Non-Fermi-Liquid Behavior in the Periodic Anderson Model

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We study the Mott metal-insulator transition in the periodic Anderson model with dynamical mean field theory (DMFT). Near the quantum transition, we find a non-Fermi-liquid metallic state down to a vanishing temperature scale. We identify the origin of the non-Fermi-liquid behavior as being due to magnetic scattering of the doped carriers by the localized moments. The non-Fermi-liquid state can be tuned by either doping or external magnetic field. Our results show that the coupling to spatial magnetic fluctuations (absent in DMFT) is not a prerequisite to realizing a non-Fermi-liquid scenario for heavy fermion systems.

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The theoretical understanding of the breakdown of the Fermi liquid paradigm observed in high T_c superconductors and heavy fermion systems remains one of the open challenges in strongly correlated physics. These systems show metallic phases with anomalous properties that cannot be accounted for by the Fermi liquid theory, which provides an adequate description of the electronic state of ordinary metals. The reason is intimately related to the strong correlation effects, originated in the localized nature of the d and f orbitals of the experimental compounds [1]. Different ideas have been proposed over the years to try to explain the origin of the non-Fermi-liquid (NFL) states, without an absolute consensus so far. However, many of these ideas share a common feature, namely, that the central ingredient is the proximity to a quantum phase transition (QPT), or a quantum critical point (QCP) [2]. In that scenario the breakdown of the Fermi liquid occurs in the neighborhood of a $T = 0$ transition between an ordered phase (e.g., antiferromagnetic) and a paramagnetic one. There, the fluctuations of the order parameter that couple to the electrons are strongest, and are viewed as the origin for the NFL state. Among those approaches we can mention the Hertz-Millis theory, where the paramagnons of the ordered phase "dress" the conduction electrons to produce the NFL features [3]. Another approach is the local quantum critical theory [4,5], which does not consider the electrons as "bystanders" but emphasizes their role in the screening of the local magnetic moments, via the celebrated Kondo effect. There, the competition between the tendency to formation of local singlets and the long wavelength magnetic fluctuations are to be considered on equal footing. This has been achieved by the formulation of an extension to the dynamical mean field theory (DMFT) approach [6], called EDMFT [7,8]. DMFT has proven to be a very useful technique to study strongly correlated electron systems when the main physical effects are local [6]. However, it is also recognized that this method lacks a proper description of the spatial magnetic fluctuations which are usually considered a crucial ingredient for the realization of a NFL state. This shortcoming is cured in EDMFT with the incorporation of a bosonic component to the effective mean field. Though that approach has provided useful insight into the physics of the problem [7–10], the solution of its mean field equations is more difficult and often requires some simplifying assumptions. We should also mention that a different and original approach to quantum criticality that goes beyond the Ginzburg-Landau theory has also been proposed [11].

In the present work we shall show that, contrary to conventional expectations, a non-Fermi-liquid state is readily obtained from the DMFT solution of the canonical model for the study of heavy fermion systems, namely, the periodic Anderson model (PAM) [12]. We shall show that, similarly to other approaches, this novel NFL state is located in the neighborhood of a QPT, but unlike the standard scenario described before, the relevant quantum transition here is a Mott transition. Thus, the present study sheds a different light onto the problem, showing that the coupling to long wavelength magnetic fluctuations (which are absent in DMFT) is not a prerequisite for the realization of a NFL scenario that captures some features observed in heavy fermion systems. *Local* temporal magnetic fluctuations alone can provide sufficient scattering to produce an incoherent metallic state. Two recent works have also reported non-Fermi-liquid states in models that generalize the PAM by introducing a finite bandwidth to the localized orbitals [13,14]. However, those approaches fundamentally differ from the present one, since they view the NFL state as the result of an orbital selective Mott transition, which is absent in the PAM. Thus, our study shows that the PAM, solved within DMFT (i.e., in the limit of infinite dimensions), may be considered as a "bare bones" or minimal approach that can qualitatively capture a physical scenario found in some NFL heavy fermion systems.

The periodic Anderson model Hamiltonian reads

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

where $p_{i\sigma}$ and $p^+_{i\sigma}$ are the destruction and creation operators for the electrons at p orbitals with energy ϵ_p and hopping parameter t. $d_{i\sigma}$ and $d^+_{i\sigma}$ are the respective operators of the nondispersive d-electron orbitals with energy ϵ_d, that we fix equal to 0 without loss of generality [15]. 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 only. For simplicity we consider the model defined on a Bethe lattice that gives a semicircular DOS for the p-electron band (at t_{pd} and $U = 0$) [6]. Its half-bandwidth is $D = 2t = 1$ and sets the units of the problem. The charge transfer energy is defined as $\Delta = \epsilon_d - \epsilon_p$, and μ is the chemical potential. At $U = 0$ and large Δ, the hybridization parameter t_{pd} permits the delocalization of the d electrons, as a narrow band forms at the Fermi energy with bandwidth $\sim t^2_{pd}/\Delta$. However, when both U and Δ are large, and the narrow band is half-filled, the periodic Anderson model can describe two different correlated insulator states: a charge transfer insulator for $\Delta < U$, and a Mott-Hubbard one for $U < \Delta$.

