anderson model, where the low-energy scale only vanishes exponentially with $U$. It is only through the requirement of a self-consistent solution that the critical value in the Hubbard model is shifted from $\infty$ to a finite value. This can be seen in NRG calculations for $U > U_c$ with a metallic solution as the starting point: the low energy scale vanishes exponentially with the number of DMFT iterations and the insulating solution is obtained only after infinite iterations.

The three-peak structure in the spectral function and the isolation of the quasiparticle peak near the transition have important consequences for the behavior of the self-energy. Figure 3 shows the imaginary part of the self-energy for the same parameters as in Fig. 2. In the insulating regime ($U = 1.1U_c$) the self-energy has a pole at zero frequency $\Sigma(z) = \frac{1}{z} + \Sigma_{\text{ren}}(z)$ ($z = \omega + i0^+$, and $\Sigma_{\text{ren}}$ denotes the remaining part of the self-energy). The weight $\alpha$ of this pole is given by

$$\alpha^{-1} = \int_{-\infty}^{\infty} d\omega \frac{A(\omega)}{\omega^2}. \quad (5)$$

It is obvious from the NRG results for the Bethe and the hypercubic lattice in Fig. 3 that the $1/z$ term emerges from a two-peak structure in the imaginary part of the self-energy when the transition is approached from the metallic side. The weight of the peaks is roughly independent of $U_c$, while the position and the width vanish with $U \rightarrow U_c$ (the position is proportional to $\sqrt{Z}$). At the transition, the two peaks collapse and give rise to a single pole with weight $\alpha$ [these features have already been discussed in Refs. [11,21]; note that the two-peak structure in $\text{Im}\Sigma(z)$ does not imply the existence of poles in $\Sigma(z)$]. This behavior is common to both lattice types studied here and it is only the $U$ dependence of the width that differs between Bethe and the hypercubic lattice.

![Fig. 3. Imaginary part of the self-energy for Bethe and hypercubic lattice for the same parameters as in Fig. 2.](image)

Note that the vanishing of the quasiparticle peak in the standard single-impurity Anderson model (which occurs for $U/\pi\Delta \rightarrow \infty$ [22]) is also associated with the collapse of a two-peak structure in the self-energy. This is observed both in the wide-band and the narrow-band limits (see [23] for a discussion of the latter case).

The two-peak structure is related to the typical three-peak structure (quasiparticle peak plus upper and lower Hubbard bands) in the spectral functions for both the single-impurity Anderson model and the infinite-dimensional Hubbard model. In both models, one has the relation

$$\Sigma(z) = z - \epsilon_d - \Delta(z) - \frac{1}{G(z)}, \quad (6)$$

with the hybridization function $\Delta(z)$. The self-energy develops peaks at the frequencies where the real and imaginary parts of $G(z)$ are small, which is the region between the quasiparticle peak and the Hubbard bands. Therefore, all calculations for the infinite-dimensional Hubbard model which give a well-pronounced three-peak structure in $A(\omega)$ necessarily produce the two-peak structure in the self-energy (examples are calculations from the QMC [8] and the noncrossing approximation [24]; at finite temperatures, the two-peak structure is broadened).

We now turn to an additional feature seen in both IPT and NRG calculations: the coexistence of metallic and insulating solutions in an interval $U_{c,1} < U < U_{c,2}$. Starting from $U = 0$, the metal-to-insulator transition occurs at the critical $U_{c,2}$ with the vanishing of the quasiparticle peak. Starting from the insulating side, the insulator-to-metal transition happens at $U_{c,1} < U_{c,2}$ (the NRG and IPT give $U_{c,1} \approx 1.25W$ for the Bethe lattice and the NRG gives $U_{c,1} \approx 1.15W$ for the hypercubic lattice).

Similar to the metallic case, a single DMFT iteration with an insulating input produces an insulating solution for any value of $U$. The insulator-to-metal transition
can be obtained only after an infinite number of DMFT iterations for \( U < U_{c,1} \). This transition is discontinuous, i.e., associated with a redistribution of spectral weight. The metallic solution at \( U_{c,1} \) shows a quasiparticle peak with \( Z = 0.1 \). The self-energy of the insulating solution shows the \( 1/z \) pole in the whole coexistence region, with a weight \( \alpha \) which goes to zero at \( U_{c,1} \). Consequently, the \( \delta \) function in \( \text{Im}\Sigma(\omega) \) does not split in a two-peak structure at \( U_{c,1} \).

The physical solution of the DMFT equations in the coexistence region is the one with the lower energy, which turns out to be the metallic one, in agreement with [9] (near the transition, the energy difference becomes too small to decide which solution has the lower energy, so that a small uncertainty remains near \( U_{c,2} \)).

In conclusion, we have investigated the zero-temperature metal-insulator transition in the Hubbard model for both the Bethe and the hypercubic lattice using a nonperturbative approach, the numerical renormalization group method. The NRG calculations show that the details of the transition are very similar in both cases despite the different lattice structure. In the Bethe lattice case, the result for the critical \( U \) is in remarkable agreement with the result from the PSCM. The NRG results (in particular, the two-peak structure in the imaginary part of the self-energy near the critical \( U \)) cannot be explained within a skeleton diagram expansion as shown in [11]. Potential problems, due to the fact that the derivation of the DMFT is based on such a skeleton diagram expansion [23], have still to be clarified.

In order to bridge the gap between \( T = 0 \) and the lowest temperatures accessible to the QMC method, the NRG has to be extended to finite temperatures (work on this is in progress). This will allow one to study the metal-insulator transition in the whole temperature range using nonperturbative methods.

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