Pseudogaps in an Incoherent Metal

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How are the properties of a metal changed by strong inelastic scattering? We investigate this question within the two-dimensional *t-J* model using extended dynamical mean field theory and a generalized noncrossing approximation. Short-ranged antiferromagnetic fluctuations lead to a strongly incoherent single particle dynamics, large entropy, and resistance. Close to the Mott transition at low hole doping a pseudogap opens, accompanied by a drop in resistivity and an increase in the Hall constant for both lower temperatures T and doping levels. The behavior obtained bears surprising similarity to properties of the cuprates.

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Most of our present understanding of the properties of metals is based on Landau's Fermi liquid theory: low-energy excitations are coherent quasiparticles with the quantum numbers of electrons. This concept has proved to be extremely successful even in systems where interactions are very strong, e.g., in liquid ^{3}He or in heavy fermion compounds. In a few classes of materials, however, most notably the cuprate superconductors, the usual Fermi liquid picture appears to break down: transport is anomalous, pseudogaps open, entropy is large, and various ordering phenomena appear to compete with each other [1–5]. This has been taken to indicate that new low-energy, long wavelength excitations like spinons and holons or more conventionally spin, charge, current, or pair fluctuations play a dominant role [1]. However, a convincing theory based on such scenarios is still missing.

In this paper, we want to follow a different and less explored route, investigating the possibility that *incoherent* and *local* excitations dominate as it might happen especially at higher T when strong quantum and thermal fluctuations driven by competing interactions decohere the fermionic excitations. Our starting point is the two-dimensional *t-J* model which describes on the one hand the physics of a doped Mott insulator and on the other hand the physics of an antiferromagnetic (AF) superexchange interaction between neighboring spins. Long range AF order gets destroyed by a few percent hole doping. The resulting spin state is characterized by short range AF correlations, and highly incoherent excitations, which are difficult to describe in any conventional many-body scheme relying on quasiparticle excitations.

A prominent feature of the underdoped cuprates is the pseudogap in the single particle [2] and particle-hole spectra. A plausible explanation for it involves the effect of finite ranged fluctuating antiferromagnetic or superconducting domains leading to a distribution of local spin gaps [6]. We will show below that there is a different source of pseudogaps arising through nearest neighbor exchange coupling and retardation effects in the presence of strong magnetic fluctuations.

Our approximation scheme, based upon the extended dynamical field theory (EDMFT) [7], see below, neglects most of the longer-range nonlocal aspects of the problem but includes the strong inelastic scattering of electrons from local magnetic fluctuations. By comparing our results to experiments on the cuprates and to numerical results for the *t-J* model, we investigate to what extent features such as the pseudogap, the large entropy, or the Hall effect can be described by a strongly incoherent metal.

Model.—The *t-J* model describes electrons in a tight-binding model subject to (i) the constraint of at most singly occupied lattice sites [effected by projected fermion creation and annihilation operators, $\tilde{c}^+_{i\sigma} = c^+_{i\sigma}(1 - n_{-\sigma})$], and (ii) to an AF spin interaction,

$$H = -\sum_{i,j;\sigma} t_{ij}\tilde{c}^+_{i\sigma}\tilde{c}_{j\sigma} + \frac{1}{2}\sum_{i,j} J_{ij}\vec{S}_i \cdot \vec{S}_j, \qquad (1)$$

where $\vec{S}_i = \frac{1}{2}\sum_{\sigma,\sigma'} \tilde{c}^+_{i\sigma}\vec{\tau}_{\sigma\sigma'}\tilde{c}_{i\sigma'}$ is the spin operator at lattice site i, $\vec{\tau}$ denotes the vector of the Pauli matrices, and t and J couple only nearest neighbors.

