Phase Diagram of the Frustrated Hubbard Model

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The Mott-Hubbard metal-insulator transition in the paramagnetic phase of the one-band Hubbard model has long been used to describe similar features in real materials like V2O3. In this Letter we investigate the antiferromagnetic phase of this model with frustration. At \( T = 0 \) we find a first-order transition from a paramagnetic metal to an antiferromagnetic insulator. We show that even in the presence of strong magnetic frustration, the paramagnetic metal-insulator transition is hidden inside an extended antiferromagnetic region. This raises the question of whether the one-band Hubbard model with frustration is sufficient to describe the phase diagram of V2O3 or similar transition metal oxides even qualitatively.

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The microscopic description of magnetism and metal-insulator transitions constitutes one of the major research activities in modern solid state theory. Especially transition metal compounds like V2O3, LaTiO3, NiS2−xSex, and the cuprates show metal-insulator transitions and magnetic order depending on composition, pressure, or other control parameters [1]. The paramagnetic insulating phase observed in these materials is believed to be a so-called Mott-Hubbard insulator due to electron-electron correlations, in contrast to Slater or band insulators like SrTiO3.

The simplest model showing both magnetism and a correlation-induced metal-insulator transition (MIT) is the one-band Hubbard model [2]

\[
H = - \sum_{i,j,\sigma} t_{ij} c_{i \sigma}^\dagger c_{j \sigma} + \frac{U}{2} \sum_{i \sigma} n_{i \sigma} n_{i \sigma}.
\]

(1)

Considerable progress in understanding the physics of this model has been achieved through the development of the dynamical mean-field theory (DMFT) [3–5]. In particular, the DMFT phase diagram for the unfrustrated Hubbard model is very well understood [4,5]. At half-filling the physics is dominated by an antiferromagnetic insulating (AFI) phase for all \( U > 0 \) with a maximum \( T_N \approx 0.15W \) around \( U \approx W \), where \( W \) is the bandwidth of the noninteracting system. For finite doping, the antiferromagnetic phase persists up to a critical doping \( \delta_c \) [6] and in addition shows phase separation [7,8]. For very large values of \( U \) the antiferromagnetic phase is replaced by a small region of Nagaoka type ferromagnetism [9–11].

Artificially ignoring the antiferromagnetic phase, a transition from a paramagnetic metal (PM) to a paramagnetic insulator (PI) becomes visible at half-filling. At \( T = 0 \) it occurs at a value of the Coulomb parameter \( U_c \approx 1.5W \) [5,6,12]. Interestingly, the transition is of first order [5,13] for \( T > 0 \) with a second order end point at \( T_c = 0.017W \) and \( U_c = 1.2W \). Note that \( T_c \ll T_N^{\text{max}} \). Since the phase diagram of V2O3 [14] looks very similar, the DMFT results for the Hubbard model have been used as a qualitative explanation [5,15].

For a proper description of this material, however, the antiferromagnetic phase below \( T_N \approx 160 \text{ K} \) [14] has to be taken into account. While for perovskites like LaTiO3 or the cuprates the cubic lattice is compatible with the bipartite Néel state, the vanadium atoms in V2O3 form a hexagonal lattice. However, the observed magnetic structure led to the suggestion of V-V dimers on a bipartite lattice hosting one electron in the antibonding molecular orbitals [16]. Furthermore, the inevitable presence of longer-ranged hopping results in a partial magnetic frustration. It was argued and generally accepted [5,15] that such partial magnetic frustration leads to the anticipated situation, where the MIT extends beyond the antiferromagnetic phase at low temperatures.

The merging of these two transitions presents an interesting problem on its own, because it is commonly believed that the magnetic transition should be of second order. Furthermore, previous results for a system with magnetic frustration show an extended antiferromagnetic metallic (AFM) phase at \( T = 0 \), preceding the transition to the AFI [5,17]. This observation suggests an appealing possibility to link the MIT in the paramagnetic phase with a transition from an AFM to an AFI.

In this Letter, we present results from a calculation using Wilson’s numerical renormalization group (NRG) approach [18] and exact diagonalization (ED) techniques [5] to solve the DMFT equations [5,19] for the one-band Hubbard model with magnetic frustration at half-filling. Frustration is introduced via suitable long-ranged hopping in the Hubbard model (1). To be precise, we use a dispersion [20]
\[\varepsilon_k = -t_1 \sum_{i=1}^{D} \cos k_i a - t_2 \sum_{i=1}^{D} \cos 2k_i a, \]  

(2)

introducing magnetic frustration while at the same time avoiding computational problems connected to a conventional next-nearest neighbor hopping. Moreover, this dispersion, adapted to the Bethe lattice [5], was also studied in previous work [5,15,17], allowing us a direct comparison with the results reported there. We show that frustration of the magnetic interactions does not lead to the previously reported sequence PM \(\leftrightarrow\) AFM \(\leftrightarrow\) AFI with an extended region of an AFM at \(T = 0\) [5,17]. Instead, we observe a first-order transition PM \(\leftrightarrow\) AFI (see also [21]). Furthermore, the reduction of \(T_N\) is too small to result in the qualitative phase diagram of \(V_2O_3\).

