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

arXiv:0704.1486v1 [cond-mat.str-el]

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**Collaborators:**

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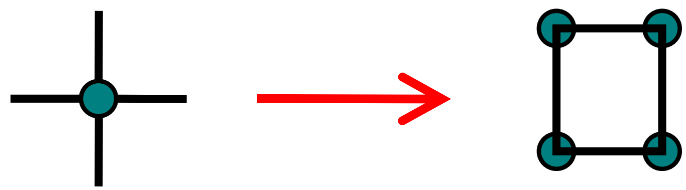
# OUTLINE

⇨ **H-Tc Superconductors**:

**Strongly correlated many-body physics** ⇨ **DMFT**

*fundamental anisotropic properties DMFT not enough !*

**DMFT**



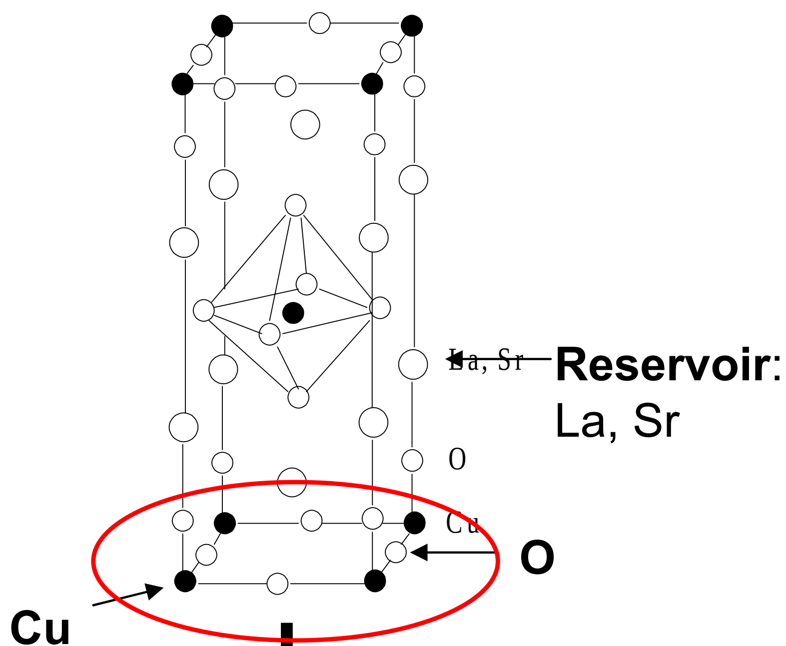
**C**ellular –**DMFT**

**2D Hubbard Model**:

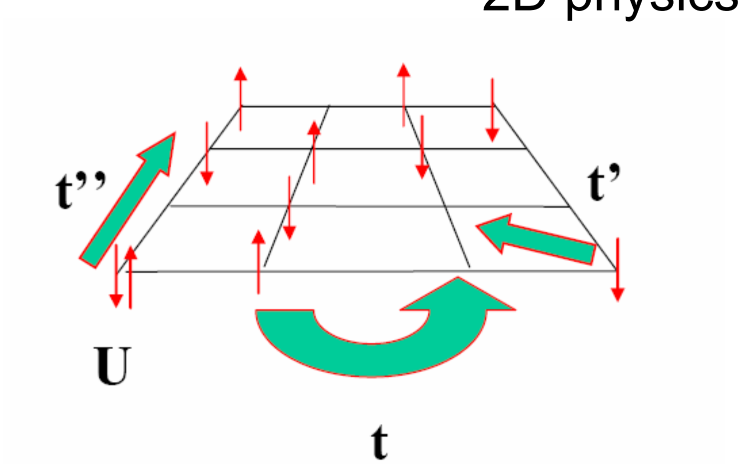
⇨
- **Normal state- Mott transition**
- **d-wave SC state**
- **nodal/antinodal dichotomy**
- **two nodal/antinodal energy-scales**

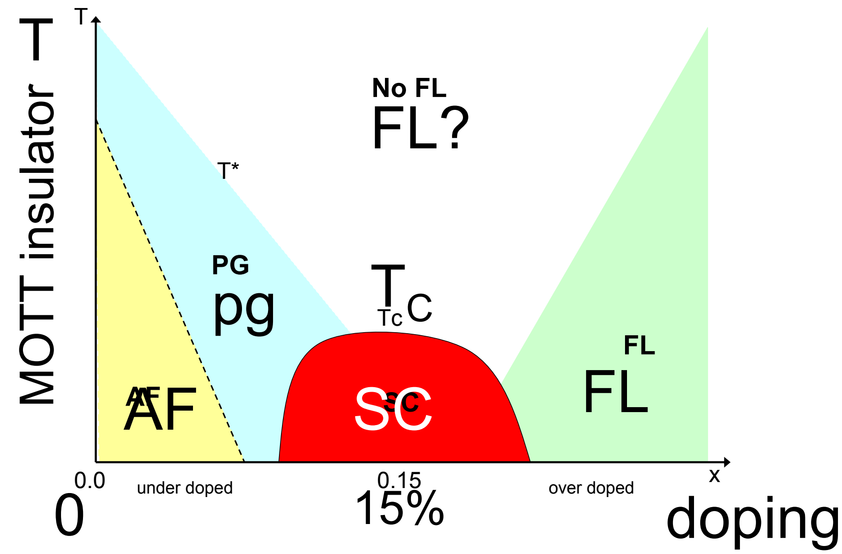
# H-Tc Superconductors Materials

## 1986 Bednorz and Muller




2D physics!



