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Metal-insulator transition by suppression of spin fluctuations

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Abstract - We have studied the metal-insulator transition in the antiferromagnetic (AF) two-plane Hubbard model in infinite dimensions as a function of the perpendicular hopping \(t_\perp\) between the two planes. In the weak-coupling regime the system undergoes a transition from a metallic to a band insulating state. For strong coupling, a transition from an AF insulating state to a singlet state occurs at \(t_\perp/t \approx \sqrt{2}\), which is consistent with a competition between intra- and inter-plane Heisenberg exchange. We calculate the spin-correlation functions of the model and show that the picture of a transition to a singlet insulating state remains valid for intermediate coupling, independent of the presence of long-range AF order. The quasiparticle peak continuously disappears due to the suppression of the local spin fluctuations by formation of the coherent singlet state. The transition is accompanied by the opening of a spin gap in the dynamical susceptibility.

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Metal-insulator transitions (MITs) are widely observed in condensed-matter systems. Metal-to-band-insulator transitions take place in weakly or uncorrelated systems and can successfully be described by an independent electron theory, such as density functional theory. An inherently different scenario emerges when electron-electron interactions become important: in such a situation the system can undergo a Mott MIT [1] due to strong electronic correlations. This has been observed in many \(d\) electron systems such as transition-metal oxides. The Mott MIT has been investigated on the two-dimensional (2D) Kagomé lattice [2] within the cluster dynamical mean-field theory (CDMFT). It was found to exhibit some unconventional properties which were attributed to the presence of geometric frustrations.

A different type of frustrated lattice is the 3D pyrochlore lattice which is a network of corner-sharing tetrahedra and is realized as a magnetic cation sublattice in several compounds such as Sm\(_2\)Se\(_4\), YMn\(_2\) [3], and LiV\(_2\)O\(_4\) [4]. While pyrochlore lattices are often discussed in the context of geometric frustrations which determine some of their essential features (see, e.g., refs. [3,4] and references therein), they have been found to exhibit a different kind of MIT: examples are the metal-to-singlet-insulator transitions found in the ruthenium oxide Hg\(_2\)Ru\(_2\)O\(_7\) [5] and in the transition metal spinel MgTi\(_2\)O\(_4\) [6]. Singlet insulator ground states are also found in quasi 1D systems such as TiOCl [7] and CuGeO\(_3\) [8] due to dimerization via a spin-Peierls mechanism. They are further characterized by the presence of a spin-gap. The formation of dynamical singlets on pairs of vanadium atoms has been proposed as the mechanism for the MIT in VO\(_2\) [9].

It is known that in the Fermi liquid state close to the Mott transition, the spectral function exhibits a characteristic three-peak structure: Two broad incoherent peaks, the Hubbard bands, are present at high energies. They coexist with the coherent quasi-particle peak at the Fermi level [10]. The latter is considered as the Abrikosov-Suhl, or Kondo resonance [11] which is a consequence of local quantum spin fluctuations. It is known that in order to have the Kondo effect, the spins need to be quantum, i.e., it cannot be obtained either in the limit of zero or infinite (classical) spins; for the latter case the double-peak structure without the Kondo resonance was demonstrated near the MIT point [12]. In fact, within a path integral approach the Kondo effect was explained as a consequence of quantum tunneling between degenerate wells of a double-well potential [13], which explicitly stresses the quantum nature of the phenomenon.

It is expected that dimerization, i.e., the singlet formation between neighboring sites leads to a quenching of the Kondo effect, since it inhibits the local singlet formation...
Fig. 1: (Color online) The two-plane Hubbard model on the Bethe lattice visualized for coordination number $z = 3$. It can be viewed as a lattice of dimers, or equivalently as two planes with opposing sites coupled by a perpendicular hopping $t_\perp$.

between the local moment and the conduction electron spins. Since the Kondo effect provides quasiparticle weight within the Mott pseudogap, tuning the dimerization is a possible mechanism for driving the MIT.

Starting from earlier works on the stacked Hubbard model, which addressed the competition between the RKKY interaction and Kondo physics [14], more recently the Mott-to-band-insulator transition was studied in the 2D bilayer Hubbard model [15]. Further studies focused on the ground-state phase diagram [16], the role of frustration and dimensionality [17] and the magnetic and transport properties for the doped case [18].

