Mott-Hubbard metal-insulator transition in d=∞

J. Schlipf(1), M. Jarrell(2), P. G. J. van Dongen(1), N. Blümer(1), S. Kehrein(3), Th. Pruschke(4), and D. Vollhardt(1), (1)Universität Augsburg, Germany, (2)University of Cincinnati, USA, (3)Harvard University, USA, (4)Universität Regensburg, Germany

Abstract

The Mott-Hubbard transition between a paramagnetic metal and a paramagnetic insulator is investigated within the infinite-dimensional Hubbard model. Recent results from high-precision quantum Monte Carlo (QMC) simulations, in particular for the phase diagram and the density of states, are discussed.

The transition is shown to be continuous down to at least $T = W/140$ (W = bandwidth). We find that the Fermi-liquid breaks down before the gap opens. Thus, for a bandwidth of 0.8 eV, the transition is continuous down to $T \approx 70$K.

Introduction

- Mott-Hubbard metal-insulator transition: transition between paramagnetic metal and paramagnetic insulator due to electronic interactions. Example: V_2O_3 doped with Cr.
- Long-standing but still not fully understood phenomenon [1].
- Standard model to describe transition: half-filled single-band Hubbard model:

$$H = -t \sum_{\langle \mathbf{ij} \rangle, \sigma} c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \, . \qquad (1)$$

- Previous study of Mott-Hubbard transition by Kotliar, Georges et al. within Dynamical Mean-Field Theory (DMFT, exact in $d=\infty$) using iterative perturbation theory (IPT) and exact diagonalization (ED) [2].

  Their conclusions:
  1. transition is *discontinuous* for all finite temperatures $T < T_{\rm IPT}$, with hysteresis due to coexisting metallic and insulating states.
  2. experimentally observed *first-order* transition in Cr-doped V_2O_3 can already be understood using a purely electronic model.

Aim of this study and results

- We re-examine nature of Mott-Hubbard transition within DMFT at $T > 0$ with very careful QMC calculations [3].
- Usually convergence is reached if rate of change of self-energy in the DMFT iteration procedure becomes small: $\eta \equiv \langle |\Delta\Sigma(i\omega_n)| \rangle_n \le 10^{-3}$.
- Straightforward implementation of QMC algorithm with this criterion indeed leads to hysteresis (→ Fig. 1).

  BUT: More accurate calculation (→ inset of Fig. 1) shows, *both* solutions at $U = 5$ are unstable; new stable solution reached after approximately 20 more iterations → smooth curve $D(U)$ *without* hysteresis.

Quasiparticle renormalization factor $Z = m/m^*$ and compressibility κ

- Mott-Hubbard transition occurs at $U = U_c$ where $Z(U)$, $\kappa(U) \to 0$ (Fig. 2).
- Resulting phase diagram: Fig. 3
- We find: *continuous* transition down to at least $T = 1/35 \simeq 0.325\, T_{\rm IPT} \simeq 70$ K.

Conclusion

- Single-band Hubbard model does not provide quantitative description of first-order metal-insulator transition in Cr-doped V_2O_3 below $T_c \simeq 380$K.
- *Continuous* metal-insulator transition (crossover) down to at least $T_{\min} \simeq 70$K.
- To quantitatively explain experiment, other degrees of freedom must also be taken into account.

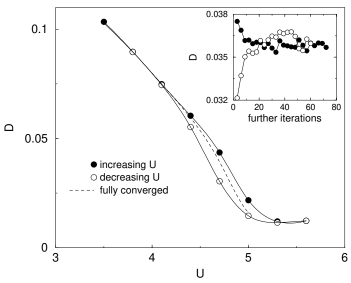

Fig. 1: QMC-results for the double occupancy D at $T = 1/20$ using the criterion $\eta \le 10^{-3}$. The error bars are smaller than the data points. All lines are guides to the eye only. Inset: Vanishing of the hysteresis as a function of the number of further iterations at $T = 0.05$, $U = 5$ and $\Delta\tau = 0.3$

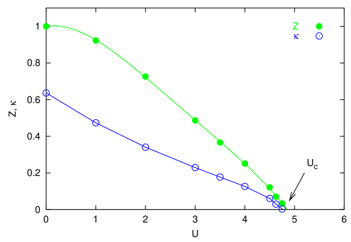

Fig. 2: Compressibility κ and quasiparticle renormalization factor $Z = m/m^*$ vs. U for $T = 1/15$. All lines are guides to the eye only.

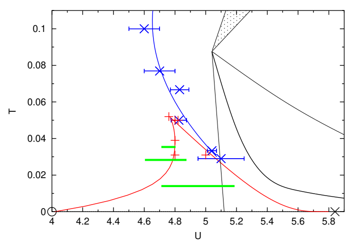

Fig. 3: Phase diagram of the Hubbard model (paramagnetic phase only). Blue crosses: continuous metal-insulator transition calculated with QMC (error bars include both the statistical errors and the uncertainty in U_c due to finite temperatures). Green horizontal lines: coexistence region within ED. Black lines: coexistence region within IPT; the line of first-order transitions ends at $T_{\rm IPT} \approx 0.088$. The shaded area above $T_{\rm IPT}$ is a crossover region. Also shown are the recent QMC results by Rozenberg et al. [4] (in red) and, for $T = 0$, the U_c-values from PSCT/NRG (X) [5,6] and RDA (O) [7].

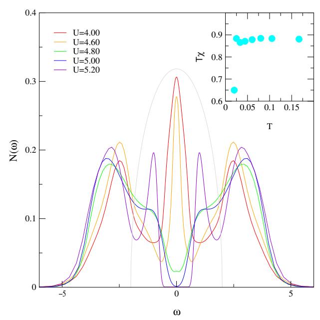

Fig. 4: QMC/MEM-results for the DOS (Bethe lattice) for various values of U at $T = 1/20$, and $\Delta\tau = 0.017$. The gap opens at $U_g \simeq 5.0$. The grey line indicates the non-interacting DOS. The temperature-dependence of the screened local moment m_s (the product of the temperature and the local susceptibility) is shown in the inset for $U = 4.8$.

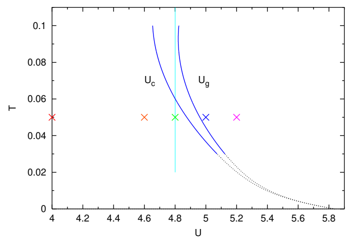

Fig. 5: Schematic phase diagram of the Hubbard model (paramagnetic phase only). The interaction values U_c and U_g correspond to the breakdown of the Fermi liquid and the opening of the gap, respectively. The vertical line (light blue) indicates the T-interval and the U-value for which the screened local moment was calculated (insert Fig. 4). The crosses indicate the U-values and the temperature for which the density of states (Fig. 4) was calculated.

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