Pseudogaps in an Incoherent Metal

K. Haule\textsuperscript{1,2}, A. Rosch\textsuperscript{2,3}, J. Kroha\textsuperscript{2} and P. Wölfle\textsuperscript{2}
\textsuperscript{1}J. Stefan Institute, P.O. Box 3000, 1001 Ljubljana, Slovenia
\textsuperscript{2}Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76128 Karlsruhe, Germany
\textsuperscript{3}Sektion Physik, LMU München, D-80799 München, Germany
(Dated: November 4, 2018)

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 non-crossing 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 and doping levels. The behavior obtained bears surprising similarity to properties of the cuprates.

PACS numbers: 71.30.+h,74.72.-h,71.10.Hf

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 been proven to be extremely successful even in systems where interactions are very strong, e.g. in liquid \textsuperscript{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, pseudo-gaps open, entropy is large and various ordering phenomena appear to compete with each other \cite{1, 2, 3, 4}. 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 \cite{5}. 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 \textit{incoherent} and \textit{local} excitations dominate as it might happen especially at higher temperatures \(T\) 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 nearest neighbor spins. Long range AF order (in 2d possible only at \(T=0\)) 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 quasi-particle excitations. The incoherent character of excitations in the cuprates is clearly seen in the high electrical resistivity, the large relaxation rates for spin and charge, and the large entropy.

Prominent feature of the underdoped cuprates is the pseudogap in the single particle \textsuperscript{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 \textsuperscript{3}. 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) \textsuperscript{4}, see below, neglects most of the longer-range non-local aspects of the problem but include 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 like the pseudogap, the large entropy or the Hall effect can be described by a strongly incoherent metal.

\textbf{Model:} The t-J model describes electrons in a tight-binding model subject to (i) the constraint of most of the longer-range non-local aspects of the problem but include 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 like the pseudogap, the large entropy or the Hall effect can be described by a strongly incoherent metal.

\textbf{Model:} The t-J model describes electrons in a tight-binding model subject to (i) the constraint of most singly occupied lattice sites (effected by projected fermion creation and annihilation operators, \(c_{i\sigma}^+ = c_{i\sigma}^{(1-n_{-\sigma})}\)), and (ii) to an AF spin interaction,

\begin{equation}
H = -\sum_{i,j;\sigma} t_{ij} c_{i\sigma}^+ \tilde{c}_{j\sigma} + \frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j
\end{equation}

where \(\vec{S}_i = \frac{1}{2} \sum_{\sigma,\sigma'} \tilde{c}_{i\sigma}^+ \tau_{\sigma\sigma'} \tilde{c}_{i\sigma'}\) is the spin operator at lattice site \(i\), \(\vec{r}\) denoting 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, \(\Sigma F(\omega) = \Sigma(\omega)\). At the same time, we will keep track of all \(\omega\)-dependences as we consider a situation where inelastic scattering is very strong. We therefore use the so-called “dynamical mean field theory” (DMFT) \textsuperscript{5, 6}. Taken as a purely local approximation, DMFT neglects the intersite \(J\) term,
the impurity orbital, numerically, e.g. using quantum Monte Carlo, the necessity model) dynamical properties can only be calculated due to the coupling by $t$ and $J$, respectively. Local correlation functions can therefore be calculated by solving the following quantum impurity model:

$$H_{\text{imp}} = \sum_{\vec{k} \sigma} E_{\vec{k}} c_{\vec{k} \sigma}^\dagger c_{\vec{k} \sigma} + V \sum_{\vec{k} \sigma} (c_{\vec{k} \sigma}^\dagger \tilde{d}_{\sigma} + h.c.) - \mu n_d + \sum_{\vec{q}} \omega_{\vec{q}} \tilde{h}_q \cdot \tilde{h}_q + I \sum_{\vec{q}} S_d (\tilde{h}_q + \tilde{h}_q^\dagger)$$

(2)