As our goal is to describe the high-T incoherent regime, we will neglect most spatial correlations, assuming that the self-energy of the electrons is local, $\Sigma_{\vec{k}}(\omega) = \Sigma(\omega)$. At the same time, we will keep track of all ω dependences as we consider a situation where inelastic scattering is very strong. We therefore use the so-called "dynamical mean field theory" (DMFT) [8,9]. Taken as a purely local approximation, DMFT neglects the intersite J term, an important source for inelastic scattering. To include its effect, we consider the so-called "extended" DMFT (EDMFT) proposed in [7]. This approximation is probably best visualized [9] by selecting a single site, the "impurity," out of the lattice. As we want to neglect spatial correlations, we can treat the surroundings as an

effective medium providing a fluctuating environment which consists both of electrons and bosonic spin fluctuations due to the coupling by t and J, respectively. Local correlation functions can therefore be calculated by solving the following quantum impurity model:

$$H_{\rm imp} = \sum_{\vec{k}\sigma} E_k c^+_{\vec{k}\sigma} c_{\vec{k}\sigma} + V \sum_{\vec{k}\sigma} (c^+_{\vec{k}\sigma} \tilde{d}_\sigma + \text{h.c.}) - \mu n_d + \sum_{\vec{q}} \omega_q \vec{h}^+_{\vec{q}} \cdot \vec{h}_{\vec{q}} + I \sum_{\vec{q}} \vec{S}_d (\vec{h}_{\vec{q}} + \vec{h}^+_{-\vec{q}}). \quad (2)$$

Here $\tilde{d}^+_\sigma$ is a projected fermion creation operator for the impurity orbital, $n_d = \Sigma_\sigma \tilde{d}^+_\sigma \tilde{d}_\sigma$ and $\vec{S}_d = \frac{1}{2} \Sigma_{\sigma,\sigma'} \tilde{d}^+_\sigma \vec{\tau}_{\sigma,\sigma'} \tilde{d}_{\sigma'}$. The (unrestricted) fermion operators $c^+_{\vec{k}\sigma}$ create a fermionic bath, the boson operators $\vec{h}^+_{\vec{q}}$ create a bosonic spin bath (local magnetic field) coupling to the impurity degrees of freedom. The effective medium, characterized by the fermion and boson energies $E_{\vec{k}}$ and $\omega_{\vec{q}}$ has to be determined self-consistently by identifying the single particle Green's function and spin susceptibility of the impurity model with the local Green's function G_{00} and local susceptibility χ_{00} of the lattice model

$$G_{00} = \sum_{\vec{k}} G_{\vec{k}}(i\omega) = \left[i\omega + \mu - \sum_{\vec{k}} \frac{V^2}{i\omega - E_k} - \Sigma(i\omega) \right]^{-1},$$
$$\chi_{00} = \sum_{\vec{q}} \chi_{\vec{q}}(i\omega) = \left[\sum_{\vec{q}} \frac{2I^2 \omega_q}{(i\omega)^2 - \omega_q^2} + \chi^{-1}_{ir}(i\omega) \right]^{-1}. \quad (3)$$

Here we use that within EDMFT the Green's function $G_{\vec{k}}$ and the spin susceptibility $\chi_{\vec{k}}$ have a simple $\vec{k}$ dependence as both the self-energy $\Sigma(i\omega)$ and the irreducible susceptibility $\chi_{ir}(i\omega)$ are taken to be independent of $\vec{k}$

$$G_{\vec{k}\sigma}(i\omega) = \frac{1}{i\omega + \mu - \epsilon_k - \Sigma(i\omega)},$$
$$\chi_{\vec{q}}(i\omega) = \frac{1}{\chi^{-1}_{ir}(i\omega) + J_q},$$

where ϵ_k and J_q are the lattice Fourier transforms of t_{ij} and J_{ij}, respectively. It follows from (3) that only the densities of states $N(\omega) = \Sigma_{\vec{k}} \delta(\omega - E_k)$ and $D(\omega) = \Sigma_{\vec{q}} [\delta(\omega - \omega_q) - \delta(\omega + \omega_q)]$ are needed and E_k and ω_q may be assumed to be isotropic in momentum space. Formally EDMFT is exact in the limit of infinite dimension, $d \to \infty$, if both t and J are scaled proportional to $1/\sqrt{d}$ [7].

The solution of the impurity problem (2) for given $N(\omega)$ and $D(\omega)$ is difficult. Even for the model without the spin boson field $\vec{h}_{\vec{q}}$ (the well-known Anderson impurity model) dynamical properties can only be calculated numerically, e.g., using quantum Monte Carlo, the numerical renormalization group, or resummations of perturbation theory like the noncrossing approximation (NCA) or the conserving T-matrix approximation [10]. Unfortunately, all of these methods except for the resummation of perturbation theory and the quantum Monte Carlo [11] method are not easily generalized to include the spin boson field $\vec{h}_{\vec{q}}$.