In this letter, we study the MIT in the $D = x$ two-plane Hubbard model at half filling. Theoretically this model is particularly appealing, since it can be solved exactly within the DMFT. The associated local Anderson impurity problem is solved using a numerically exact continuous-time quantum Monte Carlo algorithm. Hence the finite temperature results presented here are essentially exact. We will focus on the MIT in the absence of frustration, driven by tuning the coupling between dimer sites. This mechanism is rather different from the interaction-driven MIT. While increasing the perpendicular hopping in the weak-coupling regime leads to a band insulating state by separation of the bonding and antibonding bands, the transition in the correlated regime is characterized by the formation of singlets between neighboring sites, resulting in the suppression of the spectral weight at the Fermi level.

An illustration of the model is shown in fig. 1. Sites within a plane are connected by the hopping $t$ and each site is coupled to the opposing site on the other plane by a perpendicular hopping $t_{\perp}$. The model is described by the Hamiltonian

$$H = -t \sum_{\langle \langle ij \rangle \rangle} (a_{i\sigma}^\dagger a_{j\sigma} + b_{i\sigma}^\dagger b_{j\sigma}) - t_{\perp} \sum_{\sigma} (a_{i\sigma}^\dagger b_{i\sigma} + b_{i\sigma}^\dagger a_{i\sigma}) + U \sum_{\sigma} (n_{a\uparrow} n_{a\downarrow} + n_{b\uparrow} n_{b\downarrow}),$$

where the operators $a^\dagger (a)$ create (annihilate) an electron on plane $a$ and correspondingly for plane $b$. It is convenient to introduce spinors $c_{\sigma} = (a_{\sigma}, b_{\sigma})^T$ and $c_{\sigma}^\dagger = (a_{\sigma}^\dagger, b_{\sigma}^\dagger)$. The

Fig. 2: (Color online) Phase diagram of the two-plane Hubbard model on the Bethe lattice at temperature $T/t = 0.1$. The mean-field value of $t_{\perp}$ for the AF to singlet insulating transition is marked by a dashed line.

DMFT self-consistency condition for the matrix Green function is now readily shown to be [14]

$$G_{\sigma}^{-1} (i\omega_n) = \left( \begin{array}{cc} i\omega_n + \mu & -t_{\perp} \\ -t_{\perp} & i\omega_n + \mu \end{array} \right) - t_{\perp}^2 G_{-\sigma} (i\omega_n),$$

which relates the Weiss field with spin projection $\sigma$ to the Green function with opposite spin in order to account for the commensurate antiferromagnetic (AF) order within a plane. In order to obtain an AF solution, we have applied a small spin-dependent symmetry breaking field on the first DMFT iteration.

We employ the weak-coupling continuous-time quantum Monte Carlo (CTQMC) algorithm to solve the impurity problem. In brief, the basic idea is to divide the action $S = S_0 + W$ into a non-interacting Gaussian part $S_0$ and an interaction part $W$ and to expand in the interaction. In simplified notation (for a general formulation we refer the reader to ref. [19]), the Green function can be expressed as a formal perturbation series

$$G(\tau - \tau') = \frac{Z_0}{Z} (T \mathcal{C}(\tau) \mathcal{C}(\tau') \exp(-W))_0 = \sum_k \int d\tau_1 \cdots \int d\tau_k \tilde{g}(\tau_1, \cdots, \tau_k) \Omega_k (\tau_1, \cdots, \tau_k),$$

where $(\cdots)_0$ denotes the average over the unperturbed system. The quantity $\tilde{g}$ is the contribution to Green’s function for a given configuration which can be expressed as the ratio of fermionic determinants and $\Omega_k$ is a probability distribution. The Monte Carlo (MC) procedure consists in importance sampling of configurations specified by a perturbation order $k$ and, for a given order, a set of times $\tau_1, \cdots, \tau_k$. In each MC step, the contributions to the Green function are obtained as $\tilde{g}(\tau, \tau') = G_0 (\tau - \tau') - \sum_{k=1}^k G_0 (\tau - \tau) G_{ij} \cdots G_0 (\tau_k - \tau')$, where the elements of the matrix $G_{ij}$ contain the non-interacting Green functions $G_0$ evaluated at the times according to
the particular configuration. Note that while the Green functions $G(\tau - \tau') = \langle \hat{g}(\tau, \tau') \rangle$ (here and in the following $\langle \ldots \rangle$ denotes the MC-average) only depend on the time difference, the quantities $\hat{g}(\tau, \tau')$ generally do not.