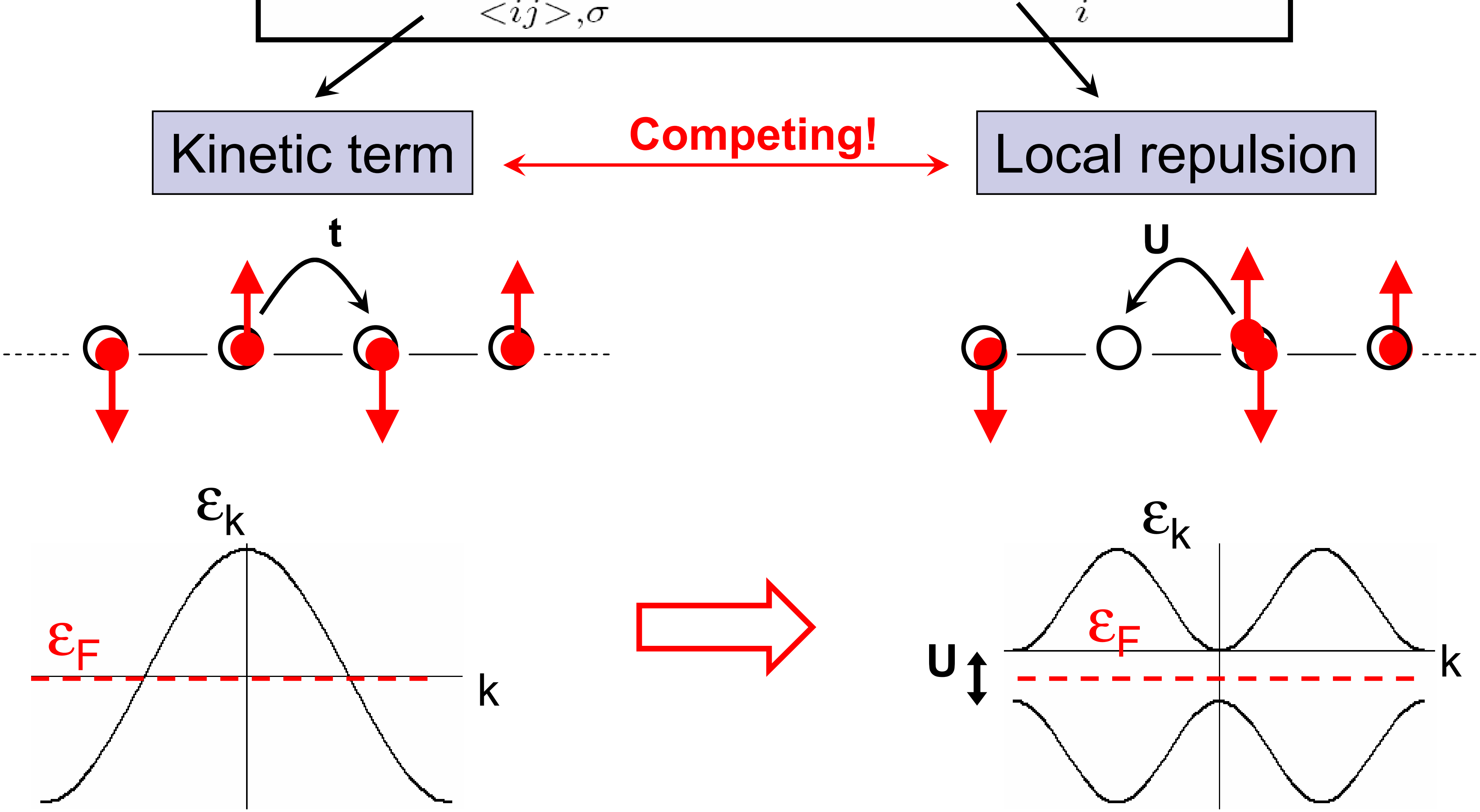

Simple theoretical

**Hubbard Model**

$$H = -t \sum_{<ij>,\sigma} (c^{+}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

# Strongly Correlated Mott Physics

$$H = -\underline{t} \sum_{<ij>,\sigma} (c^{+}_{i\sigma} c_{j\sigma} + h.c.) + \underline{U} \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

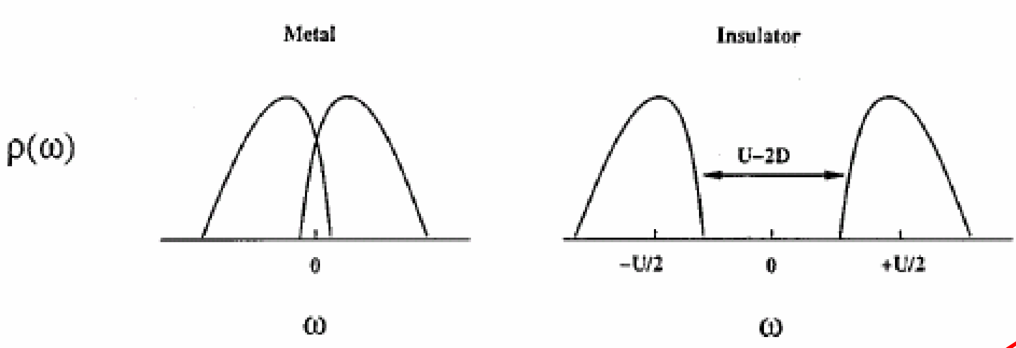


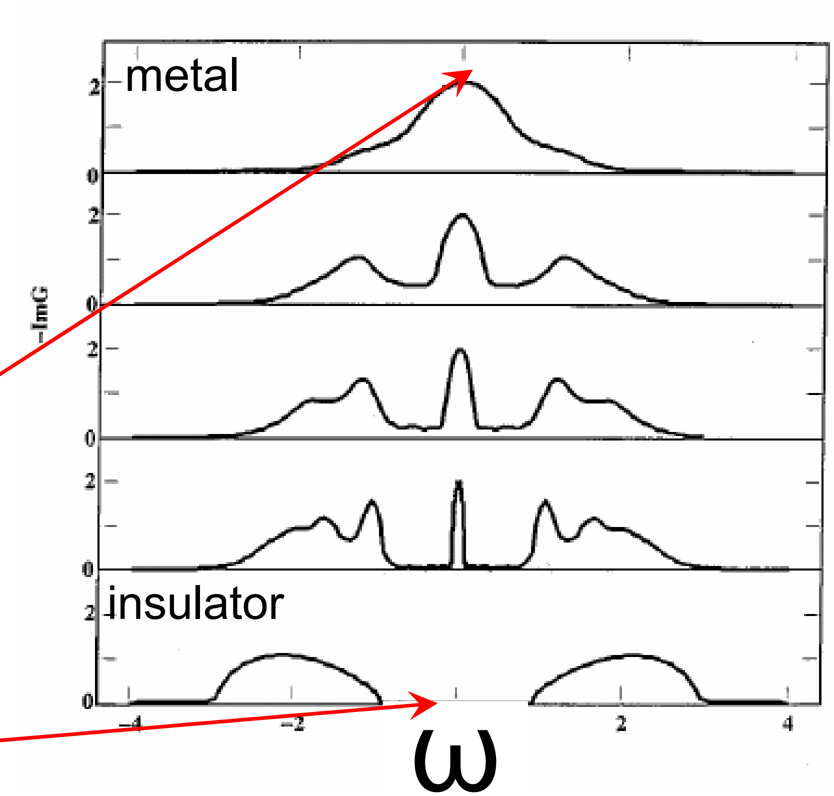
# Why **Dynamics** so important?

**e.g. Density of states- Halffilling-**
**vary interaction U**

Density of States **A(ω)**

HOW?

