Nodal/Anti-nodal Dichotomy and the Energy-Gaps of a doped Mott Insulator

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OUTLINE

H-Tc Superconductors:

- Strongly correlated many-body physics
- DMFT
- Fundamental anisotropic properties
- DMFT not enough!

2D Hubbard Model:

- Normal state - Mott transition
- d-wave SC state
- Nodal/antinodal dichotomy
- Two nodal/antinodal energy-scales
H-Tc Superconductors Materials
1986 Bednorz and Muller

Reservoir: La, Sr

2D physics!

Simple theoretical Hubbard Model

\[ H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^+ c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]
Strongly Correlated Mott Physics

\[ H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^+ c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

**Kinetic term**

**Local repulsion**

\[ \varepsilon_k \]

\[ \varepsilon_F \]

\[ U \]
Why Dynamics so important?

e.g. Density of states- Halfilling-
vary interaction $U$

HOW?

Density of States $A(\omega)$

Competition

High-low energy physics!
**Dynamical Mean Field Theory**

For a review: A. Georges et al. Rev. Mod. Phys. 68, 13 1996

\[ \Sigma(i\omega_n) = G_0(i\omega_n)^{-1} - G[\Sigma](i\omega_n)^{-1} \]

- non-interacting
- interacting
Remarks DMFT:

DMFT is exact for Dimension $= \infty$:

i) Mapping to Impurity model exact

ii) Local Self-energy $\Sigma \neq \Sigma(k)$

exact self-consistency condition

BUT

What if $\Sigma$ is $k$ dependent? (finite Dimension)
Experimental Evidence: ARPES


Quasiparticle! Quasiparticle Peak

Simple FL breaks!
**ARPES in the first quadrant of BZ**

\[ A(k, \omega \to 0) = -\frac{1}{\pi} G(k, \omega \to 0) \]

- **Hole doped**
  - (0,0) \( x = 0.05 \)
  - (\pi,\pi) \( x = 0.10 \)

- **e\(^-\) doped**
  - (0,\pi) \( x = 0.10 \)
  - (\pi,\pi) \( x = 0.05 \)

*ARPES: Armitage, Damacelli, Z. Shen, K. Shen, Hussain, Campuzano, Norman, Randeira

**K-dependent Properties**
- Local correlations needed

**Quasiparticle Peak**

**DMFT Not Enough!**
Describing K-dependence is a fundamental ingredient.

Can we improve a LOCAL DMFT?
**Cellular Dynamical Mean Field Theory**


Lattice $\rightarrow$ Superlattice

Cluster Impurity

Self consistency

$$\Sigma_{\mu\nu\sigma}(\omega_n) = G_{\mu\nu\sigma}^{-1}(\omega_n) - G_{\mu\nu\sigma}^{-1}(\omega_n, \Sigma)$$
Remarks CDMFT:

Good:
$$\Sigma = \Sigma(k)$$  →  Real Systems
D finite

Price:

i) Mapping to Impurity Model not exact
ii) Self-energy $\Sigma(k)$ approx.
OUTLINE

H-Tc Superconductors:
Strongly correlated many-body physics $\rightarrow$ DMFT
fundamental anisotropic properties $\rightarrow$ DMFT not enough!

DMFT $\rightarrow$ Cellular -DMFT

2D Hubbard Model:
- Normal state- Mott transition
- d-wave SC state
- nodal/antinodal dichotomy
- two nodal/antinodal energy-scales
2D Hubbard Model with next-nearest neighbor hopping $t'$

Impurity considered:

- CMFT output few parameters:
  - Cluster self-energy $\Sigma_{11}, \Sigma_{12}, \Sigma_{13}$
  - $\Sigma_{\text{ano}} \rightarrow < c_1^\uparrow c_2^\downarrow >$

- Preserve square lattice symmetries

- Allows to describe d-wave superconductor broken symmetry
EigenValues of the cluster $\text{Im}\Sigma_{\mu\nu}$