We now turn to the results of our MC calculations. The finite-temperature phase diagram of the double Bethe Hubbard model is depicted in fig. 2. We find essentially four different phases: For small perpendicular hopping, the system exhibits antiferromagnetism, which is also present in the decoupled lattices. In the weak-coupling regime, the system is metallic and magnetic order is suppressed for small values of $t_\perp$. For larger values of the interaction $U$ the local moments order antiferromagnetically, giving rise to an AF metal phase. Further increase of $U$ drives the system into the AF insulating phase. For $U = 0$ and larger perpendicular hopping, a transition to a band insulating phase is expected to occur at $t_\perp = W/2$ at zero temperature, where the bonding and antibonding bands (bandwidth $W = 4t$) split. From the maximum entropy density of states at the Fermi level we find a somewhat larger value for small values of $U$, due to temperature smearing of the bands. For larger values of $U$, we have determined the boundary to the insulating state by the condition that the total spin of the dimer is zero within the MC error. This yields essentially the same results as the condition of vanishing density of states at the Fermi level. For $U/t < \sqrt{2}$, the system is clearly AF insulating. For larger $U/t$, the situation is drastically different. For $U/t = 2.0$ the system is at the transition to the Mott insulating state for vanishing $t_\perp$. For small perpendicular hopping it becomes metallic and exhibits a pseudogap structure. Moreover, it displays the characteristics of an AF metal. For larger $t_\perp$ we find the Kondo resonance at the Fermi level, which is spin-split due to antiferromagnetism. At enhanced perpendicular hopping the spin-splitting disappears as the system crosses the transition line to the paramagnetic state. A gap develops again upon further increase of $t_\perp$ and finally fully opens at the metal–singlet-insulator transition line.

Let us now investigate the transition from the AF to singlet insulator in the correlated regime in more detail. We note that the MC error was negligible, i.e. considerably smaller than the symbol size, except where shown. In fig. 4 we present the magnetization on both sites of the dimers as a function of the inter-plane hopping $t_\perp$ for $U/t = 4.0$. For small $t_\perp$ we have the AF solution with a different sign of the magnetization on opposite sides of the planes. It can further be seen that in the limit of zero coupling between dimer sites, the magnetization is close to zero. For larger $t_\perp$ the DOS shows no spin polarization, while the system remains insulating. For smaller $U$, the situation is drastically different. For $U/t = 2.0$ the system is at the transition to the Mott insulating state for vanishing $t_\perp$. For small perpendicular hopping it becomes metallic and exhibits a pseudogap structure. Moreover, it displays the characteristics of an AF metal. For larger $t_\perp$ we find the Kondo resonance at the Fermi level, which is spin-split due to antiferromagnetism. At enhanced perpendicular hopping the spin-splitting disappears as the system crosses the transition line to the paramagnetic state. A gap develops again upon further increase of $t_\perp$ and finally fully opens at the metal–singlet-insulator transition line.

In fig. 3 we show some characteristic local density of states (DOS) obtained using the maximum-entropy method for two different values of the on-site repulsion $U$ and different inter-plane hoppings. For an on-site repulsion of $U/t = 4.0$ and small $t_\perp$, the system is clearly an AF insulator. The spin splitting is pronounced and the DOS displays a four peak structure. The outer peaks can be identified as the lower and upper Hubbard bands, while the inner peaks are characteristic of the AF state. At $t_\perp/t = \sqrt{2}$ these peaks have almost disappeared and the magnetization is close to zero. For larger $t_\perp$ the DOS displays a four-peak structure. The outer peaks can be identified as the lower and upper Hubbard bands, while the inner peaks are characteristic of the AF state. At $t_\perp/t = \sqrt{2}$ these peaks have almost disappeared and the magnetization is close to zero. For larger $t_\perp$ the DOS displays a four-peak structure. The outer peaks can be identified as the lower and upper Hubbard bands, while the inner peaks are characteristic of the AF state.
plane are coupled by an effective AF Heisenberg exchange $J_\perp \sim t_\perp^2 / U$. Noting that for the infinite lattice the number of bonds connecting the dimers is twice the number of bonds on a dimer, the condition for the exchange $J_\perp \sim t_\perp^2 / U$ between sites on a dimer to overcome the exchange due to hopping within the planes is $J_\perp = 2 J$, so that $t_\perp / t = \sqrt{2}$.

