Dynamical Mean Field Theory of the Antiferromagnetic Metal to Antiferromagnetic Insulator Transition

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We study the zero temperature antiferromagnetic metal to antiferromagnetic insulator transition using dynamical mean field theory and exact diagonalization methods. We find two qualitatively different behaviors depending on the degree of magnetic correlations. For strong correlations combined with magnetic frustration, the transition can be described in terms of a renormalized Slater theory, with a continuous gap closure driven by the magnetism but strongly renormalized by correlations. For weak magnetic correlations, the transition is weakly first order.

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The correlation driven metal insulator transition (MIT) or Mott transition is one of the central problems of condensed matter physics. Recently, a great deal of progress has been made in understanding the MIT using the dynamical mean field approach (DMFT), a method which becomes exact in the well-defined limit of infinite lattice coordination [1,2]. However, all studies so far have been confined to the paramagnetic metal (PM) to paramagnetic insulator (PI) transition. In this Letter, we use DMFT to study the transition from the antiferromagnetic metal (AM) to an antiferromagnetic insulator (AI) at zero temperature. The motivation for this work is twofold. Experimentally, the interaction or pressure driven MIT in V_2O_3 [3,4] and $NiS_{2-x}Se_x$ [4,5] takes place between *magnetically ordered* states. The Néel temperatures are much smaller than the respective characteristic electronic energy scales. We interpret this as a sign of reduced effective magnetic correlations as compared to estimates obtained from a simple one band Hubbard model. Close to the MIT, the behavior of physical quantities like the specific heat coefficient is, however, different in these two materials. Furthermore, measurements of the magnetic moment seem to indicate that the magnetism in V_2O_3 is much weaker than in $NiS_{2-x}Se_x$ [6]. This suggests that the strength of the magnetic correlations influences the MIT. We would therefore like to understand how magnetic correlations, which control the scale at which the spin entropy is quenched, affect the MIT and hence, various physical quantities. While we are still far from a realistic modeling of these materials (in this work we consider only commensurate magnetic order and ignore orbital degeneracy and realistic band structure), we present a simple model which, we believe, captures the generic effects of the magnetic correlations on the MIT.

We consider a simple one band Hamiltonian,

$$H = t_1 \sum_{nn\sigma} c^\dagger_{i\sigma} c_{ij\sigma} + t_2 \sum_{nnn} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - J \sum_{nn} \mathbf{S}_i . \mathbf{S}_j ; \tag{1}$$

t_1 and t_2 are nearest and next nearest neighbor hoppings, respectively, and U is the onsite Coulomb repulsion. The hoppings are parametrized as $t_1^2 = (1 - \alpha)t^2$ and $t_2^2 = \alpha t^2$, where α is the degree of frustration. A nonzero t_2 is required to obtain an AM-AI transition, because the perfect nesting present in bipartite hypercubic lattices when $t_2 = 0$, always leads to a PM-AI transition [7,8]. J is a ferromagnetic spin coupling that [9] tunes the strength of the magnetic exchange between neighboring spins. J is independent of U and t_2/t_1 and simulates reduced magnetic correlations which could stem from different physical processes like orbital degeneracy in V_2O_3 [10] or lattice structure and competing four spin interactions in $NiS_{2-x}Se_x$.

Within DMFT, in the presence of magnetic order, the single particle Green's functions on the A and B Neel sublattices have the following form:

$$G_\sigma^{-1} = \begin{bmatrix} i\omega_n + \mu_\sigma - \epsilon_2(\mathbf{k}) - \Sigma_{A\sigma} & -\epsilon_1(\mathbf{k}) \\ -\epsilon_1(\mathbf{k}) & i\omega_n + \mu_{-\sigma} - \epsilon_2(\mathbf{k}) - \Sigma_{B\sigma} \end{bmatrix}; \tag{2}$$