- **h-doped**
  - $t' = -0.3 \, t$
  - $t' = +0.3 \, t$

- **e-doped**

Eigenvalues:

$$\Sigma_A = \Sigma_{11} - \Sigma_{13}$$

$$\Sigma_B = \Sigma_{11} - 2\Sigma_{12} + \Sigma_{13}$$

$$\Sigma_C = \Sigma_{11} + 2\Sigma_{12} + \Sigma_{13}$$

Graphs showing $\text{Im}\Sigma_A$, $\text{Im}\Sigma_B$, and $\text{Im}\Sigma_C$ for different doping levels.
All information in the Green’s function

$$G(k, \omega) = \frac{1}{\omega - \varepsilon_k - \Sigma_k}$$

$$\varepsilon_k = -t (\cos k_x + \cos k_y) - t' \cos k_x \cos k_y - \mu$$

Extracting $k$-dependence ---- for example $\Sigma_k$

$$\Sigma_k = \Sigma_{11} + \frac{1}{2} \Sigma_{12} (\cos k_x + \cos k_y) + \frac{1}{4} \Sigma_{13} \cos k_x \cos k_y$$
Mott transition in the Normal State: hot/cold Spots

\[ A(k, \omega \rightarrow 0) = -\frac{1}{\pi} G(k, \omega) \]

Experiments

- **hole doped**
  - (a) \( x = 0.05 \)
  - (b) \( x = 0.10 \)

- **e- doped**
  - (a) \( x = 0.04 \)
  - (b) \( x = 0.10 \)

Theory

- **hole doped**
  - (a) \( (\pi, 0) \)
  - (b) \( (\pi, \pi) \)

- **e- doped**
  - (a) \( (0, 0) \)
  - (b) \( (\pi, 0) \)
How do we extract k-quantities?

CDMFT cluster-local theory

USE most local quantities to extract k-quantities!

Truncated Fourier Expansion

\[ \Sigma_k = \Sigma_{11} + \frac{1}{2} \Sigma_{12} (\cos k_x + \cos k_y) + \frac{1}{4} \Sigma_{13} \cos k_x \cos k_y \]
1) candidate \[ \Sigma \]

\[
\Sigma_k = \Sigma_{11} + \frac{1}{2} \Sigma_{12} (\cos k_x + \cos k_y) + \frac{1}{4} \Sigma_{13} \cos k_x \cos k_y
\]

2) candidate \[ M \]

cluster \[
\hat{M} = \frac{1}{(\omega + \mu)1 - \hat{\Sigma}}
\]

lattice \[
M_k = \frac{1}{\omega + \mu - \Sigma_k}
\]

\[
M_k = M_{11} + \frac{1}{2} M_{12} (\cos k_x + \cos k_y) + \frac{1}{4} M_{13} \cos k_x \cos k_y
\]

T. Stanescu and G. Kotliar, Phys. Rev. B 74, p.125110
QMC TEST ON 1D CHAIN
courtesy of B. Kyung

24 sites!
TEST: insulating state 2D

\[ M_k = M_{11} + \frac{1}{2} M_{12} (\cos k_x + \cos k_y) + \frac{1}{4} M_{13} \cos k_x \cos k_y \]

\[ \Sigma_k = \Sigma_{11} + \frac{1}{2} \Sigma_{12} (\cos k_x + \cos k_y) + \frac{1}{4} \Sigma_{13} \cos k_x \cos k_y \]

\[ G_{11}(\omega) = \sum_k G(k, \omega) \]

\[ \text{INSULATOR} \]

States In the Mott gap!
Normal state at small doping

5% doping

M works better!
CONSEQUENCE IS A
PSEUDO-GAP STATE!
The figure illustrates the pseudogap phenomenon in a material, with points A, B, and C indicating different experimental observations.

**Pseudogap**

\[ \delta = 0.05t \sim 0.015 \text{ eV} \]

- **T. Stanescu et al.**

- **T. Stanescu and G. Kotliar**
  *Phys. Rev. B 74, p.125110*

- **A(k,\omega)**
  *Phys. Rev. Lett. 76, 4841 (1996)*
Simple case: 2D Hubbard Model

$t' = 0$

High doping

\[ A(\omega) \]

\[ \omega \]

Insulator

\[ A(\omega) \]

\[ \omega \]

\[
H = -t \sum_{<ij>,\sigma} (c_{i\sigma}^+ c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]
Line of $G(k,0+) = 0$ at half-filling

T. Stanescu et al. cond-mat/0602280

$A(\omega)$

$\omega$

$\Delta$

$-\Delta$

$\text{Re} G(k,0) = 0$ at half-filling

$A(k,\omega)$ is even

Half-filling $n_{\text{holes}} = 1 - n_{e-} = 1/2$ + particle/hole symmetry

$$A(k,\omega) = A(\pi-k,-\omega)$$
Natural continuity into a doped Mott insulator

G(k,0⁺) = 0!