Here $\tilde{d}_{\sigma}$ is a projected fermion creation operator for the impurity orbital, $n_d = \sum_{\vec{k} \sigma} \tilde{d}_{\sigma}^\dagger \tilde{d}_{\sigma}$ and $\tilde{S}_d = \frac{1}{2} \sum_{\vec{k} \sigma} \sum_{\vec{q}} \tilde{d}_{\sigma}^\dagger \tilde{\tau}_{\vec{q}, \sigma} \tilde{d}_{\sigma}$. The (unrestricted) fermion operators $c_{\vec{k} \sigma}^\dagger$ create a fermionic bath, the boson operators $\tilde{h}_q^\dagger$ 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 Greens function and spin susceptibility of the impurity model with the local Greens function $G_{00}$ and local susceptibility $\chi_{00}$ of the lattice model

$$G_{00} = \sum_{\vec{k}} G_{\vec{k}}(i \omega) = \left[ \frac{i \omega + \mu - \sum_{\vec{k}} \frac{V^2}{i \omega - E_{\vec{k}}} - \Sigma(i \omega)}{i \omega - E_{\vec{k}}} \right]^{-1}$$

$$\chi_{00} = \sum_{\vec{q}} \chi_{\vec{q}}(i \omega) = \left[ \sum_{\vec{q}} \frac{2 I^2 \omega_{\vec{q}}}{(i \omega)^2 - \omega_{\vec{q}}^2} + \chi_{ir}^{-1}(i \omega) \right]^{-1}$$

(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 $\vec{k}$

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

where $\epsilon_k$ 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 $N(\omega) = \Sigma_q \delta(\omega - E_q)$ and $D(\omega) = \Sigma_q [\delta(\omega - \omega_q) - \delta(\omega + \omega_q)]$ are needed and $E_k$ and $\omega_q$ 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 $1/\sqrt{d}$.

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 $\tilde{h}_q$ (the well-known Anderson impurity model) dynamical properties can only be calculated numerically, e.g. using quantum Monte Carlo, the numerical renormalization group (NRG), or resummations of perturbation theory like the non-crossing approximation (NCA) or the conserving T-matrix approximation (CTMA) [9]. Unfortunately, all of these methods except for the resummation of perturbation theory and the quantum Monte Carlo method are not easily generalized to include the spin boson field $\tilde{h}_q$.

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 pseudo-particle representation, where the singly occupied state is created by pseudo-fermion (pseudo-boson) 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 $G_{h \sigma}$ of the bosonic bath. Also shown are the self-energies, the local electron Green’s function $G_{00}$ and the local susceptibility $\chi_{00}$.

![FIG. 1: The two lowest order contributions to the Luttinger-Ward functional $\Phi$ and corresponding self-energies. Only diagrams with no line-crossings are taken into account (a generalization of NCA). The broken (wavy) line denotes pseudo fermion (pseudo-boson) 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 $G_{h \sigma}$ of the bosonic bath. Also shown are the self-energies, the local electron Green’s function $G_{00}$ and the local susceptibility $\chi_{00}$.](image-url)
be calculated as a simple convolution of pseudo-particle 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 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 $T/T_c$. 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 [11], who did not find any pseudogaps. We believe this to be an artifact of their approximation 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 wavefunction 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 $\mu - \text{Re}\Sigma(\omega = 0)$ is pushed towards the edge and finally out of the lower Hubbard band [12] by strong magnetic fluctuations: this is only possible in an incoherent metal when $\text{Im}\Sigma$ 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 $\Omega$:

$$\Omega/N = \Omega_{\text{imp}} + \frac{1}{\beta} \sum_{i,\omega, \sigma} \sum_{\vec{q}} \ln \frac{G_{\vec{k}}(i\omega)/G_{00}(i\omega)}{\chi_{\vec{q}}^\sigma(\omega)/\chi_{00}^\sigma(\omega)}$$

$$-\frac{1}{2} \sum_{i,\omega, \sigma} \sum_{\vec{q}} \ln \left( \chi_{\vec{q}}^{\sigma}(\omega)/\chi_{00}^{\sigma}(\omega) \right)$$

where the impurity contribution in terms of the pseudoparticle spectral functions $A_{\sigma,b}$ is given by $e^{-\beta\Omega_{\text{imp}}} = \int d\omega e^{-\beta\omega} \left[ \sum_\sigma A_{\sigma,\sigma}(\omega) + A_{\sigma,\bar{\sigma}}(\omega) \right]$. 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 fluctuations quench the $\ln 2$ entropy of a magnetically disordered Mott insulator (for $J=0$ the entropy increases for $\delta \to 0$). Interestingly, the drop in entropy

**FIG. 2:** The local spectral function plotted versus frequency for $T = 0.06t$ and $J/t = 0.3$ for various hole-doping concentrations $\delta$. Inset: The 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) [12] 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.
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 higher doping).