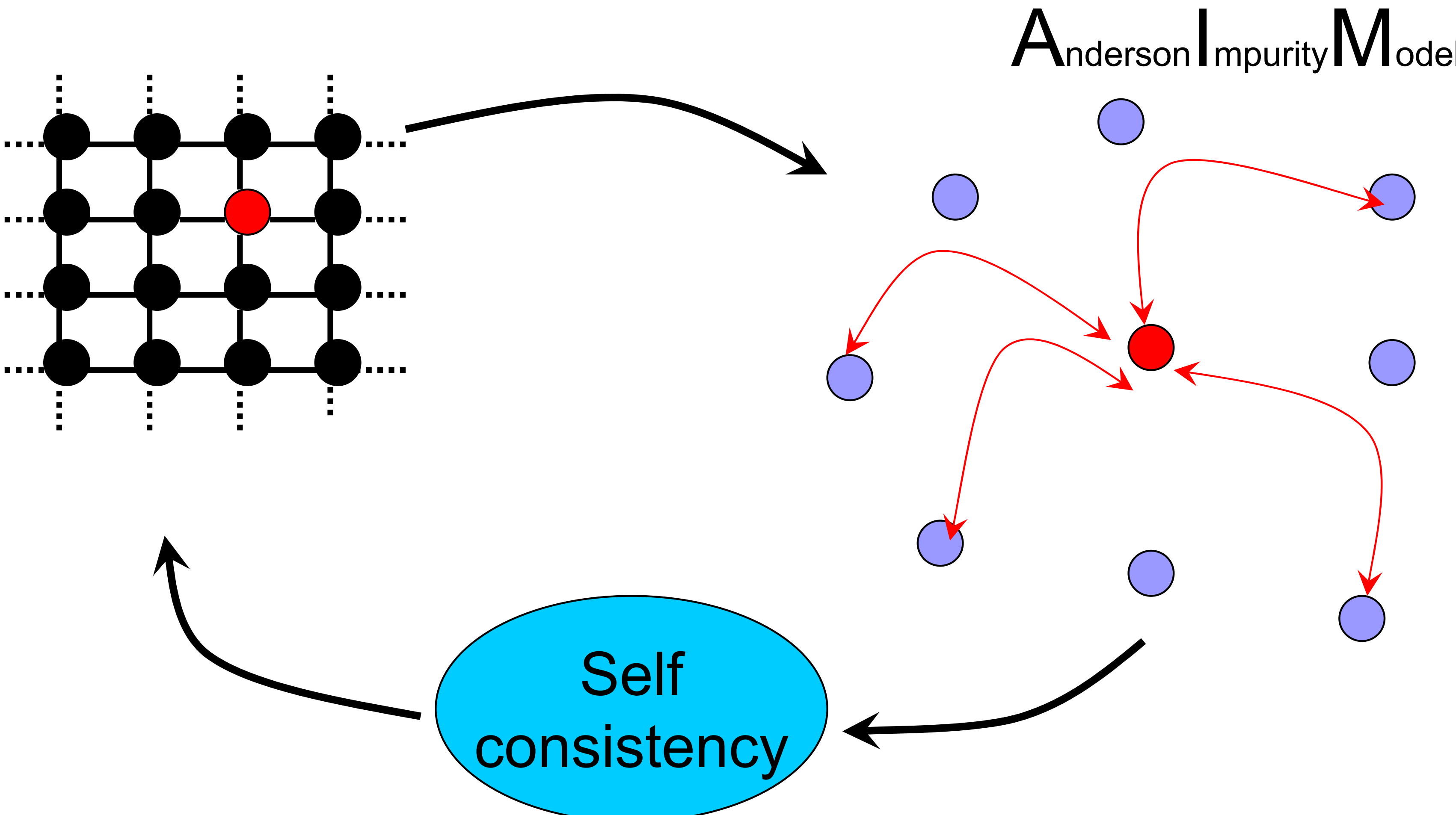



Competition
High-low energy physics!

# **D**ynamical **M**ean **F**ield **T**heory

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




$$\Sigma(i\omega_n) = \mathcal{G}_o(i\omega_n)^{-1} - G[\Sigma](i\omega_n)^{-1}$$

non-interacting

interacting

# Remarks DMFT:

DMFT is exact for $D_{imension} = \infty$:

i) Mapping to Impurity model exact

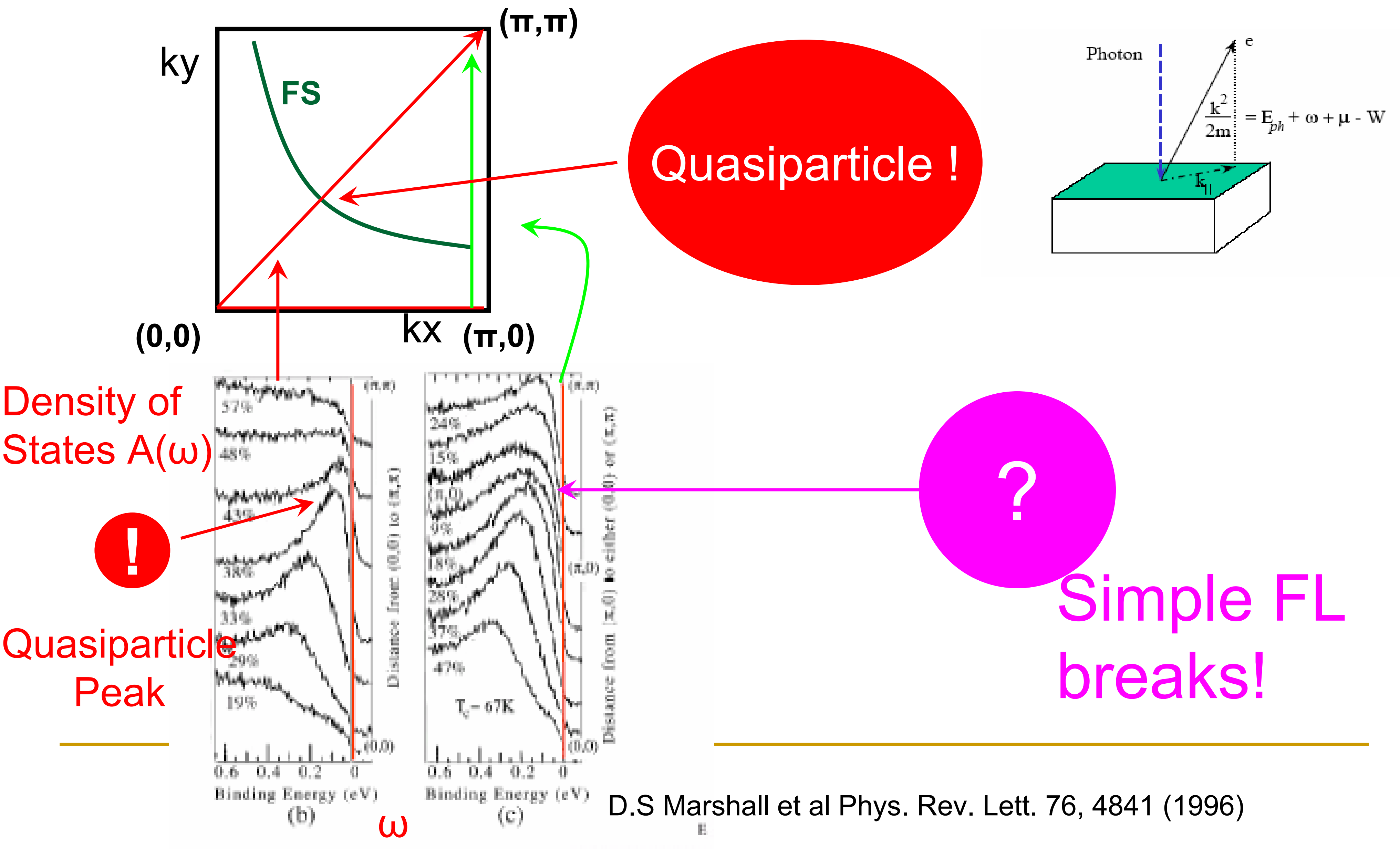
ii) Local Self-energy $\Sigma \neq \Sigma(k)$

exact self-consistency condition

BUT

**What if $\Sigma$ is k dependent? (finite D..)**

# Experimental Evidence: ARPES

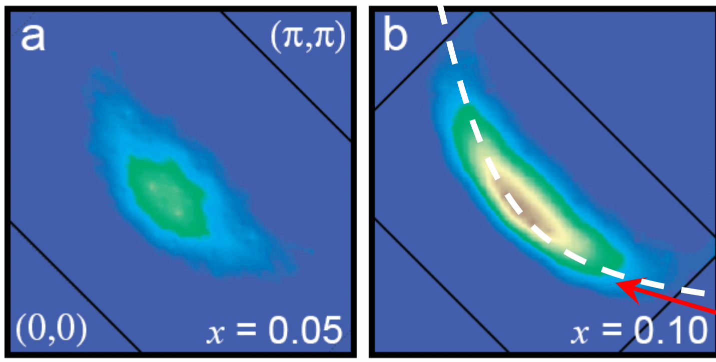



D.S Marshall et al Phys. Rev. Lett. 76, 4841 (1996)

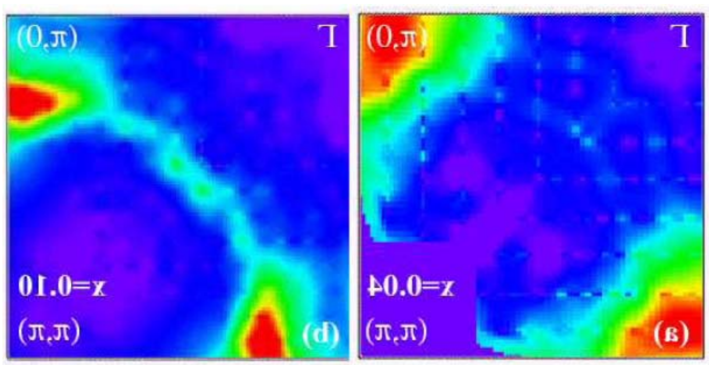
# ARPES in the first quadrant of BZ

$$A(k,\omega\to 0) = -1/\pi\, G(k,\omega \to 0)$$
*

hole doped




e⁻ doped




!

