

Metal-Insulator Transitions in the Periodic Anderson Model

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We solve the periodic Anderson model in the Mott-Hubbard regime, using dynamical mean field theory. Upon electron doping of the Mott insulator, a metal-insulator transition occurs which is qualitatively similar to that of the single band Hubbard model, namely, with a divergent effective mass and a first order character at finite temperatures. Surprisingly, upon hole doping, the metal-insulator transition is not first order and does not show a divergent mass. Thus, the transition scenario of the single band Hubbard model is not generic for the periodic Anderson model, even in the Mott-Hubbard regime.

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The metal-insulator transition in strongly correlated materials remains a central problem of modern condensed matter physics [1,2]. Great progress in its understanding was made possible by the development of new theoretical approaches such as the dynamical mean field theory [3], which is a method that becomes exact in the limit of large lattice connectivity [4]. The mean field equations can usually be tackled with a variety of numerical approaches which allow us to obtain reliable solutions and insights. In this context, the Hubbard model, which is probably the simplest model that captures a correlation driven metal-insulator transition (MIT), called Mott-Hubbard transition, has received most of the attention in the past 15 years. As a result of intense investigation, our understanding of the metal-insulator transition in that model is now profound. The studies have unveiled a scenario where, at low temperatures and moderate interaction, the half-filled Mott insulator may be driven to a correlated metallic state through a first order transition [5]. The transition can occur as a function of correlation strength, temperature, or doping. The first order line ends at finite temperature in a critical point and the critical region can be described by a Ginzburg-Landau theory [6]. This theoretical prediction was experimentally verified in experiments on V_2O_3 [7]. The Hubbard model is often considered as a minimal model for the study of rather complicated compounds such as transition metal oxides and heavy fermion systems. This is supported by the implicit assumption that the Hubbard model is expected to be the effective low energy Hamiltonian for a wider class of more realistic multiband models for strongly correlated electron systems.

On the other hand, a more realistic model which is also widely used in theoretical investigations of strongly interacting systems, though still schematic, is the periodic Anderson model (PAM). In the context of correlated electron systems, this model permits us to describe explicitly both the localized orbitals, such as the d in transition metal oxides or the f in heavy fermion systems, and their hybridization to an itinerant electron band (such as that of p orbitals of oxygen in transition metal oxides). In fact, the PAM allows us to investigate the various regimes where

Mott insulating states occur, as characterized by the Zaanen-Sawatzky-Allen (ZSA) scheme [8]. They are classified as either Mott-Hubbard insulators or charge transfer insulators. The first apply to the early transition metal oxides such as titanates and vanadates, while the second is relevant for cuprates, such as the high- T_c superconductors, and manganites, which show colossal magnetoresistance [2]. In theoretical studies, however, it is often assumed that both Mott-Hubbard and charge transfer systems may be described at low energies by a simpler one band Hubbard model Hamiltonian.

In the present work we shall test the putative validity of the Hubbard model as the effective low energy Hamiltonian of the more realistic periodic Anderson model. We shall do this within a well-defined mathematical framework, namely, the dynamical mean field theory (DMFT), that allows us to obtain essentially exact numerical solutions of the models (in the statistical Monte Carlo sense). In particular, we shall concentrate on the nature of the (paramagnetic) metal-insulator transitions that occur in the periodic Anderson model with parameters that set it in the Mott-Hubbard regime and discuss it with respect to the corresponding scenario that is realized in the one band Hubbard model case. In addition, our results should also be valuable for the interpretation of experimental spectroscopies of strongly correlated transition metal oxides that experienced fantastic improvements in the last decade. In fact, the analysis of experimental data of systems which have a mixed orbital character is not always simple when strong correlations are present. Finally, our work addresses a very relevant issue in regard of the intense effort that is currently dedicated to the implementation of *ab initio* methods for strongly correlated materials [9] which makes heavy use of the DMFT methodology [10].

Among our main results we find that in the case of the electron doped driven MIT, the scenario is indeed similar to the one realized in the Hubbard model; however, the hole doping scenario is qualitatively different. In this case, the correlated metal has a resonance peak at the Fermi energy flanked by a Hubbard band, but, unlike the Hubbard model scenario, it is not related to the formation of a

Kondo-like resonance and its mass does not diverge at the transition. Moreover, and also in contrast to the Hubbard model case, our results indicate that this metal-insulator transition is of second order as no signs of coexistent solutions were observed. We shall argue that while the metallic state in the former case is a renormalized “Brinkman-Rice” Fermi liquid [11], the latter can be interpreted as liquid of “Zhang-Rice singlets” [12].