Hence the formation of a singlet between neighboring sites on a dimer is expected as the source of the transition to the non-magnetic state. In order to prove this consideration, we have explicitly calculated the spin-correlations within our Monte Carlo procedure. To this end, we decompose the averages of spin operators into sums of four-point correlation functions. For example, for the total spin we have $(S^2) = ((S_i + S_j)^2) = \sum_{ij} (S_i \cdot S_j)$, where the sum is over the cluster sites. The product of spin operators can be further decomposed using $S_i \cdot S_j = S_i^z S_j^z + 1/2 (S_i^+ S_j^- + S_i^- S_j^+)$. Now the remaining operators can be expressed in terms of $c$-operators as $S^z = (n_i - n_i) / 2$, $S^\pm = c_i^\dagger c_i (\pm 1)$. Since the $c$-operators depend on imaginary time, e.g. the “instantaneous” correlator $(S_i^z S_j^z)$ formally has to be interpreted as the limit $\lim_{\tau \to 0} (S_i^z(\tau) S_j^z(0))$. Once expressed in terms of $c$-operators, the spin-correlators can be calculated within the CTQMC by exploiting the fact that the average in eq. (3) is over the noninteracting system. Hence the Wick theorem is applicable and the four-point correlators can be expressed in terms of an MC average over products of contributions to Green’s function: $(c_i^\dagger(\tau) c_i(\tau) c_j^\dagger(0) c_j(0)) = \langle \tilde{g}_{ij}(\tau, \tau) \tilde{g}_{ij}(0, 0) \rangle - \delta_{\tau,0} \langle \tilde{g}_{ij}(\tau, 0) \tilde{g}_{ij}(0, \tau) \rangle$, and similar for other averages.

The result of these calculations for the total spin is shown in fig. 5. The total spin $(S^z)$ of a single site is somewhat smaller than $= S(S+1) = 3/4$, but varies only slightly as a function of the perpendicular hopping.

For the total spin of a dimer, however, the situation is different. It continuously decreases as the coupling $t_\perp$ between dimer sites is increased. Our results are consistent with a total spin of zero at $t_\perp / t \approx \sqrt{2}$, thus proving our consideration that a singlet is formed between neighboring spins on opposite sites of the planes. This picture is further underlined by comparing the quantities $(S_i^z S_j^z)$ and $-(S_i^z S_j^z)$ for $i \neq j$ on a dimer as shown in the inset of fig. 5. The square of the $z$-projection of the spin decreases due to enhanced double occupancy (note that for the Hubbard model $\langle n_i n_i \rangle = 1/2 - 2 (S^z S^z)$ holds). Furthermore, we find that the correlation $(S_i^z S_j^z)$ for $i \neq j$ has negative sign, in accordance with the tendency to AF coupling between the spins. For weak coupling the on-site and inter-site correlations differ. This is expected, since spin flips destroy the correlation between sites. For larger values of the coupling however, the magnitude of the intersite correlation approaches the on-site value, showing the formation of a coherent state. In contrast to the MC error for all other measured quantities, the error of the total spin of the dimer is considerable, reflecting the fact that this quantity is strongly fluctuating in the simulation.

By tuning the perpendicular hopping between the two planes, we thus have a way of continuously varying the degree of entanglement and to form a coherent singlet state between the local moments on the dimer sites. This feature is inherent to the model due to the absence of spatial correlations within the planes. This is also reflected in the fact that the transition occurs at the mean-field value $\sqrt{2}$.

To further underline our findings, we plot the dynamical susceptibility $\chi_{\text{loc}}(\omega)$ in fig. 6 for different values of the perpendicular hopping for $U/t = 4.0$. It is obtained by analytical continuation [20] of the Fourier components of the corresponding imaginary time correlation function $\chi(\tau) = (S_\tau^z S_\tau^z(0))$. For small values of $t_\perp$, we find a pronounced peak at zero energy. This can be attributed to the Goldstone mode present in the symmetry-broken
(ordered) state. Therefore the peak diminishes as the border to the disordered state is approached by increasing the perpendicular hopping. At the same time a new feature starts to develop at higher energies at around $\omega/t \sim 1$. This energy scale is the same as the effective (in-plane) exchange $J_{\|} = 4t^2/U$. This is consistent with the fact that for $U/t = 5$ this feature occurs at $\omega/t \sim 0.8$. It can be attributed to a spin-flip transition. The opening of the spin-gap occurs at $t_{\perp}/t = \sqrt{2}$, i.e. at the same point at which the spin of the dimer vanishes.

Our results bear some resemblance to a bilayer square-lattice Heisenberg model, although the two models are quite different. Two modes exist in the spectrum corresponding to the in-phase and out-of-phase excitations of the two layers [21]. In order to compare this with our results, one should bear in mind that on the Bethe lattice there are only two $k$-points: The $\Gamma$-point ($k = 0$) and the $M$-point ($k = (\pi, \ldots, \pi)$). For the bilayer Heisenberg model the energies of the in-phase excitation at the $\Gamma$-point and the out-of-phase excitation at the $M$-point (and vice versa) are equal in the ordered state and similar in the disordered phase. Hence the two modes cannot be distinguished in our case. However, the excitation is gapless in the ordered phase in agreement with fig. 6. The out-of-phase excitation at the $\Gamma(M)$-point has the highest energy in the spectrum. Presumably the intensity is too low so that this mode is not detected. In the disordered phase the in-phase excitation at $\Gamma$ is gapped, in accordance with our results.