Quasiparticle Peak

**K-dependent Properties**

Local correlations needed

**DMFT Not Enough !**

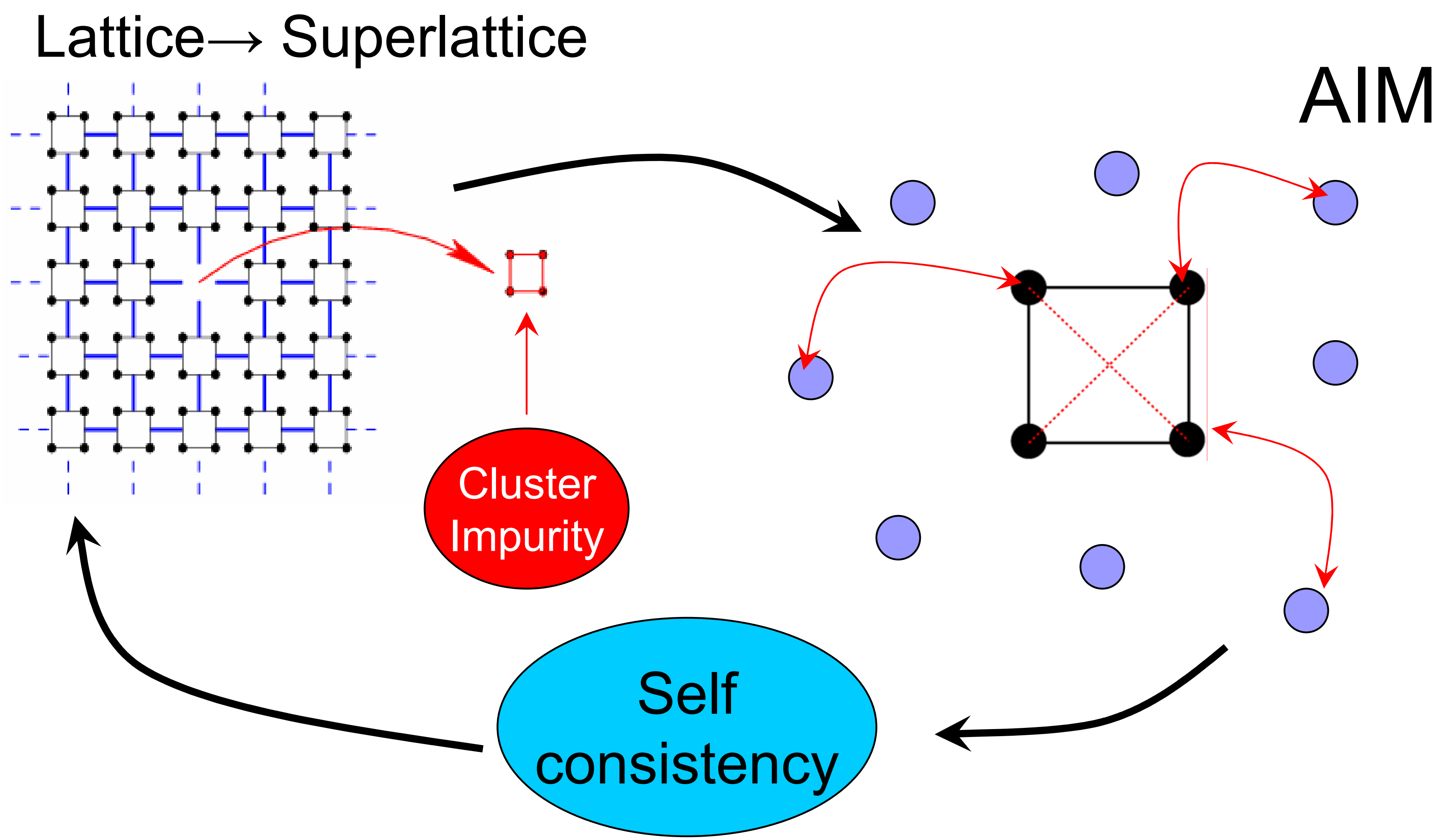
**ARPES:Armitage, Damacelli, Z. Shen, K. Shen, Hussain,Campuzano, Norman, Randeira*

Describing K-dependence is a fundamental ingredient

Can we improve a LOCAL DMFT?

# Cellular Dynamical Mean Field Theory

G. Kotliar et al. Phys. Rev Let. 87, 186401 (2001)




$$\Sigma_{\mu\nu\sigma}(\imath\omega_n) = \mathcal{G}^{-1}_{\mu\nu\sigma}(\imath\omega_n) - G^{-1}_{\mu\nu\sigma}(\imath\omega_n, \hat{\Sigma})$$

# 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

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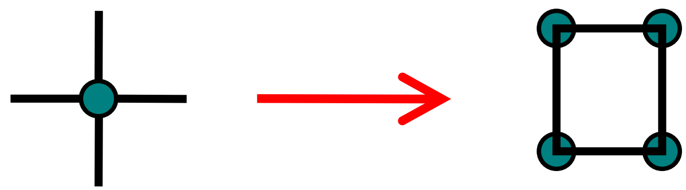
**DMFT**  **C**ellular –**DMFT**

**2D Hubbard Model**:

- **Normal state- Mott transition**
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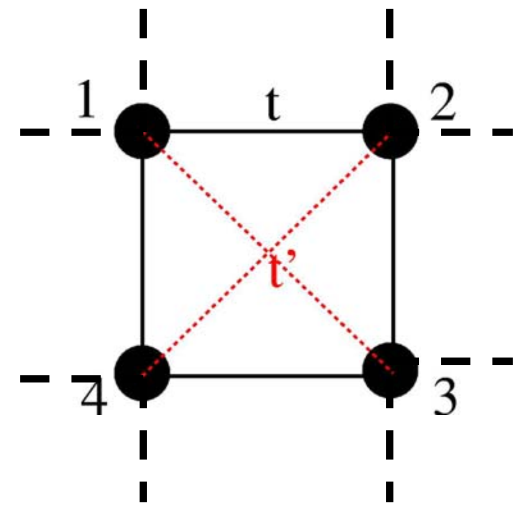
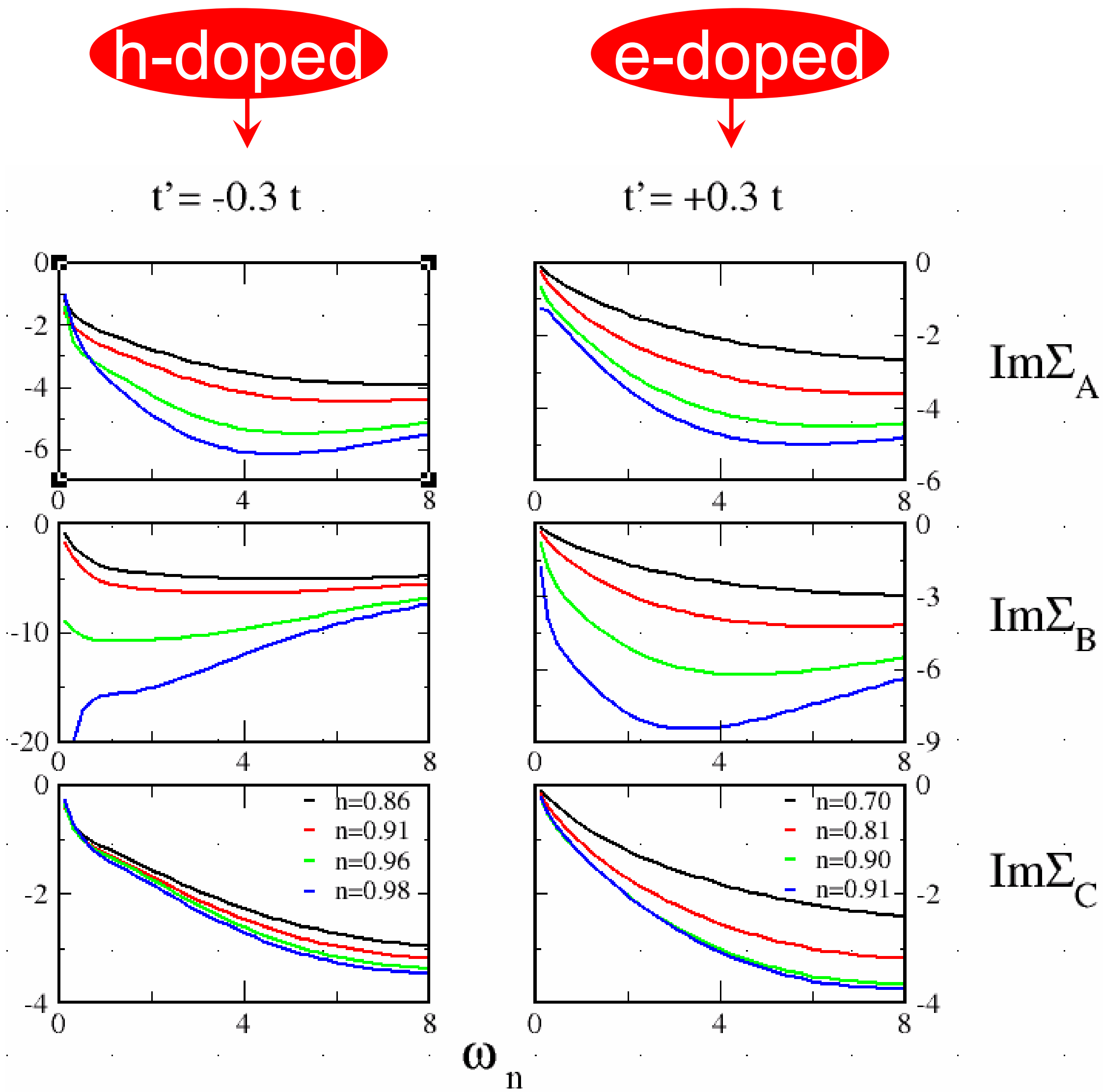
# 2D Hubbard Model with next-nearest neighbor hopping t'