The periodic Anderson model Hamiltonian reads

$$H = -t \sum_{\langle ij \rangle \sigma} (p_{i\sigma}^+ p_{j\sigma} + p_{j\sigma}^+ p_{i\sigma}) + (\epsilon_p - \mu) \sum_{i\sigma} p_{i\sigma}^+ p_{i\sigma} \\ + (\epsilon_d - \mu) \sum_{i\sigma} d_{i\sigma}^+ d_{i\sigma} + t_{pd} \sum_{i\sigma} (d_{i\sigma}^+ p_{i\sigma} + p_{i\sigma}^+ d_{i\sigma}) \\ + U \sum_i (n_{d\uparrow} - \frac{1}{2})(n_{d\downarrow} - \frac{1}{2}),$$

where the d_σ and d_σ^+ operators destroy and create electrons at nondispersive d orbitals with energy ϵ_d , p_σ and p_σ^+ destroy and create electrons at p orbitals with energy ϵ_p which form a band with hopping parameter t . The p and d orbitals are hybridized with an amplitude t_{pd} , and the electron correlations are introduced by the Coulomb interaction U on the d sites. It is customary to define the charge transfer energy $\Delta = \epsilon_d - \epsilon_p$, and μ is the chemical potential. As described in the ZSA scheme, this model predicts correlated insulating states in two very different regimes: at $\Delta \ll U$ the charge transfer insulator and at $U \lesssim \Delta$ the Mott-Hubbard insulator. The latter is relevant for the early transition metal oxides and will be the focus of the present work.

To solve the PAM using DMFT, for simplicity we adopt a Bethe lattice that corresponds to a semicircular density of states (DOS) for the p -electron band. Setting the hopping of the p electrons to $t = 1/2$, their half bandwidth is equal to one and fixes the units of the model. To set the system in the Mott-Hubbard regime, we adopt $\epsilon_d = 0$ and ϵ_p negative, so that the p band lies well below the Fermi surface and is almost full, while the occupation of the local d sites will be close to 1. The parameter t_{pd} controls the hybridization between the orbitals at each lattice site and permits the delocalization of the d electrons. In fact, a finite t_{pd} turns the “flat” band of d orbitals into a conduction band with mainly d character and bandwidth of the order of t_{pd}^2/Δ . Now, for a moderate value of the repulsion $U > t_{pd}^2/\Delta$ and an occupation of the d site n_d close to 1, one expects the conduction band to open a correlation gap and the system becomes a Mott-Hubbard insulator.

The DMFT equations are most easily derived using the cavity method [3,13], and one obtains the local effective action for the d electrons:

$$S_{\text{eff}} = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\sigma} d_{\sigma}^+(\tau) \mathcal{G}_0^{-1}(\tau - \tau') d_{\sigma}(\tau') \\ + U \int_0^\beta d\tau \left[n_{d\uparrow}(\tau) - \frac{1}{2} \right] \left[n_{d\downarrow}(\tau) - \frac{1}{2} \right], \quad (1)$$

where d_σ and d_σ^+ correspond to a given (any) site of the lattice. This equation defines the so-called associated impurity problem of the model that is subject to a self-consistent constraint that reads

$$\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \epsilon_d - \frac{t_{pd}^2}{i\omega_n + \mu - \epsilon_p - t^2 G_{pp}}.$$

The solution of the quantum impurity problem (1) gives the local d -electron Green’s function G_{dd} and defines a self-energy $\Sigma = \mathcal{G}_0^{-1} - G_{dd}^{-1}$. The local Green’s function of the p electrons G_{pp} is obtained in terms of Σ and the non-interacting semicircular DOS ρ_0 as:

$$G_{pp} = \int d\epsilon \frac{\rho_0(\epsilon)}{i\omega_n + \mu - \epsilon_p - \frac{t_{pd}^2}{i\omega_n + \mu - \epsilon_d - \Sigma(i\omega_n)} - \epsilon}.$$

We solve for these equations using two powerful, and in principle exact, numerical methods: quantum Monte Carlo (QMC) and exact diagonalization (ED) [3]. A similar methodology was used in the study of a related two-band Hubbard model [14]. The QMC is a finite temperature method and is exact in the statistical sense, while the ED is at $T = 0$ and relies on diagonalization of finite clusters and extrapolations are performed to account for the systematic finite size effects [3].