The doping driven metal-insulator transition (MIT) in the paramagnetic Mott-Hubbard insulator was the focus of our recent study [16]. The main finding was a qualitatively different scenario for the electron or hole driven transitions. In the former case the MIT was expectedly similar to the first order transition of the well studied one band Hubbard model [6]. However, in the latter case, an intriguing second order transition was found. Here, we shall study in detail the unexpected nature of this Mott transition.

Within DMFT the PAM can be mapped onto a quantum impurity problem subject to a self-consistency condition [17]. Using the cavity method [6] one obtains the effective action for the quantum impurity model:

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

where d_σ and d^+_σ destroy and create a d electron on an arbitrarily chosen site and $n_{d\sigma}$ is the occupation operator. $\mathcal{G}_0$ is the function describing the properties of the dynamical bath of the site, which is subject to the self-consistent condition,

$$\mathcal{G}^{-1}_0(i\omega_n) = i\omega_n + \mu - \epsilon_d - \frac{t^2_{pd}}{i\omega_n + \mu - \epsilon_p - t^2 G_{pp}(i\omega_n)}. \quad (3)$$

The p-electron Green function G_{pp} is written in terms of the local self-energy Σ_{pp} and the noninteracting density of states ρ^0 as

$$G_{pp}(i\omega_n) = \int d\epsilon \frac{\rho^0(\epsilon)}{i\omega_n + \mu - \epsilon_p - \Sigma_{pp}(i\omega_n) - \epsilon} \quad (4)$$

where ϵ is the single particle energy, and Σ_{pp} is obtained from the quantum impurity model self-energy $\Sigma(i\omega_n)$ of Eq. (2) [6,17],

$$\Sigma_{pp}(i\omega_n) = \frac{t^2_{pd}}{i\omega_n + \mu - \epsilon_d - \Sigma(i\omega_n)}. \quad (5)$$

To solve these equations we use two, in principle exact, numerical methods: quantum Monte Carlo (QMC) [18] and exact diagonalization with the density matrix renormalization group (ED-DMRG) [19]. The former is a finite temperature calculation and is exact in a statistical sense, while the latter is a $T = 0$ method that relies on diagonalization of large finite clusters. The comparison of the results obtained from these methods allows for a nontrivial benchmark of the numerical results. In our simulations we typically perform over 10^6 Monte Carlo sweeps in order to minimize the statistical errors.

In the main panel of Fig. 1 we show the DOS of the metallic state that results of lightly doping $\delta = 3 - n$ holes into the "parent" Mott insulator state (shown in the inset). The main features of the metallic state are its mixvalence character and the presence of a quasiparticle peak at the Fermi energy that is flanked by lower and upper Hubbard bands [16]. Within Fermi liquid theory, the key

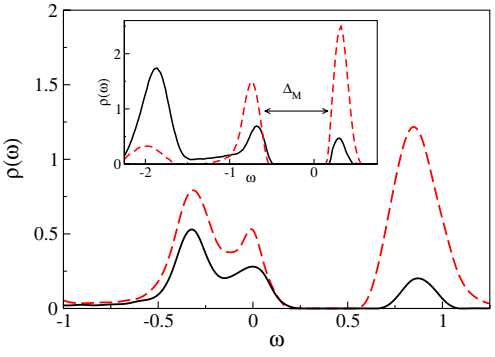

FIG. 1 (color online). Density of states for p and d electrons (solid and dashed line, respectively) from QMC data at $T = 1/128$. The doping is $\delta = 0.049$, $\mu = 0.53$, $\Delta = 1$, $U = 2$, and $t_{pd} = 0.9$. The analytic continuation is done using the maximum entropy method. Inset: DOS of p and d electrons in the Mott-Hubbard insulating phase. The chemical potential is $\mu = 1.08$ and the occupation is $n = n_d + n_p = 3$, with $n_d = 1 + \nu$, $n_p = 2 - \nu$, and $\nu = 0.14$. Δ_M denotes the Mott insulating gap.