Impurity considered:




- CMFT output few parameters:
  cluster self-energy $\Sigma_{11}, \Sigma_{12}, \Sigma_{13}$
  $\Sigma_{ano} \rightarrow < c_{1\uparrow} c_{2\downarrow} >$
- Preserve square lattice symmetries
- Allows to describe d-wave superconductor broken simmetry

# EigenValues of the cluster $\mathrm{Im}\Sigma_{\mu\nu}$

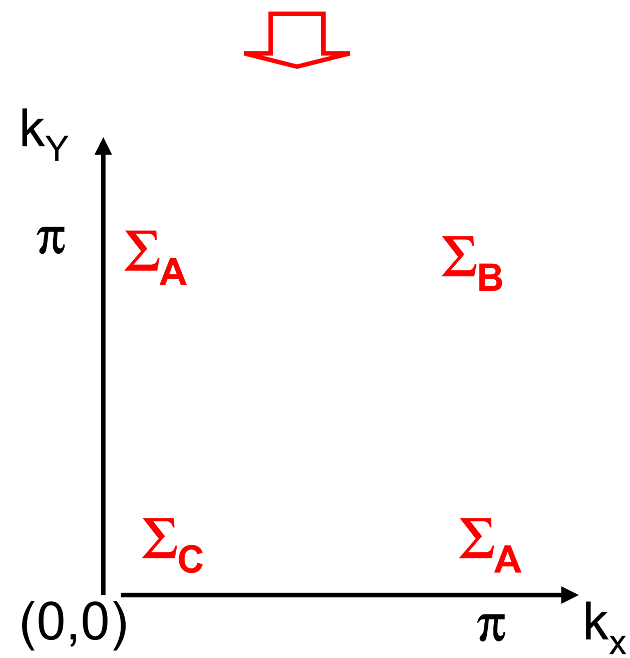



eigenvalues

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

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

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



# All information in the Green's function

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

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

<u>Extracting k-dependence</u> ---- for example $\Sigma_k$

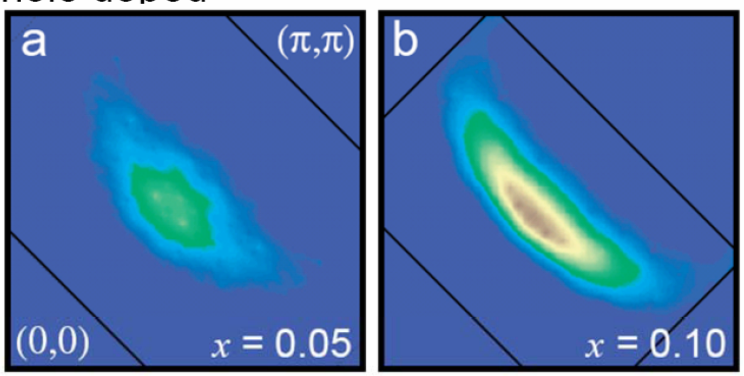
$$\Sigma_k = \Sigma_{11} + \frac{1}{2}\Sigma_{12}(\cos k_x + \cos k_y) + \frac{1}{4}\Sigma_{13} \cos k_x \cos k_y$$

# *Mott transition in the Normal State: hot/cold Spots*

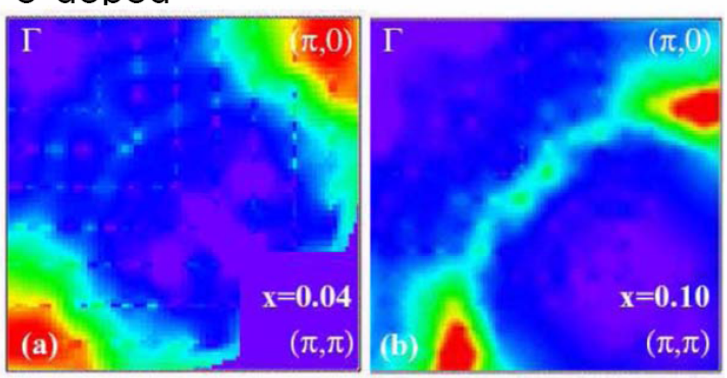
## $A(k,\omega \to 0) = -1/\pi\, G(k,\omega)$

Experiments

hole doped

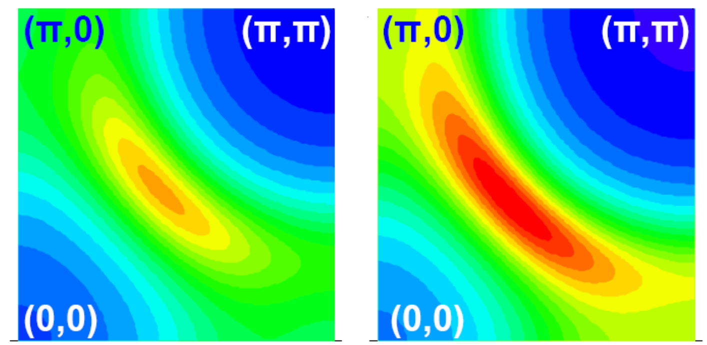



$e^-$ doped

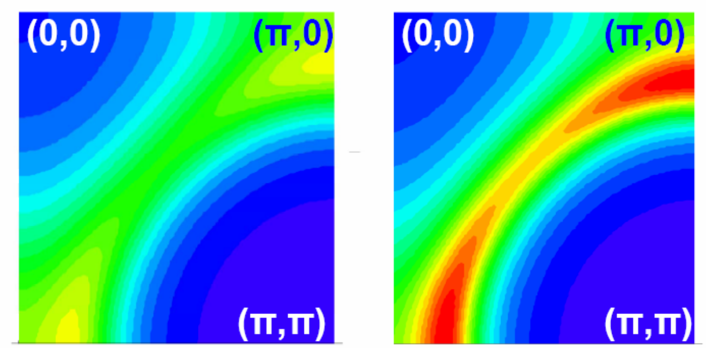



Theory

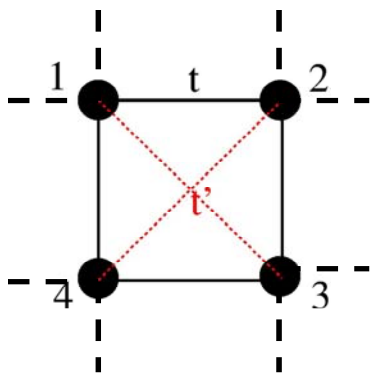
hole doped




e- doped



# How do we extract k-quantities?




CDMFT **cluster-local** theory

USE **most local** quantities to extract k-quantities!