Coexistence of poles and zeroes
BROKEN FS IN A(k,0)

FS Poles in G(k,0⁺)

Topol. FS transit.
OUTLINE

H-Tc Superconductors:

- Strongly correlated many-body physics \( \Rightarrow \) DMFT
- Fundamental anisotropic properties \( \text{DMFT not enough} \)

\[ \text{DMFT} \quad \rightarrow \quad \text{Cellular – DMFT} \]

2D Hubbard Model:

- Normal component - Mott transition
- \text{d-wave} SC state
- Nodal/antinodal dichotomy
- Two nodal/antinodal energy-scales
d-wave SC with CDMFT

Kancharla et al. cond-mat/0508205

AIM with d-wave SC bath

\[
H_{\text{imp}} = \sum_{\mu\nu\sigma} E_{\mu\nu\sigma} c_{\mu\sigma}^\dagger c_{\nu\sigma} + \sum_{m\sigma} \epsilon_m^\alpha a_{m\sigma}^\dagger a_{m\sigma}^\alpha \\
+ \sum_{m\mu\sigma} V_m^\alpha a_{m\mu\sigma}^\dagger (c_{\mu\sigma} + \text{h.c.}) + U \sum_{\mu} n_{\mu\uparrow} n_{\mu\downarrow} \\
+ \sum_{\alpha} \Delta^\alpha (a_{1\uparrow}^\alpha a_{2\downarrow}^\alpha - a_{2\uparrow}^\alpha a_{3\downarrow}^\alpha + a_{3\uparrow}^\alpha a_{4\downarrow}^\alpha - a_{4\uparrow}^\alpha a_{1\downarrow}^\alpha \\
+ a_{2\uparrow}^\alpha a_{1\downarrow}^\alpha - a_{3\uparrow}^\alpha a_{2\downarrow}^\alpha + a_{4\uparrow}^\alpha a_{3\downarrow}^\alpha - a_{1\uparrow}^\alpha a_{4\downarrow}^\alpha + \text{h.c.}).
\]

\[
F_{\mu\nu} \equiv -T \langle c_{\mu\downarrow}(\tau)c_{\nu\uparrow}(0) \rangle
\]

Self-consistency

\[
\hat{G}_c(\tau, \tau') = \begin{pmatrix}
\hat{G}_{\uparrow}(\tau, \tau') & \hat{F}(\tau, \tau') \\
\hat{F}^\dagger(\tau, \tau') & -\hat{G}_{\downarrow}(\tau', \tau)
\end{pmatrix}
\]
d-wave SC state supported!

\[ \text{dSc non-zero } P_d = \langle c^\uparrow c^\downarrow \rangle \text{ in the 2D Hubbard Model} \]

S.S. Kancharla et al, cond-mat/0508205
M. Civelli et al. cond-mat/0704.1486v1

Anomalous \( \Sigma_{\text{ano}} \neq 0 \), low energy non-momotonic in doping \( \delta \)

Very important!
Σ cluster-Eigenvalues

superconducting

normal

\[ \Sigma \]

\[ \text{Im} \Sigma \to 0 \]

Fermi Liquid
Superconducting Green’s function
Nambu’s notation

\[ G^{-1}_{k\sigma}(\omega) = \begin{pmatrix} \omega - \varepsilon_k - \Sigma_{\sigma}^{\text{nor}}(k, \omega) & -\Sigma_{\sigma}^{\text{ano}}(k, \omega) \\ \Sigma_{\sigma}^{\text{ano}}(k, \omega) & \omega + \varepsilon_k + \Sigma_{\sigma}^{\text{nor}}(k, -\omega)^* \end{pmatrix} \]

quasi-particle particle band

\[ \varepsilon_k = -t(\cos k_x + \cos k_y) - t' \cos k_x \cos k_y - \mu \]
Periodization procedure

Normal component set $\sum_{\text{ano}} = 0$

$$G_{11}(\omega) = \sum_k G(k, \omega)$$

5% doping

Better M
Periodization procedure $\Sigma_{\text{ano}} \neq 0$

Superconducting component

$$\text{Im} G^{11}_{\sigma}(k, \omega) \approx \mathcal{Z}_{\text{nod}} \delta \left( \omega - \sqrt{v^2_{\text{nod}} k^2_{\perp} + v^2_{\Delta} k^2_{\parallel}} \right)$$

Only the nodal point is gapless

$$N(\omega) = -\frac{1}{\pi} \sum_k \text{Im} G^{11}_{\sigma}(k, \omega) \sim \frac{1}{\pi} \frac{\mathcal{Z}_{\text{nod}}}{v_{\text{nod}} v_{\Delta}} \omega$$

Spectrum Linearized!

