Pseudogaps in the incoherent metal phase of hole doped Mott insulators

P. Wölfle,
Universität Karlsruhe

Collaborators:  K. Haule, Rutgers University
               A.Rosch, Universität Köln
               J. Kroha, Universität Bonn
• Concept of an incoherent metal

• Extended dynamical mean –field theory (EDMFT) of the t-J model

• Novel mechanism of pseudogap formation close to a Mott insulator
Motivation

Physics of the cuprates

• strong fluctuations of spin, charge (stripes), Cooper-pairs, ...

• quasi particle description possible? strongly modified Fermi liquid or novel quasiparticles, e.g. spin-charge separation?

• alternative: no quasi particles, highly incoherent excitations?

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Describing incoherent excitations

- dominating inelastic processes $\rightarrow \omega$ dependence essential

- momentum-dependence less important
  $\rightarrow$ dynamical mean field theory (DMFT)

- source of incoherence: scattering from collective fluctuations
  $\rightarrow$ extended DMFT

$\Sigma(k, \omega) \sim \Sigma(\omega)$
Methods: EDMFT

Extended dynamical mean field theory (EDMFT)
Si, Smith (1996), Kajuter (1996)

t-J model: 
\[ H = - \sum_{\langle i,j \rangle, \sigma} (t_{ij} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + H.c.) + \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

- electrons hop only on empty site, no double occupancy: \( t_{ij} \)
- spins exchange-coupled to n.n. spins: \( J_{ij} \)
- neglect all momentum dependence \( \leftrightarrow \) map onto effective impurity model (exact in limit \( d \Rightarrow \infty \))

- select arbitrary site
- treat rest as bath
- electrons hop from bath to impurity \( \rightarrow \) fermionic bath (DMFT)
- exchange coupling of local spin to neighboring spins \( \rightarrow \) bosonic bath (EDMFT)
  - fluctuating magnetic field
Methods: Selfconsistent impurity model

\[ H_{\text{BDMFT}} = \sum_{k,\sigma} E_k c_{k\sigma}^+ c_{k\sigma} + V \sum_{k,\sigma} (c_{k\sigma}^+ d_{\sigma} + \text{h.c.}) - \mu n_d + \sum_q \omega_q h_q^+ \cdot h_q + I \sum_q S_d \cdot (h_q + h_q^+) \]

Fermionic bath

\[ G_{\text{bath}}(i\omega) = \sum_k \frac{1}{i\omega - E_k} \]

Bosonic bath

\[ G_h(i\omega) = \sum_q \frac{2\omega_q}{(i\omega)^2 - (\omega_q)^2} \]

Selfconsistency condition

\[ G_{\text{imp},\sigma}(i\omega) = -\int d\tau e^{i\omega \tau} \langle T_\tau d_\sigma(\tau) d_\sigma^+(0) \rangle = G_{\text{loc},\sigma}(i\omega) = \sum_k G_{k,\sigma}(i\omega) \]

\[ \chi_{\text{imp},\alpha}(i\omega) = \int d\tau e^{i\omega \tau} \langle T_\tau S_\alpha(\tau) S_\alpha(0) \rangle = \chi_{\text{loc},\alpha}(i\omega) = \sum_q \chi_{q,\alpha}(i\omega) \]

\[ G_{k,\sigma}(i\omega) = \frac{1}{i\omega + \mu - \epsilon_k - \Sigma_{\sigma}(i\omega)} \]

\[ \chi_{q,\alpha}(i\omega) = \frac{1}{J_q + M_\alpha(i\omega)} \]

\[ V^2 G_{\text{bath}}(i\omega) = i\omega + \mu - G_{\text{imp},\sigma}^{-1}(i\omega) - \Sigma(i\omega) \]

\[ I^2 G_h,\alpha(i\omega) = M_\alpha(i\omega) - \chi_{\text{imp},\alpha}^{-1}(i\omega) \]

\[ \epsilon_k, J_q : \text{n.n. hopping/exchange c. on square lattice} \]
Methods: Generalized NCA

• Solving impurity problem by conserving diagrammatic method

• Pseudoparticle representation: \( d_\sigma = b^+ f_\sigma \), \( b^+ b + \sum f^+_\sigma f_\sigma = 1 \)

• Generating functional \( \Phi \)

\[
\Phi = \Phi_0 + \frac{1}{2} \Phi_2
\]

\[
\Sigma_f = \Sigma_f^0 + \Sigma_f^1, \quad \Sigma_b = \Sigma_b^0 + \Sigma_b^1
\]

\[
V^2 G_{\text{loc}} = V^2 G_{\text{loc}}^0 + V^2 G_{\text{loc}}^1, \quad -\Gamma^2 \chi_{\text{loc}} = -\Gamma^2 \chi_{\text{loc}}^0
\]

Fermion bubble is zero in the paramagnetic state

Here: only paramagnetic phase
Results: Local spectral function (J dependence)

- small hole doping $\delta = 1\%$
- $J = 0$ (DMFT) no pseudogap
- increasing $J$: pseudogap develops
- width of pseudogap: $J$ (for $J > T \ln[1/\delta]$)
Results: Local spectral function (doping dep.)