Truncated Fourier Expansion

e.g. $$\Sigma_k = \Sigma_{11} + \frac{1}{2}\Sigma_{12}(\cos k_x + \cos k_y) + \frac{1}{4}\Sigma_{13} \cos k_x \cos k_y$$

# 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 cumulant

cluster

$$\hat{\mathrm{M}} = \frac{1}{(\omega + \mu)\mathbf{1} - \hat{\boldsymbol{\Sigma}}}$$

lattice

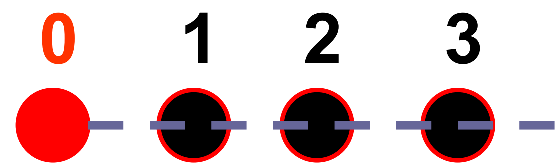
$$M_k = \frac{1}{\omega + \mu - \Sigma_k}$$

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

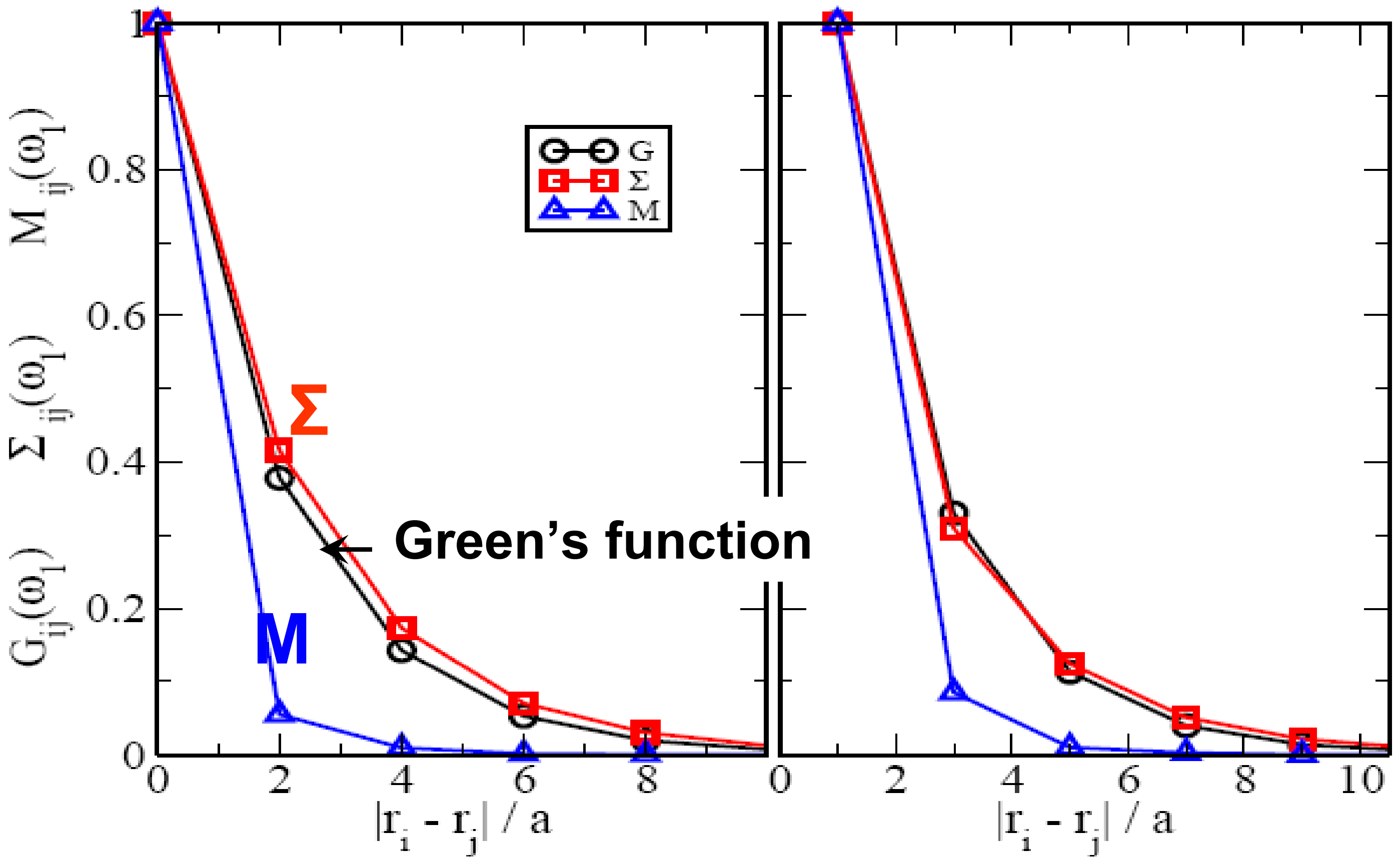
**T.Stanescu et al.** ***Ann. of Phys., Vol. 321, 2006, p.1682***
**T. Stanescu and G. Kotliar,** ***Phys. Rev. B 74, p.125110***

# QMC TEST ON 1D CHAIN

courtesy of B. Kyung




24 sites!



