Zero temperature metal-insulator transition in the infinite-dimensional Hubbard model

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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 quasiparticle weight, spectral function and self-energy are discussed for Bethe and hypercubic lattice. In both cases, the metal-insulator transition is found to occur via the vanishing of a quasiparticle resonance which appears to be isolated from the Hubbard bands.

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The Mott-Hubbard metal-insulator transition 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. The mechanism driving the Mott-Hubbard transition is believed to be the local Coulomb repulsion 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:

$$H = -t \sum_{<ij>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} c_{i\uparrow}, \quad (1)$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) denote creation (annihilation) operators for a fermion on site $i$, $t$ is the hopping matrix element and the sum $\sum_{<ij>,\sigma}$ 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), a very detailed analysis of the phase diagram of the infinite dimensional Hubbard model became possible. The Iterative Perturbation Theory (IPT) results of gave a first order metal-insulator transition at finite temperatures. The transition is occurring within a coexistence region of metallic and insulating solutions extending from $T = 0$ up to $T^* \approx 0.02W$ ($W$: bandwidth). On approaching the metal-insulator transition from the metallic side (i.e. on increasing $U$), the authors of found a quasiparticle peak with vanishing spectral weight which becomes isolated from 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 has been questioned by various authors. The criticism is partly based on the fact that the IPT is essentially 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.

Non-perturbative 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 J. Schlipf et al. gave no indications for a first order transition at finite $T$. The experimentally found first order transition in certain transition metal oxides can therefore not 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’ has been shown by S. Kehr in 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) where the opening of the gap and the vanishing of the quasiparticle peak was 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 non-perturbative 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 non-perturbative 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 has been introduced by Wilson for the Kondo problem and has been applied by Krishna-murthy et al. to the impurity Anderson model. It has been later shown that the NRG allows for a very accurate calculation of dynamical properties of various impurity models. This is important be-
cause 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 [18,19]). One therefore expects that the NRG gives equally accurate results for the effective impurity 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 so 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 groundstate (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 Bethe and hypercubic lattice are

$$\rho_B(\varepsilon) = \frac{1}{2\pi} \sqrt{4 - \varepsilon^2} \quad : |\varepsilon| \leq 2,$$

$$\rho_{hc}(\varepsilon) = \frac{1}{\sqrt{2\pi}} \exp \left(-\frac{\varepsilon^2}{2}\right).$$

The effective bandwidth $W = 4\sqrt{\int d\varepsilon \rho(\varepsilon)\varepsilon^2}$ 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 semi-elliptic density of states $\rho_B$).

Fig. 1a shows the $U$-dependence of the quasiparticle weight

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

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

Fig. 1b shows the NRG-result for the Bethe lattice together with results from calculations using the Random Dispersion Approximation (RDA) [2] and the IPT [3]. The NRG and RDA results agree very well up to $U \approx 2.5$ but the NRG gives a long tail in the $Z(U)$-curve ending at a critical $U_c$ which is considerably larger than the $U_{c,RDA} \approx W$. 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 starts to deviate from the NRG result already for very small values of $U$. It has been found earlier that the critical $U$ is overestimated by the IPT ($U_{c,\text{IPT}} \approx 1.65W$ [3]) and that the Projective Self-consistent Method (PSCM) [20] gives a lower $U_{c,\text{PS}} \approx 1.46W$ 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 $U \approx 4.5$ [3]. The critical values obtained from the QMC (e.g. $U_{c,\text{QMC}} = (1.26 \pm 0.01)W$ for $T = 1/30$) are smaller than those from the NRG and the $U_{c,\text{QMC}}(T)$-curve shows a negative slope, a consequence of the higher spin-entropy of the insulating phase.

The spectral functions $A(\omega)$ for Bethe and hypercubic lattice are compared in Fig. 2 for $U = 0.8U_c$, $U = 0.99U_c$ and $U = 1.1U_c$ (for details of the numerical calculations, see [13]). Although the semi-elliptic 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 has been observed in the IPT calculations for the Bethe lattice [3]. Consequently, the gap appears to open discontinuously at the critical $U$. 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.
The term ‘preformed gap’ is frequently used to describe the behavior seen in Fig. 2 although it is not clear whether a ‘preformed gap’ only means a strong suppression of spectral weight between the Hubbard bands (as seen in both NRG and IPT) or an exact vanishing of the spectral function in a finite interval. Using the latter definition, it is not possible to decide within a numerical approach (like NRG, QMC or IPT) whether the system shows a ‘preformed gap’ or not.

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. Fig. 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 $\Sigma(z) = \frac{\omega}{z} \Sigma_{\text{rem}}(z)$ ($z = \omega + i0^+$, $\Sigma_{\text{rem}}$ denotes the remaining part of the self-energy). There are several possibilities how the $1/z$-term in $\Sigma(z)$ develops when the transition is approached from the metallic side. One possibility would be that $\alpha$ is zero at the transition ($U = U_c$) and then increases continuously with increasing $U$. This imposes some constraints on the form of the spectral function because the weight $\alpha$ of the pole in the insulating regime is given by

$$\alpha^{-1} = \int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\mathcal{A}^{\text{pot}}(\omega)}{\omega^2}.$$  \hspace{1cm} (5)

If one assumes a powerlaw $\mathcal{A}^{\text{pot}}(\omega) \propto |\omega|^r$ for small $\omega$, the exponent has to satisfy $r \leq 1$ for $\alpha$ to vanish at the transition.

The other possibility is what is seen in the NRG-results for the Bethe and hypercubic lattice in Fig. 3. The $1/z$-term emerges from a two-peak structure in the imaginary part of the self-energy. The weight of the peaks is roughly independent of $U$, while the position and the width vanish with $U \to U_c$ (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 [11,21]; note that the two-peak structure in Im$\Sigma$ 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 $\omega$, that differs between Bethe and hypercubic lattice.

Note that the vanishing of the quasiparticle peak in the standard single impurity Anderson model (which occurs for $U/\pi \Delta \to \infty$ [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 limit (see [22] 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 single impurity Anderson model and the infinite dimensional Hubbard model. In both models, one has the relation

$$\Sigma(z) = z - \varepsilon_d - \Delta(z) - \frac{1}{G(z)},$$  \hspace{1cm} (6)

with the hybridization function $\Delta(z)$. The self-energy develops peaks at the frequencies where real- and imaginary part 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 $\mathcal{A}(\omega)$ necessarily produce the two-peak structure in the self-energy (examples are calculations from the QMC [8] and the Non Crossing Approximation [23]; 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).

The coexistence of metallic and insulating solutions is probably connected to the structure of the self-energy at $T = 0$. When $U$ is reduced below $U_{c,2}$, the $\delta$-function peak in the imaginary part of the self-energy does not split into the two-peak structure which is found for the metallic solution. The $\delta$-function peak only vanishes when its weight $\pi\alpha$ vanishes which happens at a lower value of $U$ (the $U_{c,1}$). The $U$-dependence of $\alpha$ near $U_{c,1}$ is difficult to determine and it is presently not clear whether $\alpha$ vanishes continuously or not.

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 [1] (near the transition, the energy difference becomes too small to decide which solution has the lower energy, so that a small uncertainty remains near $U_{c,2}$). The coexistence of solutions therefore does not play a role at $T = 0$ and can be neglected.

In conclusion, we have investigated the zero-temperature metal-insulator transition in the Hubbard model for both Bethe and hypercubic lattice using a non-perturbative 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 Projective Self-consistent Case. 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 [25] 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 to study the metal-insulator transition in the whole temperature range using non-perturbative methods.

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