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# Metal-insulator transition in the infinite-dimensional Hubbard model

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## Abstract

The nature of the Mott-Hubbard metal-insulator transition in the infinite-dimensional Hubbard model is investigated by quantum Monte Carlo simulations down to temperature  $T = W/140$  ( $W =$  bandwidth). Calculating with significantly higher precision than in previous work, we show that the hysteresis below  $T_{\text{IPT}} \simeq 0.022W$ , reported in earlier studies, disappears. Hence the transition is found to be *continuous* rather than discontinuous down to at least  $T = 0.325T_{\text{IPT}}$ . We also study the changes in the density of states across the transition, which illustrate that the Fermi liquid breaks down before the gap opens.

**Keywords:** condensed matter physics; correlated electron systems; quantum Monte Carlo; metal-insulator transition

## 1 Introduction

The explanation of the nature of the Mott-Hubbard metal-insulator transition, i.e., the transition between a paramagnetic metal and a paramagnetic insulator, is one of the classic and fundamental problems in condensed matter physics [1, 2, 3]. Metal-insulator transitions of this type are, for example, found in transition metal oxides with partially filled bands near the Fermi level. For such systems band theory typically predicts metallic behavior. The most famous example is  $\text{V}_2\text{O}_3$  doped with Cr [4]. In particular, in  $(\text{V}_{0.96}\text{Cr}_{0.04})_2\text{O}_3$  the metal-insulator transition is *first-order* below  $T_c \simeq 380\text{K}$  [4], with discontinuities in the ratio of the lattice parameters and in the conductivity, accompanied by hysteresis.

The Mott-Hubbard transition is caused by electron-electron repulsion. The fundamental features of this transition are traditionally expected [1, 4] to be explainable in terms of the half-filled single-band Hubbard model [5],

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{\mathbf{i}} n_{i\uparrow} n_{i\downarrow},$$

which describes electrons hopping on a lattice with amplitude  $t$ , interacting with each other through on-site Coulomb repulsion  $U$ .

On the basis of this model the Mott-Hubbard transition was studied intensively over the last 35 years. Early approaches could only describe high-energy features [6] or low-energy features [7] of the model correctly. A unified approach, treating all energy scales on the same footing, has recently become possible within the Dynamical Mean-Field Theory (DMFT) [8], which provides the exact solution of the Hubbard model in the limit of infinite dimensionality (or coordination number) [9]. The still complicated structure of the self-consistent DMFT-equations makes an analytic solution untractable and hence one has to resort to approximate techniques, such as iterated perturbation theory (IPT), exact diagonalization (ED) of small systems, quantum Monte-Carlo (QMC) simulations, or, at  $T = 0$ , the projective self-consistent technique (PSCT) [8, 10] or the numerical renormalization group (NRG) method [11].

In the last few years, Georges, Kotliar and collaborators performed investigations of the metal-insulator transition scenario within the DMFT, employing IPT, ED, QMC, and PSCT, finding the transition to be *discontinuous* for all temperatures  $T < T_{IPT}$ , with hysteresis involving coexisting metallic and insulating states. In their scenario, the quasiparticle weight disappears abruptly and the gap between the Hubbard bands opens discontinuously as a function of  $U$ . Hence these authors argued that the experimentally observed metal-insulator transition in  $V_2O_3$  can already be understood using a purely electronic correlation model. NRG studies [11] also found hysteresis which agrees with the results of the PSCT [10]. Nevertheless, the existence of a preformed gap at  $T = 0$  and the corresponding separation of energy scales on which the PSCT is based were recently disputed [12]. Finally, a *continuous* transition with a considerably lower  $U_c$  was found in a cluster approach [13] and, most recently, within the random dispersion approximation (RDA [2, 14]). Clearly the Mott-Hubbard transition scenario is still very controversial.

We re-examine the nature of the metal-insulator transition within DMFT by performing finite-temperature auxiliary-field QMC calculations. The usage of two different codes reduces possible systematic errors. For the Hubbard model at half-filling, there is no “minus-sign problem”.

## 2 Vectorization, Parallelization and Performance

The computationally intensive part of our calculations, the solution of the quantum impurity problem, is performed using the algorithm of Hirsch and Fye [15]. For details concerning the implementation and computational cost, see the contribution by Held et al.