$\epsilon_{1,2}(\mathbf{k})$ are the dispersions corresponding to t_1 and t_2. $\sigma = 1, 2$ refer to the spin up and down states, m the staggered magnetization, and $\mu_\sigma = [\mu - \frac{U}{2} + (-1)^\sigma Jm]$ is the shifted chemical potential. Σ are the self-energies which are momentum independent within this approximation. The local Green's functions $G_{ii\sigma}$ depend on the sublattices (A and B) and obey $G_{A1} = G_{B2} \equiv G_1(i\omega_n)$, $G_{A2} = G_{B1} \equiv G_2(i\omega_n)$. Similarly, $\Sigma_{A1} = \Sigma_{B2} \equiv \Sigma_1(i\omega_n)$ and $\Sigma_{A2} = \Sigma_{B1} \equiv \Sigma_2(i\omega_n)$. The Σ and G are obtained from an Anderson impurity model

$$H_{\text{imp}} = \sum_{l\sigma} \epsilon_{l\sigma} d^\dagger_{l\sigma} d_{l\sigma} + \sum_{l\sigma} V_{l\sigma} (d^\dagger_{l\sigma} f_\sigma + \text{H.c.}) - \mu_\sigma \sum_\sigma f^\dagger_\sigma f_\sigma + U n_{f\uparrow} n_{f\downarrow} \tag{3}$$

describing an f electron hybridizing with a bath of conduction electrons d, via the spin-dependent hybridization

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functions

$$\Delta_\sigma(i\omega_n) = \sum_l \frac{V_{l\sigma}^2}{i\omega_n - \epsilon_{l\sigma}}, \tag{4}$$

where ω_n are the Matsubara frequencies. The Δ_σ obey self-consistency conditions that can be expressed in terms of the noninteracting density of states [2], G_1 and G_2 (which are also the impurity Green's functions). Here, we restrict ourselves to the Bethe lattice with a noninteracting density of states, $D(\epsilon) = \frac{2}{\pi D^2}\sqrt{D^2 - \epsilon^2}$ where $D = \sqrt{2}\,t$ is the half bandwidth. The self-consistency conditions take the following simple form

$$\Delta_\sigma(i\omega_n) = \frac{t_1^2}{2} G_{-\sigma}(i\omega_n) + \frac{t_2^2}{2} G_\sigma(i\omega_n). \tag{5}$$

Note that (5) is independent of the sign of t_2. We consider only the half-filled case, which due to a special particle hole symmetry of the impurity problem: $d_{l\sigma}^\dagger \to d_{l-\sigma}$, $d_{l\sigma} \to d_{l-\sigma}^\dagger$, $f_\sigma \to f_{-\sigma}^\dagger$, $f_{l\sigma}^\dagger \to f_{-\sigma}$, and with $(\epsilon, V)_{l\sigma} \to -(\epsilon, V)_{l-\sigma}$ requires that $\mu = U/2$.

To obtain G_1 and G_2, we use the algorithm of Ref. [11] which uses the zero temperature Lanczos method to compute the Green's functions of the impurity model given by (4) and iterate the model until the self-consistency given by (5) is achieved. Though the results to be presented were obtained for the case where the bath was represented by $N = 5$ sites, several of them were checked for $N = 7$ to establish the results seen for $N = 5$. The typical number of iterations for robust convergence varied between 50–65. Below, we discuss the substantially different behaviors seen in the cases of strong and weak magnetic correlations (induced by J).

Strong magnetic correlations: $J = 0$.—This is the case where the system has substantial antiferromagnetic correlations despite being magnetically frustrated. This frustration arises from the next nearest neighbor antiferromagnetic exchanges generated by t_2. For small U, the system is in the paramagnetic phase. As U increases beyond a critical U_{cm}, antiferromagnetic moments develop and the spin up and down spectral functions $\rho_\sigma(\omega) = (-1/\pi)\,\mathrm{Im}G_\sigma(\omega)$ are no longer equal. ρ_1 has more spectral weight in the upper Hubbard band than in the lower Hubbard band and vice versa for ρ_2. The low frequency Kondo-like resonance in $\rho_\sigma(\omega)$ is no longer centered around $\omega = 0$ but is split into two peaks centered around some $\pm\omega_0$ with a minimum at $\omega = 0$. This can be attributed to the fact that the effective staggered magnetic field generated when antiferromagnetism develops, splits the quasiparticle bands. Moreover, unlike in the paramagnetic case, the height of the resonance is not pinned at the value of the noninteracting density of states but decreases with increasing U. As U approaches a critical U_{MIT}, the density of states $\rho_\sigma(\omega = 0) \to 0$. For $U \geq U_{\mathrm{MIT}}$, a gap opens continuously and the system becomes insulating.