The investigation of magnetic properties in the DMFT is straightforward [5]. In the case of the Néel state as a natural first choice, the system is divided into \(A\) and \(B\) sublattices, which results in a matrix structure of the DMFT equations [5]. An antiferromagnetic Néel order then corresponds to a finite staggered magnetization \(m_S > 0\) with \(m_A = m_S\) and \(m_B = -m_S\).

While in the DMFT for the paramagnetic state, the lattice structure enters only via the free density of states (DOS) [5], the matrix structure in the Néel state can lead to the challenging problem of a numerical \(k\) summation. The attempt to use the limit of an infinite coordination number as a means to evaluate the \(k\) sums introduces artificial band tails that can mask interesting physical effects like a MIT in the magnetically ordered phase [22].

Such computational problems can be avoided by adapting the dispersion (2) to the Bethe lattice, resulting in the DMFT equations [5,17]

\[G_{A\sigma}(z) = \frac{1}{z + \mu - \Sigma_{A\sigma}(z) - \frac{\Delta}{4} G_{B\sigma}(z) - \frac{\Delta}{4} G_{A\sigma}(z)},\]

\[G_{B\sigma}(z) = \frac{1}{z + \mu - \Sigma_{B\sigma}(z) - \frac{\Delta}{4} G_{A\sigma}(z) - \frac{\Delta}{4} G_{B\sigma}(z)},\]

(3)

which contain magnetic frustration and lead to a DOS with compact support.

In the paramagnetic case, Eqs. (3) reduce to those of a standard Bethe lattice, which, for example, result in the well-studied Mott transition. Furthermore, despite the frustration introduced, the system is still particle-hole symmetric. Especially for half-filling, this feature reduces the numerical effort quite drastically.

In the presence of magnetic frustration, the Néel state is not the only possible magnetic order. We nevertheless believe that our results capture the essential changes in the physics introduced to the Hubbard model by magnetic frustration on the level of the DMFT. Note that in \(D \leq 2\) the true lattice structure and nonlocal fluctuations invalidate the DMFT results.

Invoking the symmetry \(G_{A\sigma}(z) = G_{B\sigma}(z)\) valid for the Néel state, Eqs. (3) reduce to two coupled nonlinear equations that we solve iteratively. In the course of the iterations, the quantity \(\Sigma_{\sigma}(z)\) has to be calculated from the solution of a generalized single impurity Anderson model [5]. For that task we employ the NRG [8,18,23].

Let us first discuss the results for the magnetization as a function of \(U\) for \(T = 0\). In the following, we fix \(t_2/t_1 = 1/\sqrt{3} \approx 0.58\) [24] and use the bandwidth \(W = 2(t_1^2 + t_2^2)^{1/2}\) of the noninteracting system as our energy scale. The NRG results in Fig. 1 (circles) show a completely different behavior as compared to the ED data (diamonds) from Ref. [17]. Instead of a continuous increase of the staggered magnetization \(m_S\) for \(U > U_c = 0.4W\) as suggested by both a Hartree calculation (crosses) and the data from Ref. [17], we find a jump in \(m_S\) at a considerably larger \(U_c = 0.9W\). To clarify this discrepancy, we performed ED calculations, resulting in the triangles shown in Fig. 1. We find good agreement with our NRG results, the transition systematically approaching the NRG curve with increasing system size in the ED.

The explanation for why the same method leads to qualitatively different results lies in a rather strong dependence on details of the numerical procedure, e.g., the largest frequency \(\omega_{\text{max}}\) in the calculation of \(G(i\omega)\) or the choice of initial values for the generation of the parameters of the effective Anderson impurity model [5]. The triangles shown in Fig. 1 were obtained using \(\omega_{\text{max}} = 40\pi\) and fixed initial values in each DMFT step. Initializing the ED with results from the previous DMFT iteration leads to a solution similar to Ref. [17], which, however, has a higher total energy. Thus, choosing the numerical procedure in the ED such that it gives the lowest possible total energy leads to results consistent with the NRG. The NRG, on the other hand, is stable with respect to changes in the parameters controlling its numerical accuracy.