Sum selects Nodal area only

Better $\Sigma$!
Periodizing recipe:

- **Nodal point** → periodize $\Sigma$

  $\iff$ In particular d-wave gap

  \[ \Sigma^{\text{ano}}(k, \omega) = \Sigma^{\text{ano}}_{12}(\omega) (\cos k_x - \cos k_y) \]

- **Anti-nodal point** → periodize $M$

  as in the normal state case
EXPERIMENTS: ARPES SPECTRA

\[
A(\omega) = -\frac{1}{\pi} \text{Im} G^{11}_\sigma(k, \omega)
\]

Optimal doping

\[\text{doping} \quad \downarrow\]

\[\text{Tc} = 50 \text{K} \quad \text{Tc} = 40 \text{K} \quad \text{Tc} = 30 \text{K}\]
Question: one or two energy-gaps?


See e.g. discussion Science Dec 2006
Quasi-particle Spectra CDMFT

\[ \Sigma_{\text{ano}} = 0 \]

pseudo-gap!

\[ \Sigma_{\text{ano}} \neq 0 \]

asymmetry
At the node I have a quasiparticle

\[ G_{k\sigma}^{-1}(\omega) = \left( \begin{array}{cc} \omega - \varepsilon_k - \Sigma_{\sigma}^{\text{nor}}(k, \omega) & -\Sigma_{\text{ano}}^{\alpha}(k, \omega) \\ -\Sigma_{\text{ano}}^{\alpha}(k, \omega) & \omega + \varepsilon_k + \Sigma_{\sigma}^{\text{nor}}(k, -\omega)^* \end{array} \right) \]

We can attempt a standard Fermi-Liquid Expansion at low energy

\[ \xi_k^0 \equiv \varepsilon_k + \text{Re}\Sigma_{\sigma}^{\text{nor}}(k, 0) \]

\[ Z_{\text{nod}} = (1 - \partial_\omega \text{Re}\Sigma_k(\omega))^{-1} \bigg|_{\omega=0} \]

\[ v_{\text{nod}} = Z_{\text{nod}} |\nabla_k \xi_k^0| \]

\[ v_\Delta = Z_{\text{nod}} |\nabla_k \Sigma_{\text{ano}}^{\alpha}(k)| \]
Nodal velocities - standard Fermi Liquid Analysis

\[ \xi_0 \equiv \varepsilon_k + \text{Re}\Sigma^{nor}(k, 0) \]
\[ Z_{nod} = \left| 1 - \delta \omega \text{Re}\Sigma_k(\omega) \right|^{-1}_{\omega=0} \]
\[ v_{nod} = Z_{nod} |\nabla_k \xi_0| \]
\[ v_\Delta = Z_{nod} |\nabla_k \Sigma^{ano}(k)| \]

Local density of states

\[ \text{Im} G^{11}_{\sigma}(k, \omega) \approx Z_{n_{od}} \delta \left( \omega - \sqrt{v_{n_{od}}^2 k_{\perp}^2 + v_{\Delta}^2 k_{\parallel}^2} \right) \]

\[ N(\omega) = -\frac{1}{\pi} \sum_k \text{Im} G^{11}_{\sigma}(k, \omega) \sim \frac{1}{\pi v_{n_{od}} v_{\Delta}} \omega \]

2 ENERGY GAPS!

From quasi-particle spectra we measure gaps!

Anti Nodal GAP

PHOTOEMISSION EXP

Nodal GAP

Anti Nodal GAP

Nodal GAP

pseudo GAP

CONCLUSIONS

◊ Used **Cellular DMFT** to study the strongly correlated many body systems:

**H-Tc Superconductor materials**

◊ **2D Hubbard Model**, **Nomal State**
  a “mottness” region at small doping: PG, arcs FS

◊ **Anomalous d-wave SC state**
  - notal/antinodal dichotomy
  - 2 energy-gaps!: PG+ superconducting gap
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