# TEST: insulating state 2D

**Σ**
**M**

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

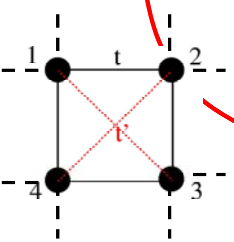
periodize

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

**$G_k(\omega)$**

cluster

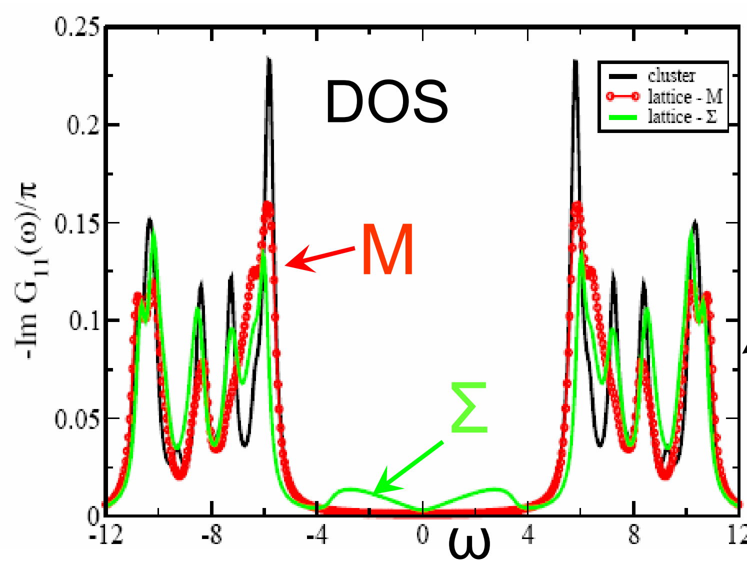
K-space




local

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

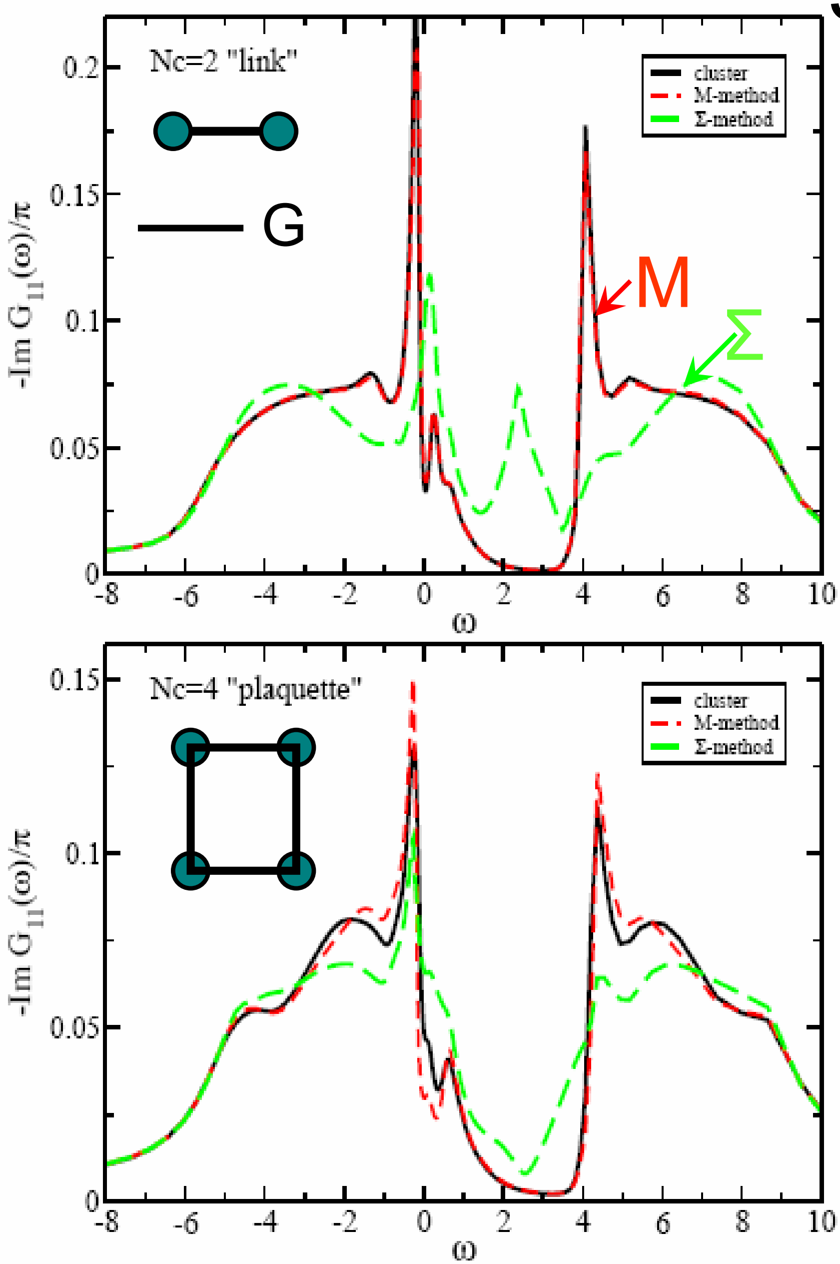
**Σ**
**States**
**In the**
**Mott gap!**

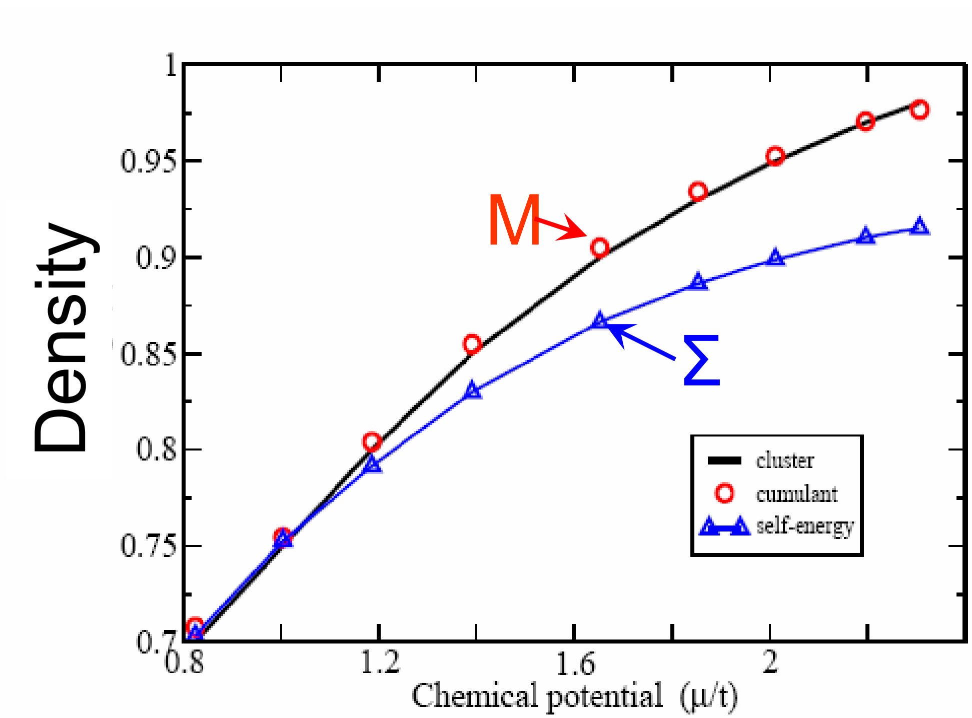



INSULATOR

# Normal state at small doping

5% doping

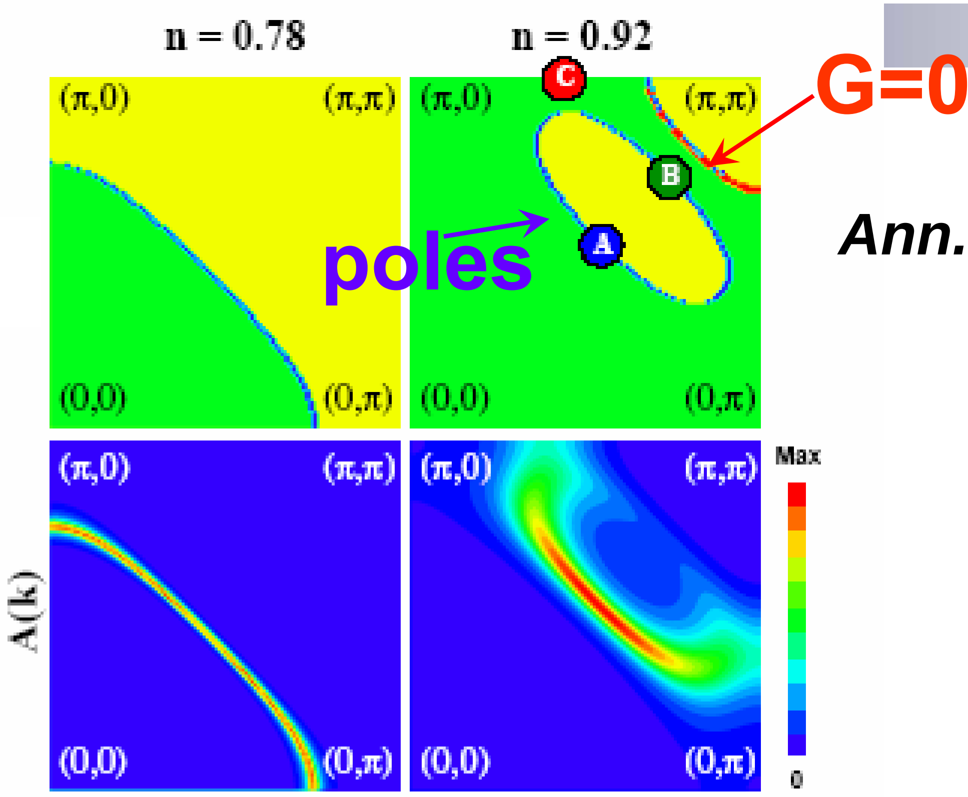



M works better!