concept is that the one-particle excitations near the Fermi energy, the "quasiparticles", are long lived entities. In consequence, the imaginary part of their self-energy should go to zero as $\omega \to 0$. More precisely, $\Sigma(i\omega_n) \approx i\omega_n a + b$ for small ω_n, with a and b real constants. Quite surprisingly, however, the self-energy of the metallic peak of Fig. 1 does not have this property. In Fig. 2 we show the numerical results for various paramagnetic metallic states obtained by small doping of the Mott insulator. The main panel shows the large finite intercept of $\mathrm{Im}\Sigma_{pp}$ that reveals the NFL nature of the states. Therefore, the metallic peak at the Fermi energy of Fig. 1 is not due to quasiparticles but rather to incoherent (i.e., short lived) excitations. In the lower inset of Fig. 2 we show the extrapolated value of $\mathrm{Im}\Sigma_{pp}(\omega \to 0)$ that is an estimate of the resistivity $\rho(T)$. Contrary to what is expected for a metal, the resistivity increases with decreasing T. At higher doping, however, it crosses over to conventional metallic (i.e., Fermi liquid) behavior. This feature is in qualitative agreement with experiments in various NFL heavy fermion compounds [1]. The coherence temperature scale T_{coh}, below which the Fermi liquid behavior is obtained depends on δ. It is computed from the local spin susceptibility χ_{loc} and is given by the x-axis intercept of $1/\chi_{\mathrm{loc}}(T) \sim T + T_{\mathrm{coh}}$. Physically, it corresponds to the Kondo quenching of the local magnetic moments. We found that T_{coh} decreases with decreasing doping, and becomes vanishingly small at low δ. This feature is reminiscent of the phenomenon of exhaustion, where few conduction electrons have to screen a large number of spins. It has been extensively investigated in the Kondo lattice model [20,21] and also in the PAM [22–24]. The exhaustion is usually realized in the limit where the number of local electrons is restricted to unity, so to represent a spin at every lattice site, while the number of conduction electrons is taken vanishingly small. Here, in contrast, as Fig. 1 shows, we are in a more mix-valence situation where the number of p carriers (holes) is not very small and never vanishes (it is $\nu = 0.14$ at $\delta = 0$, and increases further with doping). Nevertheless, in the present case also the exhaustion physics is in fact responsible for the vanishing T_{coh}. One should realize, however, that the relevant number of "conduction electrons" is not given by the finite nominal p-hole occupation, but by δ which is the number of doped carriers to the (mix-valance) Mott insulator state.

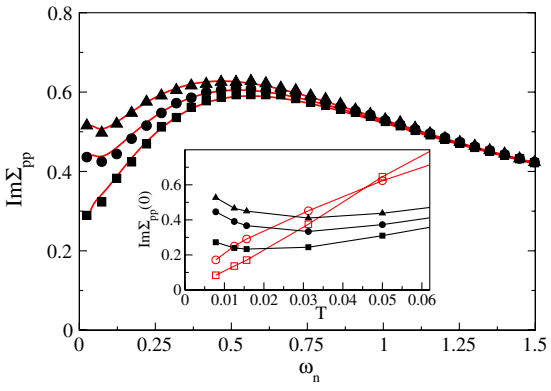

FIG. 2 (color online). Imaginary parts of the p-electron self-energy $\mathrm{Im}\Sigma_{pp}(i\omega_n)$ in the NFL state, from QMC calculations at $T = 1/128$. The hole doping is $\delta = 0.016$ (squares), $\delta = 0.049$ (circles), $\delta = 0.093$ (triangles), and $\mu = 0.58$, 0.53, and 0.48, respectively. Solid line is the same quantity from ED-DMRG. The ED-DMRG data are obtained for large finite clusters of 40 sites and are plotted down to the frequency of the lowest energy pole. Inset: inverse scattering time $\mathrm{Im}\Sigma_{pp}(\omega \to 0)$ as a function of temperature. The black symbols are for the same values of δ as in the main panel. Open symbols are for higher doping $\delta = 0.44$ (circles) and 0.62 (squares) with $\mu = 0.23$ and 0.13, respectively. Note that the inverse scattering time goes to 0 in the Fermi liquid state.

Another important difference with respect to the standard exhaustion scenario is the stability of the present NFL regime regarding magnetic ordering. The exhaustion regime is usually found to be unstable towards magnetic phases [22]. Here, in contrast we find that the NFL regime is largely paramagnetic, except at very low dopings and temperatures, where the system becomes an antiferromagnetic metal (AFM). The reason for the magnetic stability of the NFL regime can be argued to result from the magnetic frustration due to competing magnetic interactions. On one hand, neighboring localized electrons in the Mott state interact via the superexchange mechanism, that follows from the mapping of the narrow band to the Hubbard model. This interaction is antiferromagnetic and is responsible for the AFM state that is found in the limit of very low hole doping. On the other hand, there is also a competing ferromagnetic interaction induced by hole doping. The doped holes need to delocalize to lower their kinetic energy, but they are subject to a strong on-site magnetic binding to the local moments [16]. Therefore, in order to hop, they need the local moments of the neighbor sites to have the same magnetic orientation as the one in its current site. These competing magnetic interactions lead to unquenched local dynamical fluctuations of the magnetic moments down to the vanishingly small T_{coh}, that provide the source for the NFL scattering.