We will therefore employ a conserving approximation in which infinite classes of Feynman diagrams are resummed. We are aiming at a level of approximation corresponding to NCA for the usual Anderson model. In order to effect the projection onto the sector of Hilbert space without double occupancy of the local energy level we use a pseudoparticle representation, where the singly occupied state is created by pseudofermion operators f^+_σ, $\sigma = \uparrow, \downarrow$, whereas the empty orbital is created by a boson operator b^+. Since the local level is either empty or singly occupied, the operator constraint $Q = b^+ b + \Sigma_\sigma f^+_\sigma f_\sigma = 1$ has to be satisfied at all times, which can be enforced by adding a term λQ to the Hamiltonian (2) and taking the limit $\lambda \to \infty$. The projected local electron operators in (2) may then be replaced by $\tilde{d}_\sigma = b^+ f_\sigma$, turning the problem into a many-body system of pseudofermions f_σ and slave bosons b, interacting with the fermions $c_{\vec{k}\sigma}$ and bosons $\vec{h}_{\vec{q}}$ of the bath.

It is essential that in any approximation one stays within the physical Hilbert space and does not violate the constraint. Therefore, we employ a "conserving approximation" specified by a generating Luttinger-Ward type functional Φ from which all self-energies and correlation functions are obtained. We employ the simplest conserving approximation by considering only the lowest order diagrams in V and I (see Fig. 1) using that the effective hybridization V and the exchange field I are small compared to the bandwidth $8t$. Within our conserving approximation, both the local Green's function of the physical electron and the local susceptibility can be calculated as a simple convolution of pseudoparticle Green's functions without vertex corrections (Fig. 1).

It is important to note that our approximation scheme does not include the vertex corrections needed to describe

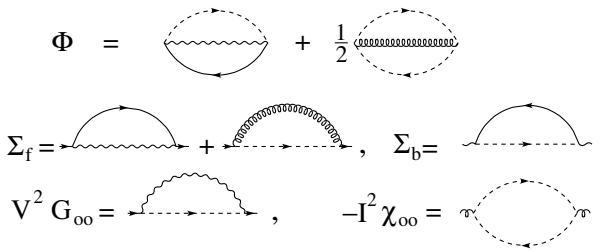

FIG. 1. The two lowest order contributions to the Luttinger-Ward functional Φ and corresponding self-energies. Only diagrams with no line crossings are taken into account (a generalization of NCA). The broken (wavy) line denotes pseudofermion (pseudoboson) Green's function $G_{f\sigma}$ (G_b), and the solid lines represent the conduction electron Green's functions $G_{c\sigma}$, the curly line the correlator $G_{h\alpha}$ of the bosonic bath. Also shown are the self-energies, the local electron Green's function G_{00}, and the local susceptibility χ_{00}.

correctly how the effective interactions with the bosonic and fermionic bath renormalize each other. It therefore cannot be expected to capture correctly the behavior at low T especially close to the quantum critical point where AF order is destroyed by doping [11]. We believe, however, that in the incoherent high-T regime which is the focus of our study it is unlikely that such vertex corrections change the physics qualitatively. On a Bethe lattice, our EDMFT equations surprisingly are identical to those of a t-J model with fully *random* J, as studied within a systematic large M expansion by Parcollet and Georges [12], who did not find any pseudogaps. We believe this to be an artifact of their approximation which uses a Bose-condensed slave boson $\langle b \rangle$ therefore missing the incoherent part of the spectral function. For small doping, the EDMFT equations do not have a solution at lowest T when the magnetic correlation length gets exponentially large. This is *not* an artifact of our diagrammatic approach and has also been observed in [13], where a model equivalent to ours in the case of zero doping has been investigated using quantum Monte Carlo simulations.

Results.—What happens when inelastic scattering is increased by switching on a finite J? The effect is strongest at small doping as shown in the inset of Fig. 2: Spectral weight is pushed below the Fermi energy E_F and a well-pronounced pseudogap of width J opens. At $T = 0.06t$ the pseudogap closes for $\delta \sim 10\%$ as shown in Fig. 2.