We shall begin our discussion with the behavior of the density of states of the model in different regimes. For $U = 0$ and at $t_{pd} = 0$ the system is an insulator since neither the d orbitals at the Fermi energy can conduct (because they are localized), nor can the p band conduct (because it is full and well beneath the Fermi surface). At a finite hybridization t_{pd} , however, the system becomes metallic, as the p and d orbitals form a partially filled band at the Fermi energy with mixed p and d character. In Fig. 1 we show the comparison of the p - and d -electron DOS. The one carrying most of the spectral intensity at low frequencies is the d -electron DOS $\rho_d(\omega)$, since the bare atomic energy of the d orbitals is at the Fermi energy. The lower panel of the figure shows the dramatic effect of correlations; when the interaction U is increased, a rather large gap opens in the DOS at the Fermi energy, driving the system to a Mott insulator state. The gap is of order U and results from the high energetic cost of double occupation of the d site. An interesting effect is that the size of the Mott gap Δ_M may be substantially renormalized. In the inset of Fig. 1 we show the variation of $\Delta_M(U)$ upon increasing the distance of the p band with respect to the d -electron energy. Notice that the gap $\Delta_M(U)$ is always smaller than the bare U and becomes equal only asymptotically when $\epsilon_p \rightarrow -\infty$. This renormalization effect is of relevance to the difficult problem of the determination of the effective value of U in realistic *ab initio* calculations using DMFT [9].

The Mott insulator can be destabilized by either particle or hole doping. Therefore, the system has two doping driven metal-insulator transitions. In the one band Hubbard model, the two transitions have the same character; however, as we shall see, this is not the case in the

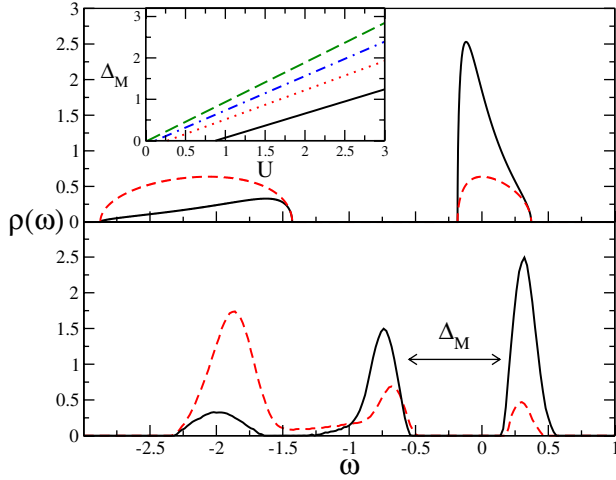


FIG. 1 (color online). Density of states for the p and d electrons (dashed and solid line) for $\Delta = 1$, $t_{pd} = 0.9$. Upper panel shows the $U = 0$ case with $\mu = 0.529$ that gives a total occupation of three particles below the Fermi energy. The lower panel shows analytically continued QMC data for the Mott insulator state with $U = 2$, $T = 1/64$, and $\mu = 1.079$ that gives $n_{\text{tot}} = 3$. The double arrow head line indicates the large Mott gap Δ_M . The inset shows $\Delta_M(U)$ for different positions of the of the p -electron band $\epsilon_p = -6, -3, -2, -1$ (top to bottom). The results are obtained with ED of finite clusters of N_s sites and the data shown are for the limit $N_s \rightarrow \infty$.

present model. In Fig. 2 we show the occupation n_d and n_p of the d and p sites for $U = 2$. The plateaux that appear around $0.7 \lesssim \mu \lesssim 1.2$ indicate the onset of the incompressible Mott insulating state when correlations are strong. While the Mott insulator is associated with the energy cost of doubly occupying the local d orbital, it is interesting to notice that the Mott plateau does not occur exactly at $n_d = 1$ but at a higher value, which depends on the hybridization. The Mott state is in fact found when the total number of particles per unit cell is exactly equal to three. Thus, the object that becomes localized due to the strong correlations is not simply a d electron, but a composite object with mixed d and p character. The inset of the figure shows the phase diagram in the U - μ plane that maps the region of the Mott insulator phase and the transition lines to correlated metallic states.