Another important question is the existence of an antiferromagnetic metallic solution of the DMFT equations. Figure 2 shows the NRG results for the DOS for

![Graph showing staggered magnetization](image-url)
$T = 0$ and spin-up on an $A$ lattice site. Because of particle-hole symmetry the DOS for spin-down on $A$ sites (or spin-up on $B$ sites) can be obtained by $\omega \rightarrow -\omega$. The full and dashed lines represent the AFI solution for $U \leq U_c$ and the PM solution for $U > U_c$, respectively. Clearly, the magnetic solution is insulating with a well-developed gap at the Fermi energy. Quite generally, we were not able to find a stable AFM solution at $T = 0$.

The discontinuity in the staggered magnetization $m_s$ at the transition PM $\rightarrow$ AFI implies a first-order transition and the existence of a hysteresis region.

Indeed, starting from the paramagnet at $U \ll U_c$ and increasing $U$ results in a magnetization curve different from the one obtained by starting at $U \gg U_c$ and decreasing $U$. This is apparent from Fig. 3 (main panel, full lines) where a region of hysteresis can be observed in the staggered magnetization for temperature $T = 0.0155W$. At the same time the total DOS at the Fermi energy $A(t) = A_t(t) + A_i(t)$ shows hysteresis between metallic and insulating behavior in exactly the same $U$ region. Note that because of the finite temperature the DOS at the Fermi level is not exactly zero in the Neél state, but strongly reduced as compared to the metal [13].

It is, of course, important to verify that the hysteresis found for small $U$ is not some kind of artifact. This can most conveniently be shown by looking at the transition at large $U$. Because of the mapping of the Hubbard model to a Heisenberg model in this regime, one should expect the transition to be of second order, with the staggered magnetization vanishing continuously like $m_s \propto \sqrt{T_N - T}$ when approaching $T_N$ from below. That this is indeed the case is apparent from the inset of Fig. 3, where we show the squared staggered magnetization as a function of $T$ for $U/W = 2$. The transition is thus of second order with the expected mean-field exponent in this region of the phase diagram.

Collecting the results for the transitions and the hysteresis region for different temperatures leads to the phase diagram in Fig. 4.

An enlarged view of the region showing the coexistence of PM and AFI is given in the inset, where the full line represents the transition PM $\rightarrow$ AFI with increasing

$U$ and the dashed line the transition AFI $\rightarrow$ PM with decreasing $U$. These two lines seem to merge at a value of $U = W$ for this particular value of $t_2$, with a critical temperature for this end point $T_c = 0.02W$. Note that, even in the presence of such a sizable $t_2$, the antiferromagnetic phase still completely encompasses the paramagnetic MIT (dotted lines in the main panel of Fig. 4 [13]).

It is, of course, interesting to see how the magnetic phase evolves with increasing $t_2$ and, in particular, how its boundary crosses the paramagnetic MIT. We find that increasing $t_2$ does not change the form of the magnetic phase in Fig. 4 qualitatively, but mainly shifts the lower critical $U$ and decreases the maximum $T_N$. The calculated estimates for those two quantities as a function of $t_2$ lead
to the schematic evolution of the phase diagram presented in Figs. 5(a)–5(c). Here, only the true phase boundaries are shown. A direct calculation of the free energy at finite temperatures is presently not possible with the NRG method, so we cannot calculate the actual transition line separating the paramagnetic and AF phases. The transition lines in Figs. 5(a)–5(c) are therefore a guide to the eye only. For the Mott transition, the position of the actual transition line has been calculated in Ref. [25].

Figure 5(a) shows the qualitative phase diagram corresponding to Fig. 4 with the line of first-order transitions ending in a critical point. Upon further increasing the value of $t_2$, the first-order transition lines from both the PM $\rightarrow$ AFI and the Mott transition cross [Fig. 5(b)], thus exposing a finite region of the Mott insulator and a transition PI $\rightarrow$ AFI. Finally, for even higher values of $t_2$, the PM $\rightarrow$ AFI transition at $T = 0$ approaches the Mott transition and $T_N$ is reduced significantly [Fig. 5(c)]. Note that in the limiting case $t_2 = t_1$ the AFI phase completely vanishes due to the structure of the DMFT Eqs. (3). However, for $t_2 \rightarrow t_1$ there is always a finite antiferromagnetic exchange $J \propto (t_1^2 - t_2^2)/U$, which is sufficient to stabilize an antiferromagnetic ground state for $U > U_c$ of the Mott transition.

From these results we conclude that a one-band Hubbard model with frustration alone is not sufficient to even qualitatively reproduce the phase diagram of materials like $V_2O_3$. In particular, the Mott transition extends beyond the AFI region only for unphysically large values of $t_2$.

The question remains whether it is possible at all to reproduce qualitatively the scenario observed in $V_2O_3$ within some kind of one-band model. Based on our results reported here, we believe that one has to take into account additional degrees of freedom, for example, phonons (within a Holstein-Hubbard model) or orbital degeneracies (within a multiband Hubbard model).

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24. This value is the same as the one used in [5,17].