A plot of the staggered magnetization m versus U is shown in Fig. 1. U is in units of t in all the figures. m increases monotonically with U. It seems to increase as

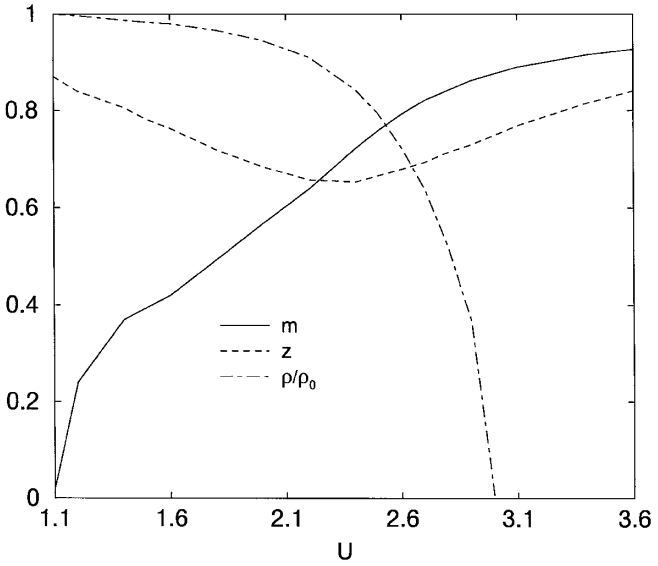

FIG. 1. The magnetization m, z and the normalized density of states at the Fermi level $\rho(0)/\rho_0(0)$ versus U for $t_2/t_1 = 0.57$ ($\alpha = 0.25$) with $U_{\mathrm{MIT}} = 3.0t$.

$(U - U_{cm})^{1/2}$ close to U_{cm} and does not exhibit any special feature at the MIT. Note that though m is quite large at the MIT and increases with increasing t_2/t_1, it saturates only when one is well into the insulating phase. Unlike the paramagnetic case where $\mathrm{Im}\Sigma$ diverges as $(i\omega_n)^{-1}$ at the MIT, in the presence of antiferromagnetism, the self-energy does not show any anomalous behavior across the MIT. To obtain an insight into the nature of the MIT, we use the following low energy parametrization of Σ_σ

$$\Sigma_{1,2}(i\omega_n) = \pm h + \left(1 - \frac{1}{z}\right) i\omega_n, \tag{6}$$

where h is the staggered field generated by the interactions. In the magnetic case, the factor z (which is the quasiparticle residue in the paramagnetic case and goes to zero at the PM-PI transition), is nonmonotonic and remains nonzero even in the insulating phase (cf. Fig. 1). In terms of the local Green's functions, Σ_σ is determined by the following expression on the Bethe lattice

$$G_\sigma^{-1} + \Sigma_\sigma = i\omega_n + \mu_\sigma - \frac{t_1^2}{2} G_{-\sigma} - \frac{t_2^2}{2} G_\sigma. \tag{7}$$

Using (6) in (7) and continuing to real frequencies, we obtain the low frequency spectral functions

$$\rho_{1,2}(\omega) = \rho(0)\left[1 \pm \frac{\omega}{hz}\right], \tag{8}$$

where $\rho(0)$ is the density of states at the Fermi level and is given by

$$\rho(\omega = 0) = \frac{2}{\pi D^2}\sqrt{D^2 - \left(\frac{h}{\alpha}\right)^2}. \tag{9}$$