Our Fortran programs have been designed for vector supercomputers. They vectorize to a high degree, since the computationally intensive parts are matrix operations. Within each iteration of the self-consistency cycle, the Monte Carlo calculation of the impurity problem can be performed in parallel on, typically, 8-32 processors. The communication overhead of this coarse-grain type of parallel execution is negligible, leading to optimal scaling for large problems. Parallelization on the level of each matrix/vector operation is presently not necessary, due to the moderate memory requirements. On the VPP 700, our programs execute at a speed of 1 GFlops per processor, i.e., half the theoretical peak performance.

## 3 Results and Discussion

We focus on the paramagnetic phase of the Hubbard model with a semi-elliptical non-interacting density of states (DOS). The bandwidth is chosen as  $W = 4$ . Experience shows that, for most purposes, convergence is reached if the rate of change of the self-energy in the DMFT iteration procedure becomes small, i.e., if  $\eta \equiv \langle |\Delta \Sigma(i\omega_n)| \rangle_n \leq 10^{-3}$ . Straightforward implementation of the QMC algorithm with this convergence criterion indeed leads to hysteresis in, e.g., the double occupancy  $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$  at  $T < T_{IPT}$ , showing metallic and insulating solutions for the same value of  $U$ . However, adding approximately 20 more iterations merges *both* solutions to a new stable solution. Thus we obtain a smooth curves  $D(U)$  *without* hysteresis.

We also studied the quasiparticle renormalization factor  $Z = m/m^*$  and the compressibility  $\kappa$ . We locate the Mott-Hubbard transition at the interaction strength  $U_c$  where  $Z(U)$  and  $\kappa(U)$  essentially vanish. The resulting phase diagram is plotted in Fig. 1. According to IPT, the transition which occurs below  $T = T_{IPT} \simeq 0.088$  is discontinuous. By contrast, we find a *continuous* transition down to at least  $T = 1/35 \simeq 0.325 T_{IPT}$ .

We calculated the density of states using the Maximum Entropy Method and found that the interaction  $U_c$  coincides with the collapse of the quasi-particle peak in the spectrum. An actual gap opens only at  $U_g > U_c$ . We expect the Mott-Hubbard transition to be a smooth but rapid crossover between  $U_c$  and  $U_g$ . However, a first-order transition at  $T < T_{min} \equiv 1/35$  cannot, at present, be ruled out.

We conclude that the single-band Hubbard model does not provide a quantitative description of the first-order metal-insulator transition in Cr-doped  $V_2O_3$  below  $T_c \simeq 380K$ , since (for a realistic choice of 0.8 eV for the

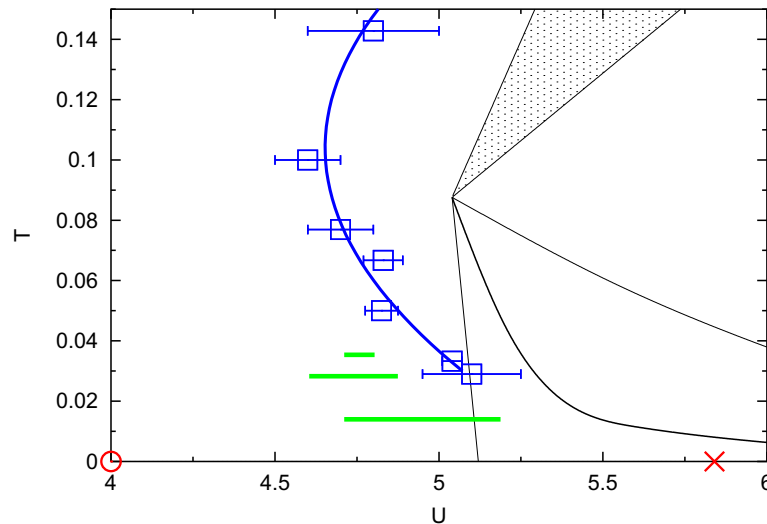


Figure 1: Phase diagram of the Hubbard model (paramagnetic phase only). Blue squares: continuous metal-insulator transition calculated with QMC. Broad green horizontal lines: coexistence region within ED [8]. Black thin lines: coexistence region within IPT; the line of first-order transitions (full curve) ends at  $T_{IPT}$  [8]. The shaded area above is a crossover region. Shown in red are the  $U_c$ -values from PSCT/NRG (X) [10] and RDA (O) [14].

bandwidth) we find a *continuous* metal-insulator transition (crossover) down to at least  $T_{\min} \simeq 70\text{K}$ . Thus, in order to quantitatively explain the experiment, other degrees of freedom must also be taken into account.

For publications [16], see: <http://www.physik.uni-augsburg.de/theo3/publications.shtml>

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