It is tempting to compare our results to experiments in the pseudogap phase of the cuprates. One should, however, keep in mind that in the cuprates nonlocal effects do play an important role, as is evident from the momentum dependence of the pseudogap. Furthermore, it is important to stress that we do *not* see a pseudogap in the local susceptibility [while a pronounced gap exists in $\chi_{\mathbf{q}}(\omega)$ for momenta $\mathbf{q}$ away from (π, π)]. However, it is interesting to ask which qualitative features can be understood as a purely local effect. For example, our approximation scheme explicitly *excludes* the possibility that the reduction of the density of states at E_F is created by the adjustment of the electronic wave function to some small magnetic or superconducting domains. The observation that a pseudogap can arise in an incoherent metal with purely *local* correlations is one of the main results of this paper. In our approach, the pseudogap opens when the renormalized chemical potential $\mu - \mathrm{Re}\Sigma(\omega = 0)$ is pushed towards the edge and finally out of the lower Hubbard band [14] by strong magnetic fluctuations: this is possible only in an incoherent metal when $\mathrm{Im}\Sigma$ is sufficiently large.

How does this physics manifest itself in other physical quantities? We calculate the entropy as a crude measure for the relevance of incoherent excitation from the free energy Ω:

$$\Omega/N = \Omega_{\mathrm{imp}} + \frac{1}{\beta}\sum_{i\omega,\sigma}\sum_{\vec{k}} \ln[G_{\vec{k}}(i\omega)/G_{00}(i\omega)] - \frac{1}{2}\frac{1}{\beta}\sum_{i\omega,\alpha}\sum_{\vec{q}} \ln[\chi^{\alpha\alpha}_{\vec{q}}(i\omega)/\chi^{\alpha\alpha}_{00}(i\omega)], \qquad (4)$$

where the impurity contribution in terms of the pseudoparticle spectral functions $A_{f,b}$ is given by $e^{-\beta\Omega_{\mathrm{imp}}} = \int d\omega e^{-\beta\omega}[\sum_\sigma A_{f\sigma}(\omega) + A_b(\omega)]$. The entropy $S = -\partial\Omega/\partial T$ as a function of doping for various T is shown in Fig. 3. First of all, one realizes that it is rather large even at the lowest temperature of $T/t = 0.1$, an indication for strong correlations and a rather incoherent state. The overall magnitude of S compares surprisingly well with both exact diagonalization and experiments in LSCO (see Fig. 3). Furthermore, it follows the general trend that entropy is reduced both for large doping where the system should become more coherent and at low doping where magnetic correlations quench the ln2 entropy of a magnetically disordered Mott insulator (for $J = 0$ the entropy increases for $\delta \to 0$). Interestingly, the drop in entropy

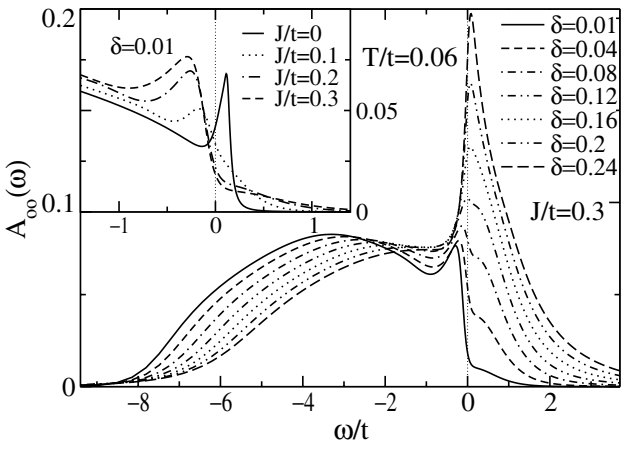

FIG. 2. Local spectral function plotted versus frequency for $T = 0.06t$ and $J/t = 0.3$ for various hole-doping concentrations δ. Inset: Local spectral function for four different $J/t = 0$, 0.1, 0.2, and 0.3 and $T = 0.06t$ for a doping of $\delta = 0.01$. The evolution of a pseudogap of width J is clearly visible.