In Fig. 3 we show the DOS for the p and d electrons in the metallic states that are obtained by either particle or hole doping of the Mott insulator. In both cases one finds that the DOS clearly show the emergence of a correlated small quasiparticle peak at the Fermi energy. The occurrence of a narrow quasiparticle peak at the Fermi energy that is flanked by large Hubbard bands which are separated by an energy of order U is a hallmark result of the solution of the Hubbard model within DMFT [3]. Thus, one may be led to conclude that the MIT in the PAM shares the same qualitative features. Rather surprisingly, this expectation is only fully confirmed for the case of particle doping, but the MIT scenario in the hole doped case is strikingly different.

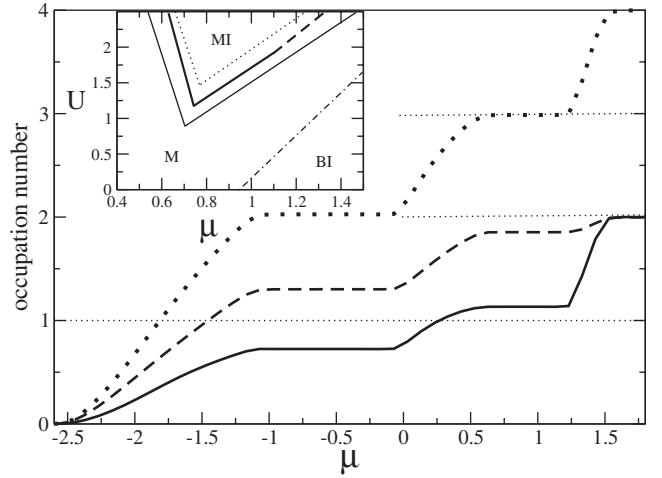


FIG. 2. n_d (solid line), n_p (dashed line), and n_{tot} (dotted line) as a function of μ , for $U = 2$. The data are from QMC at $\Delta = 1$, $t_{pd} = 0.9$, and $T = 1/64$. The plateaux at $n_{\text{tot}} = 2$ and 4 are band insulator (BI) states. The one at $n_{\text{tot}} = 3$ is the Mott insulator (MI). The inset shows the phase diagram in the U - μ plane. The boundary lines are for $T = 1/20$ (dotted line), $T = 1/64$ (thick solid line), and $T = 0$ (thin solid line). The dashed thick line segment at $T = 1/64$ denotes the region of the MIT boundary where the QMC data show coexistence of a metal and an insulating solution. The $T = 0$ data are from extrapolated ED calculations. This method is not suited for the study of coexistence of solutions at $T = 0$. The dash-dotted line denotes the transition from a metal (M) to the band insulator (BI) at $n_{\text{tot}} = 4$.

Upon particle doping of the Mott insulating state, we have confirmed that there is a small region of parameters at the MIT boundary where two coexistent solutions, one metallic and one insulating, are found. In addition, the numerical solutions show critical slowing down of the convergence speed of the self-consistency close to the transition. These two features were also observed in the previous studies of

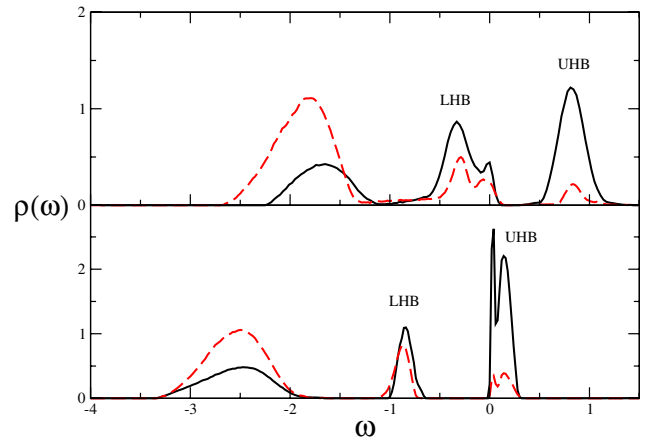


FIG. 3 (color online). Density of states of p and d electrons (dashed and solid line) for $U = 2$, $\Delta = 1$, $t_{pd} = 0.9$, and $T = 1/64$, as obtained from QMC. Upper panel: $\mu = 0.554$, which corresponds to tiny hole doping. Lower panel: $\mu = 1.234$, which corresponds to tiny particle doping.