Note that $\rho(0)$ does not depend on z. Since h increases monotonically with U, $\rho(0)$ decreases with increasing U in the magnetically ordered phase. This yields a critical

value $h_c = \alpha D$ where $\rho(0) \to 0$ and a gap opens continuously. This is the point at which the MIT occurs. We, therefore, see that the MIT is of a very different nature and there are no Kondo resonances which disappear discontinuously at the MIT. Our results indicate that in the vicinity of U_{MIT}, h increases linearly with U, implying that $\rho(0)$ vanishes as $(U_{\mathrm{MIT}} - U)^{1/2}$ as we approach the transition from the metallic side.

Using Eqs. (6), (8), and (9), the linear coefficient of the specific heat γ is found to be

$$\frac{\gamma}{\gamma_0} = \frac{2}{z}\sqrt{1 - \frac{h^2}{D^2\alpha^2}}, \tag{10}$$

where $\gamma_0 = \frac{\pi k_B^2}{3D}$ with $2\gamma_0$ being the specific heat coefficient of the noninteracting problem. We see that the basic physics controlling the behavior of the specific heat in the antiferromagnetic phase is the competition between the increase of $m^* \propto [1 - \frac{\partial\Sigma(i\omega_n)}{\partial i\omega_n}] = z^{-1}$ (m^* is the effective mass in the paramagnetic case) and the decrease of the density of states $\rho(0)$. Though m^* initially increases, its increase is cut off by the staggered magnetization (cf. Fig. 1). When the staggered magnetization m is large the decrease in $\rho(0)$ is the dominant effect, whereas the first effect dominates when the magnetism is weak. The latter is true in the case of the paramagnetic MIT, where m^* and γ are both $\propto z^{-1}$ and diverge as $z \to 0$ at the transition. This divergence is related to the fact that there is a residual entropy in the insulating phase resulting from the spin degeneracy at every site. However, this degeneracy is lost in the case where the insulator is also an antiferromagnet. Consequently, z remains nonzero and $\gamma \to 0$ as $(U_{\mathrm{MIT}} - U)^{1/2}$ at the MIT. As anticipated, we see in Fig. 2 that γ increases with U for small m and decreases for larger moments.

We can generalize the above argument to a lattice with a realistic dispersion $E_{\mathbf{k}} = \epsilon_1(\mathbf{k}) + \epsilon_2(\mathbf{k})$. The Fermi surface of the noninteracting system is defined by $E_{\mathbf{k}_F} = 0$. When U is turned on, the dispersions of the quasiparticles change and are given by the poles of the Green's function given by (2). From the preceding analysis, we can say that the main effect of interactions is to modify the band dispersion in the following manner: $E_{\mathbf{k}} = z[\epsilon_2(\mathbf{k}) \pm \sqrt{\epsilon_1(\mathbf{k})^2 + h^2}]$. In the noninteracting case ($h = 0$ and $z = 1$), the two bands overlap and there is no gap at the Fermi surface. For small U, in the paramagnetic phase, there is no gap in spectrum but the bands are slightly renormalized by the factor z. When antiferromagnetism sets in, the nonzero h changes the band curvature and the renormalized bands start moving away from each other, reducing the Fermi surface area. This reduction in the area is given by $\rho(0)/\rho_0(0)$ (Fig. 1). For small h, there are regions where the bands overlap and there is no gap in the system. At a critical value $h = h_c$, a gap opens up in the spectrum as the Fermi surface shrinks to zero, signaling the MIT.