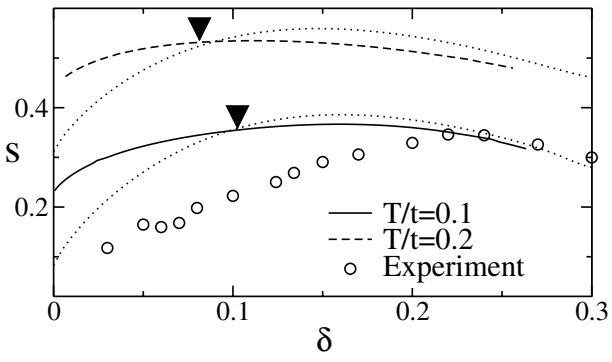

FIG. 3. Entropy as a function of doping for $J = 0.3t$, $T = 0.1t$ and $T = 0.2t$ compared to results from exact diagonalization (dotted lines) [15] and experiments in LSCO [3] at $T \sim 0.07t$. The triangles mark the doping below which a pseudogap starts to open in the spectral function.

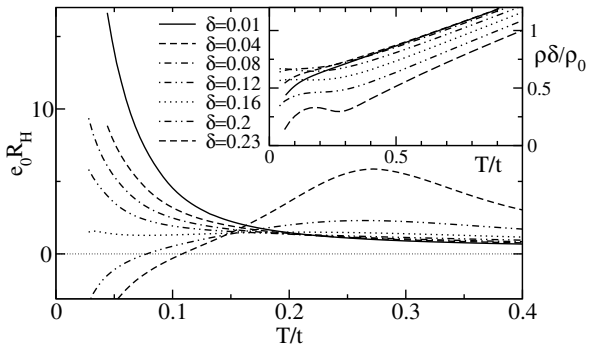

FIG. 4. T dependence of R_H for $J = 0.3t$. For small doping and $T \to 0$, R_H approaches the value $1/(e_0\delta)$ expected for a single hole in a t-J model [5,17]. Inset: T dependence of the resistivity multiplied by doping δ. The linear T behavior for high T flattens for $\delta > 0.1$ for T of the order of J. For $\delta < 0.1$ the resistivity drops in the regime where a pseudogap opens.

towards low doping occurs precisely when the pseudogap starts to open in the spectral function (note that in the experiment both the opening of the pseudogap and the drop in entropy occur at somewhat higher doping).

How is transport affected by the pseudogap? Within EDMFT, there are no vertex corrections to the conductivities σ_{xx} and σ_{xy} which can therefore be directly calculated from the spectral functions [14,16]. In the inset of Fig. 4 the T dependence of the resistivity is shown for various dopings. For high T, ρ depends linearly on T, an effect which is not related to the coupling to the bosonic environment as it is also seen in DMFT [9]. For small doping, the resistivity is proportional to $1/\delta$: only the holes doped into the Mott insulator can transport charge. At the scale of J the resistivity saturates, probably due to the strong inelastic scattering from spin fluctuations. Such a behavior is *not* observed in experiments in the cuprates, possibly an indication that nonlocal effects and vertex corrections are important for transport. Note, however, that in the regime where the pseudogap forms, i.e., for $\delta < 0.1$, the resistivity actually shows a clear drop which is reminiscent of what is seen experimentally [4].

In Fig. 4 the T dependence of the Hall constant R_H is displayed for various dopings. We find a strongly growing positive R_H with decreasing temperature for small dopings and an almost flat variation for moderate δ. In the limit of small δ and low T the universal relation $R_H = \frac{1}{e\delta}$ is approached [5,17], an indication that Luttinger's theorem is not applicable in this incoherent regime which cannot be described by moderately excited Fermi quasiparticles. Note that the rise of R_H towards low T seems to happen when the pseudogap opens – in underdoped cuprates a strong increase of R_H with falling temperature is observed upon entering the pseudogap regime [5] (the drop of R_H close to T_c or a plateau for low T and small δ is not seen in our results). In the absence of the coupling to the bosonic bath, i.e., within DMFT, both the pseudogap [9] and such an upturn [16] are absent.

In conclusion, we have investigated the properties of a highly incoherent metal close to a Mott insulator subject to strong magnetic fluctuation. Even purely local magnetic fluctuations change the physics qualitatively at small doping: they suppress the entropy and induce a pseudogap by driving the chemical potential out of the lower Hubbard band. This leads to an increase of the Hall constant and a drop in the resistivity. These features are reminiscent of the behavior seen in the pseudogap phase of the cuprates. This might indicate that some of the physics in the cuprates could reflect properties of a highly incoherent metal with dominating local fluctuations. An interesting open question is to what extent properties of such an incoherent metal are universal and independent of the details of inelastic scattering mechanisms.

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