How is transport affected by the pseudogap? Within EDMFT, there are no vertex corrections to the conductivities $\sigma_{xx}$ and $\sigma_{xy}$ which can therefore be directly calculated from the spectral functions $\sigma_{xx}$ and $\sigma_{xy}$ [14]. In the inset of Fig. 3 the $T$-dependence of the resistivity is shown for various dopings. For high $T$, $\rho$ depends linearly on $T$, an effect which is not related to the coupling to the bosonic environment as it is also seen in DMFT [8]. For small doping, the resistivity is proportional to $1/T$; only the holes doped into the Mott insulator can transport charge. At the scale of $T$ 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 non-local 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 [1].

In Fig. 3 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 dopings. In the limit of small doping and low $T$ the universal relation $R_H = \frac{1}{12}\pi^2 \frac{H}{R} T^2$ is approached [1], 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 in the regime where the pseudogap opens – in underdoped cuprates a strong increase of $R_H$ with falling temperature is observed upon entering the pseudogap regime [8] (the drop of $R_H$ close to $T_c$ is obviously not included in our theory). In the absence of the coupling to the bosonic bath, i.e. within DMFT, both the pseudogap [8] and such an upturn [14] are absent.

In conclusion, we have investigated the properties of a highly incoherent metal close to a Mott insulator subject to strong magnetic fluctuations. 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.

We acknowledge helpful discussions with E. Abrahams, J. Bonča, A. Georges, G. Kotliar, O. Parcollet, Q. Si and especially P. Prelovšek. Part of this work was supported by the Ministry of Education, Science and Sport of Slovenia, FERLIN (K.H.) and the Emmy-Noether program of the Deutsche Forschungsgemeinschaft (A.R.).

---

[1] P.W. Anderson, *The Theory of Superconductivity in High Tc Cuprates* (Princeton University Press, Princeton, 1997).
[2] A. Ino *et al.*, Phys. Rev. B 65, 094504 (2002); J.C. Campuzano, *et al.* Physica B 259-261, 517 (1999).
[3] J. W. Loram *et al.*, J. of Phys. and Chem. of Solids 59, 2091 (1998); J.R. Cooper and J.W. Loram, J. Phys. I France 6, 2237 (1996).
[4] T. Timusk and B. Statt, Phys. Rep. 62, 61 (1998); J.R. Cooper and J.W. Loram, J. Phys. I France 6, 2237 (1996).
[5] A. Rosch, Phys. Rev. B 64, 174407 (2001) and references therein.
[6] Q. Si and J.L. Smith, Phys. Rev. Lett. 77, 3391 (1996); H. Kajuter, PhD thesis, Rutgers University (1996); J.L. Smith and Q. Si, Phys. Rev. B 61, 5184 (2000).
[7] W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).
[8] A. Georges, G. Kotliar, W. Krauth, and M.J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996).
[9] T. A. Costi, J. Kroha, and P. Wölfle, Phys. Rev. B 53, 1850 (1996); J. Kroha and P. Wölfle, cond-mat/0105491.
[10] Q. Si, S. Rabello, K. Ingersent, and J. L. Smith, Nature 413, 804 (2001).
[11] O. Parcollet and A. Georges, Phys. Rev. B 59, 5341 (1999); S. Sachdev and J. Ye, Phys. Rev. Lett. 70, 3339 (1993).
[12] K. Haule, PhD thesis, (2002).
[13] J. Jaklic and P. Prelovšek, Phys. Rev. Lett. 77, 892 (1996).
[14] P. Prelovšek, Phys. Rev. B 55, 9219 (1997).
[15] E. Lange and G. Kotliar, Phys. Rev. B 59, 1800 (1999).