This similarity is a consequence of the fact that at large values of $U$, the model approximately maps to a Heisenberg model (note, however, that for the bilayer square lattice model, the mean-field value of the critical exchange is $J_{\|}/J_{\perp} = 4$ as opposed to 2 for the Bethe lattice) and the physics is dominated by the spin degrees of freedom. In this regime, the transition is an order-disorder transition between the two insulating phases.

We now investigate the more interesting case of the metal-insulator transition which takes place for intermediate $U$ as $t_{\perp}$ is varied. In order to study the interplay between the spin and charge degrees of freedom, we consider an on-site repulsion of $U/t = 1.5$. The spin-correlations are shown in fig. 7. The local moment is considerably smaller than in fig. 5. Notably, the transition to the singlet state is not observed at $t_{\perp}/t = \sqrt{2}$, since the Heisenberg picture is no longer valid for this value of $U$. Nevertheless a transition to a singlet state still takes place as the total spin goes to zero at $t_{\perp}/t \gtrsim 2.1$.

For this value of $U$ the magnetization vanishes already for small $t_{\perp}$ and the transition takes place in the paramagnetic phase, as shown in the inset of fig. 7. We note however, that qualitatively the same behavior is observed for the AF-metal-to-singlet-insulator transition which takes place in a narrow region of the phase diagram (cf. fig. 2).

In fig. 7, we also show the density of states at some characteristic points close to the point where a singlet is formed. The DOS is not spin-polarized as we are deep in the paramagnetic regime. For small $t_{\perp}$, we find the usual three-peak structure. This structure is visible over a broad range of $t_{\perp}$ values. By further increasing $t_{\perp}$, the coherent peak at the Fermi level disappears and a pseudogap starts to develop. This signals the quenching of the Kondo effect due to the singlet formation between dimer sites, which inhibits the formation of the local Kondo singlet between the local moment and the conduction electron spins. We find that the pseudogap develops continuously as the perpendicular hopping increases. Most notably, the gap is fully opened for $t_{\perp}/t \gtrsim 2.1$, i.e. where the total spin reaches zero within the MC error. The spectral weight provided by the local spin fluctuations which lead to the Kondo effect is suppressed as the singlet on the dimer is formed. Stated another way, the singlet formation leads to electron localization. The pseudogap formation is also observed in the AF metal regime, i.e. for larger values of $U$, where magnetism survives up to the point where the singlet is formed. The insulating phase can thus be understood as a singlet insulator for all values of $U$. The downturn of the transition line separating the metallic insulating state was attributed to the broadening of the bands through the correlations in ref. [16]. Here it can also be understood from the fact that for increasing $U$ the local moments are less screened and the exchange $J_{\perp}$ becomes more effective in forming the singlet.

In fig. 8 we show the dynamical susceptibility for $U/t = 1.5$ and various values of $t_{\perp}$. The interplay between spin and charge degrees of freedom leads to a more complicated behavior compared to the case of large $U$. Here the Goldstone mode at zero energy is absent since the system is in the disordered (paramagnetic) phase for the values of $t_{\perp}$ used in this figure. The spectrum is gapped for $t_{\perp}/t \gtrsim 2.1$. The width of the gap is of the order of the in-plane exchange and the separation between the
two peaks is consistent with the on-site repulsion $U$. The spin gap opens at the same point as the charge gap in our simulations.

To conclude, we have presented numerically exact results for the two-plane Hubbard model on the Bethe lattice in infinite dimensions. We have mapped out the finite temperature phase diagram and found a metal-to-insulator transition as the perpendicular hopping between the two planes is increased. By explicit calculation of the total spin of the dimers, we have shown that a singlet is formed between the localized moments. Hence the insulating state in the correlated regime can be characterized as a singlet-insulator phase. This is underlined by the formation of a spin gap in the local dynamical susceptibility. The spectral weight at the Fermi level was found to continuously decrease as local spin fluctuations responsible for the Kondo effect are gradually suppressed by the singlet formation.

It is further interesting to study the metal-insulator transition on the two-dimensional bilayer Hubbard model. We have recently developed a method that allows to treat spatial correlations beyond DMFT [22]. Within a cluster formulation [23], the local singlet formation can be treated explicitly, while long- and short-range correlations are treated perturbatively on the same footing. This allows to systematically study how spatial correlations within the planes modify the present results.

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