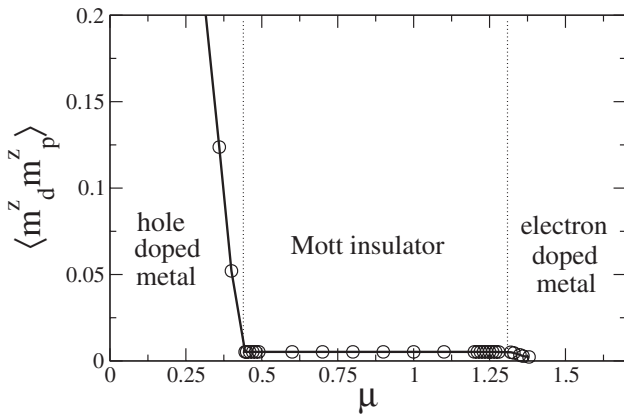


FIG. 4. $\langle m_d^z m_p^z \rangle$ as a function of μ , for $U = 2$, $\Delta = 1$, $t_{pd} = 0.9$. The results are obtained from ED with a cluster of 16 sites.

the finite T first order MIT in the Hubbard model [6]. In contrast, in the hole doped case ($n_{\text{tot}} < 3$) we found no trace of coexistent solutions down to $T = 1/128$. The solution seems to be always unique, which implies that the transition is of second order, i.e., through a quantum critical line in the U - μ plane.

Insight on the physical reason for the qualitative difference observed upon particle or hole doping is obtained from the behavior of the observables that measures the d - p correlations. In Fig. 4 we show the behavior of magnetic correlation between the d and p electrons $\langle m_d^z m_p^z \rangle = \langle (n_{d\uparrow} - n_{d\downarrow})(n_{p\uparrow} - n_{p\downarrow}) \rangle$ across the metal-insulator transitions. As the results show, the value of $\langle m_d^z m_p^z \rangle$ is sizable on the hole doped metal, while it becomes negligible on the particle doped side. In the particle doped case $\langle m_d^z m_p^z \rangle$ is negligible because the p band is already full and the extra particles mainly go to occupy d sites. Thus, the p sites do not get an induced magnetic moment and they cannot screen the magnetic moment of the local d sites. Thus the magnetic correlations develop directly among neighboring d orbitals. These correlations are of antiferromagnetic character due to the superexchange mechanism and are analogous to those created between neighboring sites in the Hubbard model case. Thus we can understand that for particle doping the character of the MIT in the periodic Anderson and Hubbard models is in fact the same; the p sites merely allow the charge fluctuation (and thus the delocalization) of the d electrons, but they do not couple magnetically and do not screen the local moments.

In striking contrast, upon hole doping the scenario is quite different. In this case, the system finds it is energetically favorable to create holes in the p band and magnetically bound the holes to the local moment of the correlated d site. This feature is reminiscent of the “Zhang-Rice” singlet formation [12] and leads to the emergence of a quasiparticle peak at the Fermi energy as the singlets delocalize.

In conclusion, we have investigated the doping driven metal-insulator transition in the periodic Anderson model in the Mott-Hubbard regime. We found that the size of the Mott gap can be significantly renormalized by hybridization effects. In addition, we found that while both correlated metallic states at small doping show a small quasiparticle peak at the Fermi energy, the nature of the MIT is qualitatively different on each side. In the particle doped side, the quasiparticle peak is associated with a Kondo-like resonance and the MIT shares the same qualitative nature of the first order transition found in the one band Hubbard model. In contrast, on the hole doped side, the quasiparticle peak is associated with the formation of “Zhang-Rice” singlets and the transition is second order. Thus, our study demonstrates that, even in relatively simple situations, the one band Hubbard model should not be automatically considered the low energy effective model of more complicated multiorbital systems. The investigation of the physical nature of the “Zhang-Rice” correlated metal is a very interesting problem open for future investigations.

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