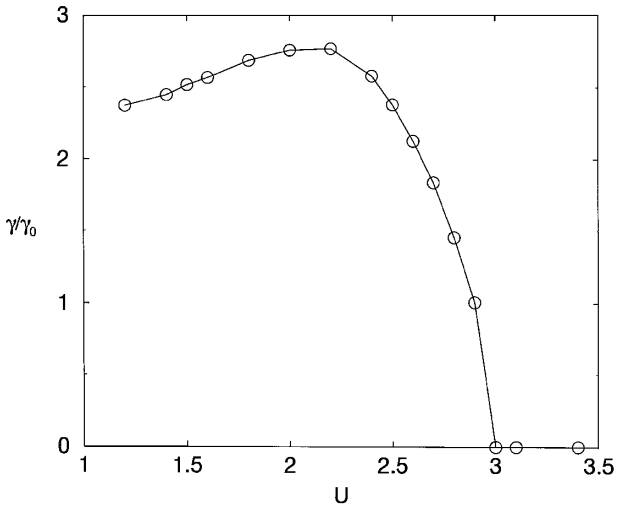

FIG. 2. The linear coefficient of the specific heat γ plotted in units of γ_0 (defined in the text) vs U for $t_2/t_1 = 0.57$ ($\alpha = 0.25$, $U_{\mathrm{MIT}} = 3.0t$).

Weak magnetic correlations: $J \neq 0$.—The previous scenario was characterized by relatively weak electron correlations, in the sense that the quasiparticle residue z near the transition was at most 0.65, indicating that a relatively high fraction of the spectral weights remain coherent. This can be understood in simple qualitative terms. When the magnetic correlations are strong, the relatively large antiferromagnetic exchange produces a large magnetization, which in turn reduces the double occupancy. All the spin entropy is quenched by the spin ordering, and the presence of a hopping in the same sublattice favors coherent quasiparticle propagation. To access the strongly correlated regime, where z is small and most of the spectral function is incoherent, we turn on a nonzero J. Its effect is only through the μ_σ term in (7) and is equivalent to a shift $h \to h - Jm$, which reduces m and hence increases U_{MIT} as suggested by (9).

We studied the case $t_1^2 = 0.95t^2$ and $t_2^2 = 0.05t^2$ ($t_2/t_1 = 0.22$). For $J = 0$, this system shows the usual band MIT discussed in the previous section, in the vicinity of $U = 2t$. By choosing a $J(U)$, cf. inset of Fig. 4, such that the magnetic moment remains very small for a large regime of U as shown in Fig. 3, we move the MIT to $U = 3.8t$. In the antiferromagnetic metallic phase, the Kondo-like resonance discussed earlier, persists in the spectral function up to $U = 3.8t$ and disappears suddenly at the transition. We also find that the slope, z, decreases to values much smaller than was seen in the band transition picture as shown in Fig. 3. z decreases until the moment becomes sufficiently large and stops its reduction. In the insulator, which still resembles the band insulator, the self-energy is analytic and one can define a z.

We find that z and m jump at the transition. This jump in conjunction with the discontinuous disappearance of the resonance mentioned earlier, is reminiscent of a first order transition. On retracing the insulating solution as a function of decreasing U, we find that there is coexistence. The insulator survives down to $U = 3.4t$ and there is a

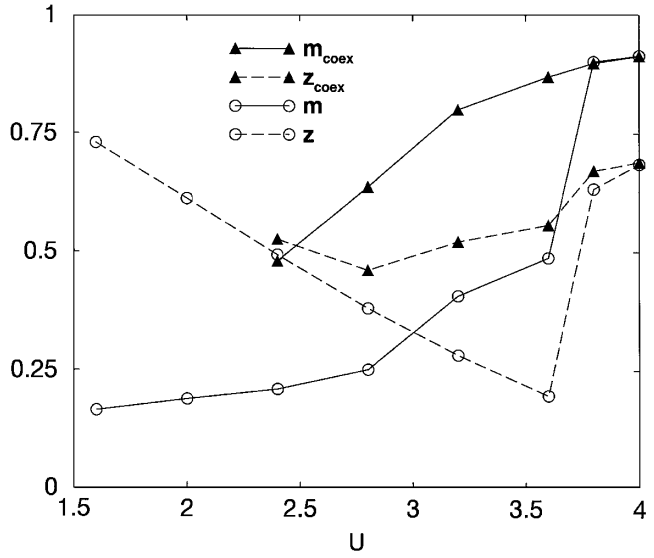

FIG. 3. m (bold line) and z (dashed line) vs U for the case of small frustration $t_2/t_1 = 0.2$ ($\alpha = 0.05$) with J varying as a function of U. $U_{\mathrm{MIT}} = 3.8t$ in this case. The subscript coex denotes the coexistent solution.