Doping dependence:
- Pseudogap starts to open at $\delta < 10\%$
- Result weakly dependent on bare DOS, 2d/3d...
Results: Spectral function $A(k, \omega)$ \(\delta=0.20\)

White lines correspond to noninteracting system
Results: Spectral function $A(k, \omega)$ \( \delta=0.10 \)

White lines corresponds to noninteracting system
Results: Spectral function $A(k, \omega) \delta=0.02$

White lines corresponds to noninteracting system

$T=0.06t$

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Results: Violation of Luttinger’s theorem

Incoherent Metal

- **incoherent** metal: Luttinger’s theorem strongly violated
- chemical potential moves **inside** Mott gap
- holes virtually in Mott gap → pseudogap
- pseudogap: **incoherent** metal close to Mott insulator
Results: Spin excitation spectrum

Susceptibility

no pseudogap in local susceptibility

but: gap at typical $q$-vectors
no gap, very large peak at $(\pi, \pi)$
Methods: Extended Dynamical Cluster Approximation

\[ G^{-1}_{0}(\pi,0) \]

\[ \chi^{-1}_{0}(\pi,\pi) \]

\[ \chi^{-1}_{0}(0,0) \]

\[ \chi^{-1}_{0}(0,\pi) \]

\[ G_{loc} = \sum_{K} \sum_{k \in K} \frac{1}{\omega + \mu - \epsilon_k - \Sigma_K} \]

\[ \chi_{loc} = \sum_{Q} \sum_{q \in Q} \frac{1}{M_Q + J_q} \]

\[ G_{K} = \sum_{k \in K} \frac{1}{\omega + \mu - \epsilon_k - \Sigma_K} = \frac{1}{\omega + \mu - \langle \epsilon_k \rangle_K - \Sigma_K - \Delta_K} \]

\[ \chi_{Q} = \sum_{q \in Q} \frac{1}{M_Q + J_q} = \frac{1}{M_Q + \langle J_q \rangle_Q - \chi^{-1}_{0}Q} \]
Results: Excitation spectra in cluster approx.

Extended dynamical cluster approximation (2x2 cluster)

(work in progress)

$A_{loc}(\omega)$ in EDCA

Local susceptibility in EDCA

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Extended dynamical cluster approximation (2x2 cluster)

Results: Local spectral functions

\[ T/t = 0.12 \]
\[ J/t = 0.3 \]
Results: Comparison of local spectral functions

- EDMFT
- EDCA 4 sites
- ED 16 sites

$c_h \sim 0.06$

$T/t = 0.15$

$c_h \sim 0.12$

$T/t = 0.1$

$c_h \sim 0.18$

$c_h \sim 0.24$
Results: $k$-dependent spectral functions

Extended dynamical cluster approximation (2x2 cluster)

\[
\begin{align*}
A_{(0,0)}(\omega) \\
A_{(0,\pi)}(\omega) \\
A_{(\pi,\pi)}(\omega)
\end{align*}
\]

$\delta=0.05$
$T=0.12$
$I=0.3$
Results: k-dependent spectral functions

Extended dynamical cluster approximation (2x2 cluster)

\[ T/t = 0.12 \]

\[ \delta = 0.01 \]
Results: k-dependent selfenergy

Extended dynamical cluster approximation (2x2 cluster)
Results: Fermi surfaces

Extended dynamical cluster approximation (2x2 cluster)
Results: Local spin excitation spectra

Extended dynamical cluster approximation (2x2 cluster)

(work in progress)

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Results: Local spin excitation spectrum

Extended dynamical cluster approximation (2x2 cluster)
Results: Spin excitation spectrum at $q=(\pi,0)$

Extended dynamical cluster approximation (2x2 cluster)
Results: Static susceptibility from EDMFT and EDCA
Results: Resistivity and Hall effect

- resistivity $\rho(T) \sim 1/\delta$
- $\rho(T)$ drops when pseudogap opens
- saturation for larger doping?
- Hall constant $R_H$ rises sharply when pseudogap opens
- for $\delta \to 0$, $T \to 0$ universal value of Hall constant $R_H = 1/(e\delta)$
  exact for single hole in t-J model (Prelovšek, 1996)
Results: Electrical resistivity

Extended dynamical cluster approximation (2x2 cluster)
Results: Resistivity and Hall effect

Results: Entropy

![Graph showing results for EDMFT+NCA and ED 20 sites comparison with experimental data.](image)

- EDMFT+NCA
- ED 20 sites

Exact diagon.:
Jaklič & Prelovšek, 1995
Experiment: LSCO (T/t~0.07)
Cooper & Loram
Results: Instability of EDMFT solution in $d=2$

Critical magnetic fluctuations at low $T$ drive solution onto unphysical sheet:

Flat DOS of exchange couplings $N_J(\varepsilon) = (1/8J), \ |\varepsilon| < 4J$

$\chi_{\text{loc}}(\omega) = (1/8J) \ln\{|4J+M(\omega)|/|4J-M(\omega)|\} = \chi' + i \chi''$

Inverting this relation

$M = 4J \ (v+1)/(v-1), \ \text{where} \ v = \exp(8J \chi) = v' + iv''$

The imaginary part of $v$, $v'' = \exp(8J \chi') \sin(8J \chi'')$, will change sign if $8J \chi'' > \pi$. Since $\chi''$ grows with decreasing $T$:

Violation of causality at $T < T_{\text{inst}}$

This instability will be shifted to lower $T$ in a cluster approximation
Conclusions

- incoherent metal regime described by EDMFT
- pseudogaps in incoherent metal close to Mott insulator phase
- robust result, weakly dep. on approx., band structure, scatt. mech.
- local theory: most mechanisms for pseudogap excluded by construction
- some features reminiscent of cuprates

Does a universal incoherent phase exist?

Open questions:
- Analytical model?
- Low temperatures (cluster EDMFT)?
- Superconductivity? (Maier, 2003)
- Charge/spin order?

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