Figure 3 condenses our results into a δ-T phase diagram. The intensity plot shows the magnitude of the scattering rate $\mathrm{Im}\Sigma_{pp}(\omega \to 0)$, which is a measure of the NFL character of the system. We observe that conventional metallic (i.e., Fermi liquid) behavior occurs in two dark regions. The one at low δ corresponds to the small AFM phase that we mentioned before, while the one at higher δ is the Fermi liquid state that is realized beneath T_{coh} due to conventional Kondo screening. In between these two regimes we find the strong NFL behavior of the system.

The normal metal behavior in the AFM phase is easy to understand. As soon as the magnetic moments become Néel ordered the doped carriers have no problem to form coherent electronic waves. Thus, a direct implication of this observation is that if one induces magnetic order, the

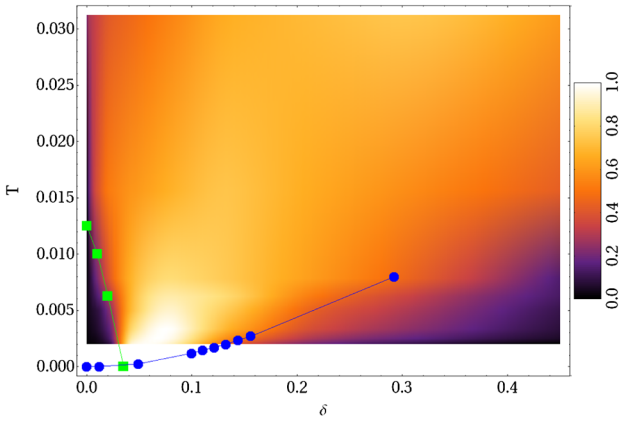

FIG. 3 (color online). Intensity plot of the scattering rate $\mathrm{Im}\Sigma_{pp}(\omega \to 0)$ as a function of doping δ and T. For visualization, the scattering rates are normalized to $\max\{\mathrm{Im}\Sigma_{pp}(\omega_n)\}$ at each (δ, T). The line with squares at low δ is T_{Neel} and gives the AFM phase boundary. (The $T = 0$ data point is obtained from ED.) The line with circle dots denotes the numerical estimate for the crossover scale T_{coh}. It is obtained from the extrapolation of the low T behavior of $1/\chi_{\mathrm{loc}}(T)$ (see text).

NFL state should become normal. To test this hypothesis we have mapped out the phase diagram as function of the external magnetic field B and T at a small fixed doping. The results are shown in Fig. 4 which displays the intensity plot of the computed scattering rate. At $B \to 0$ we find a small dark normal metal region that corresponds to the AFM state discussed before. At large B the strong magnetic field induces ferromagnetic order of the local moments and, as expected, the metallic state is normal. Interestingly, in the intermediate B region, a NFL regime emerges which can be understood as resulting from the competition between the magnetic interactions.

To conclude, we have studied the NFL regime that is realized upon doping a Mott insulator state in the periodic Anderson model within the dynamical mean field theory.

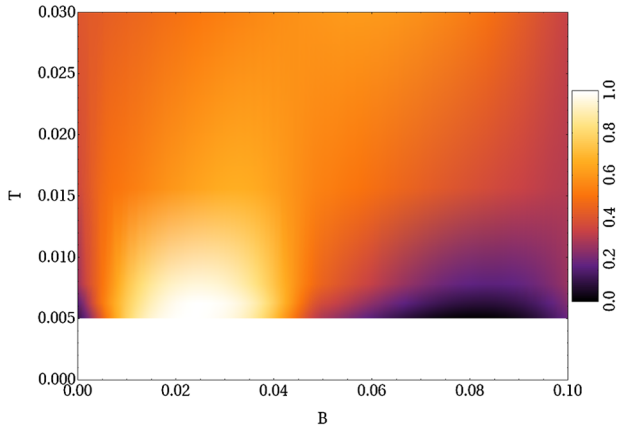

FIG. 4 (color online). Intensity plot of the scattering rate $\mathrm{Im}\Sigma_{pp}(\omega \to 0)$ as a function of external magnetic field B and T, at fixed doping $\delta = 0.01$. For visualization, the scattering rates are normalized to $\max\{\mathrm{Im}\Sigma_{pp}(\omega_n)\}$ at each (B, T).

The NFL behavior is originated in the strong *local* magnetic scattering of the doped carriers by unquenched fluctuating moments. This is in contrast to other approaches where the NFL state results from scattering by spatial magnetic fluctuations. We find that both doping and magnetic field allow us to tune into the NFL regime, in qualitative agreement with some of the non-Fermi-liquid phenomenology observed in heavy fermion systems.

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