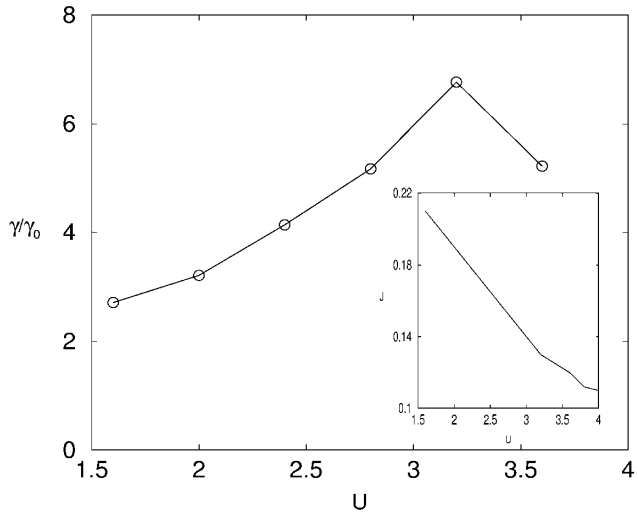

FIG. 4. γ vs U for the case of small frustration $t_2/t_1 = 0.2$ with J varying as a function of U ($U_{\mathrm{MIT}} = 3.8t$). The inset shows J vs U.

MIT of the pure band kind at that point and the solution goes over to one which is a metallic antiferromagnet but with a much higher value of the moment m and a much larger z. This metallic solution disappears around $U = 2.4t$, i.e., it becomes unstable to ferromagnetism. We find that the features discussed above persist for constant J if it is comparable to the antiferromagnetic exchange in the vicinity of the MIT. In addition, J should be chosen such that m is small in the metal and that it does not make the system unstable to ferromagnetism. We have calculated the double occupancies in both these solutions and find that the metal with the smaller moment has higher double occupancy. In this weak magnetic correlation regime, we find that the specific heat coefficient γ is strongly enhanced; cf. Fig. 4. This scenario is reminiscent of the behavior seen in V_2O_3 [3]. Note that at the MIT, there is a finite gap which is much smaller than the Hubbard gap. Also, coherent quasiparticle peaks survive albeit with very small weight. These coherent peaks are asymmetric about $\omega = 0$ in both G_1 and G_2. Close to $U = 4.1t$ these peaks vanish completely and one is left only with the incoherent Hubbard band structures. In the coexistent solution, as U is reduced, the gap closes continuously and the weight of these two coherent peaks increases continuously.

To summarize, the character of the AM-AI transition is very different from the PM-PI. We find that the strength of the magnetic correlations controls the nature of the MIT. In the limit of strong magnetic correlations, the transition takes place as a renormalized Slater transition, i.e., up to a multiplicative factor which remains finite at the transition, a gap opens continuously and $\gamma \to 0$ continuously, as the MIT is approached from the metallic side.

This is similar to the observations reported in $NiS_{2-x}Se_x$ [5,12] where the moment close to the MIT on the metallic side is sufficiently large so as to make the transition smooth. On the other hand, when antiferromagnetism in the metallic phase is suppressed, a new scenario emerges: the gap from the insulating side remains finite at the MIT, and a substantial enhancement of the specific heat is observed when the MIT is approached from the metallic side. Our results indicate that the transition is weakly first order. This scenario is reminiscent of $V_{2-y}O_3$ [3] where the moment is very small and γ is large and nonzero at the transition. Our results are consistent with our interpretation that the magnetism in V_2O_3 is weaker than in $NiS_{2-x}Se_x$. The simple model presented here captures some of the most important features of the transitions seen in many compounds and could be developed further to interpret other experimental observations [4].

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