# CONSEQUENCE IS A

# PSEUDO-GAP STATE!

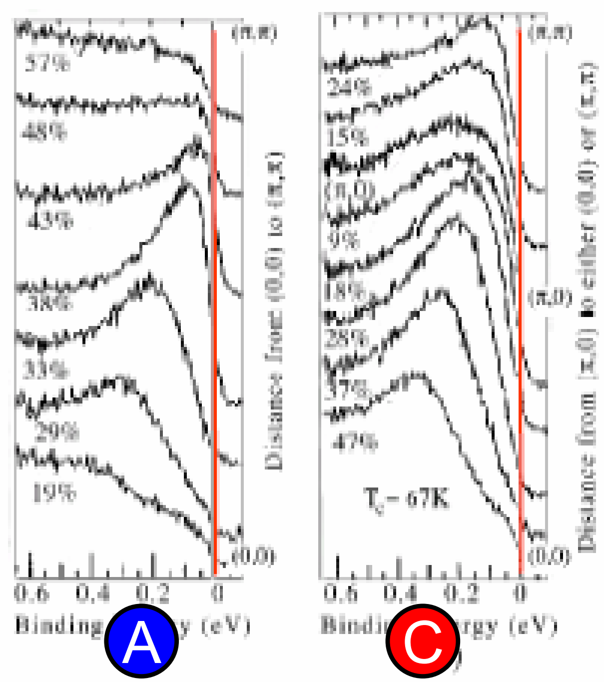


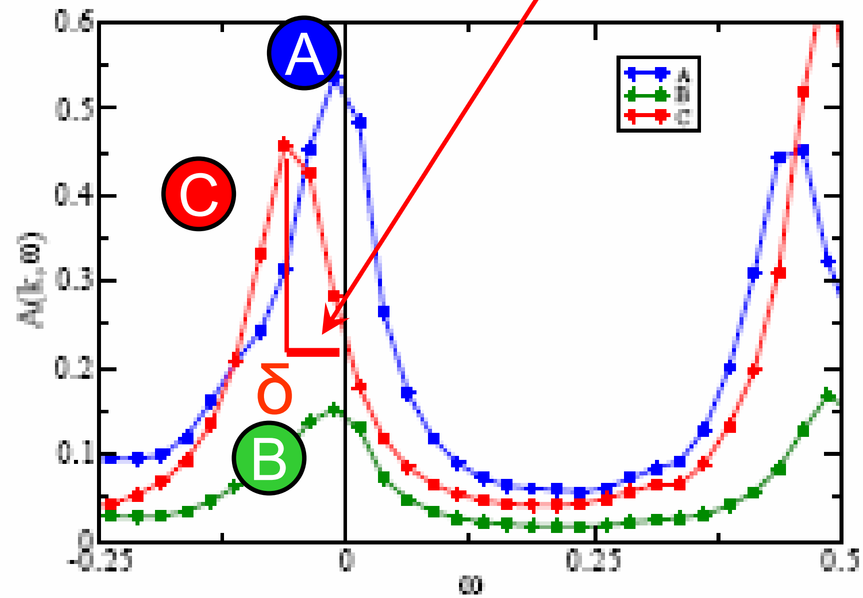

**T.Stanescu et al.**
***Ann. of Phys., Vol. 321, 2006, p.1682***

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

Pseudogap
δ=0.05t~ 0.015 eV

**A(k,ω)**
**Exp.**



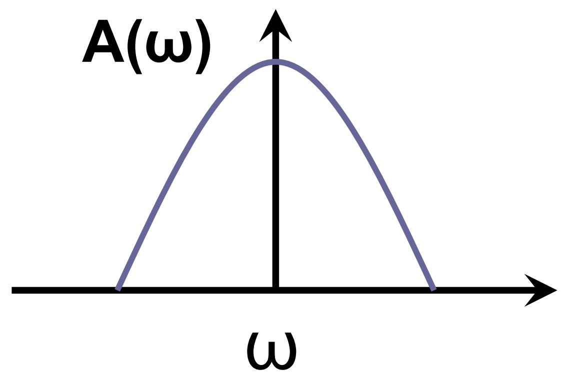

D.S Marshall et al Phys. Rev. Lett. 76, 4841 (1996)

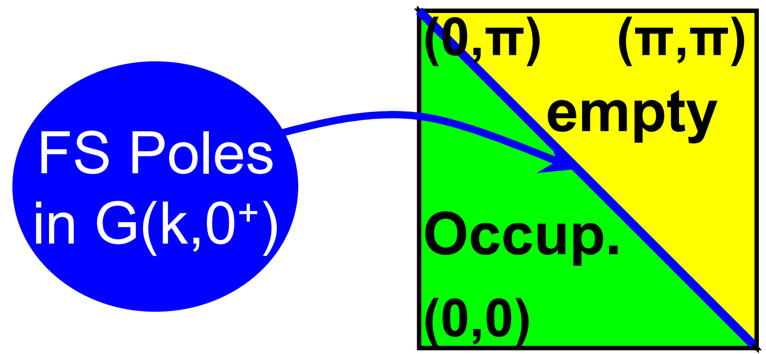
# Simple case: 2D Hubbard Model

t'=0

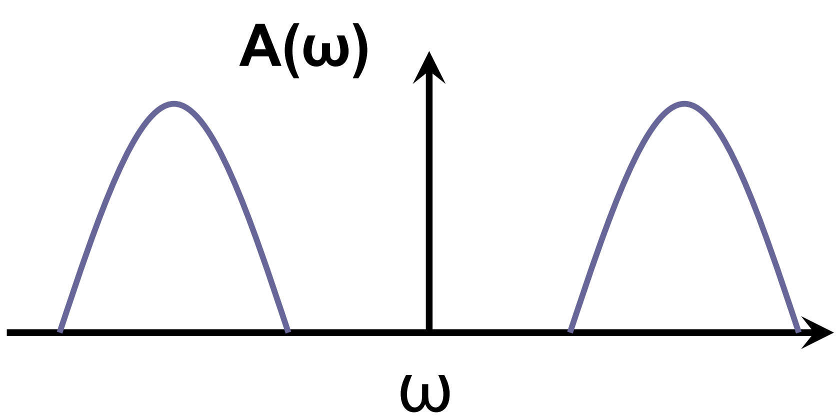
$$H = -t \sum_{<ij>,\sigma} (c^{+}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

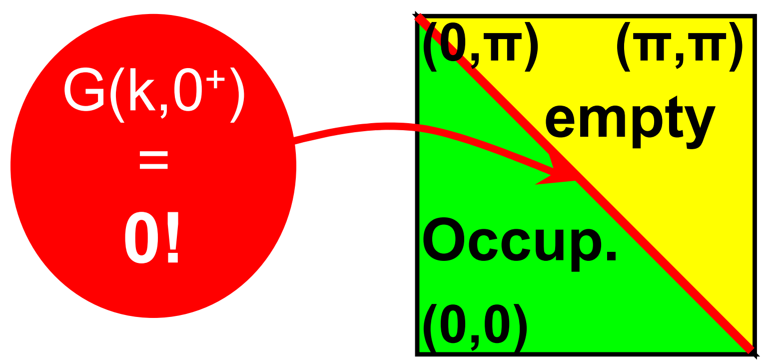
**High doping**



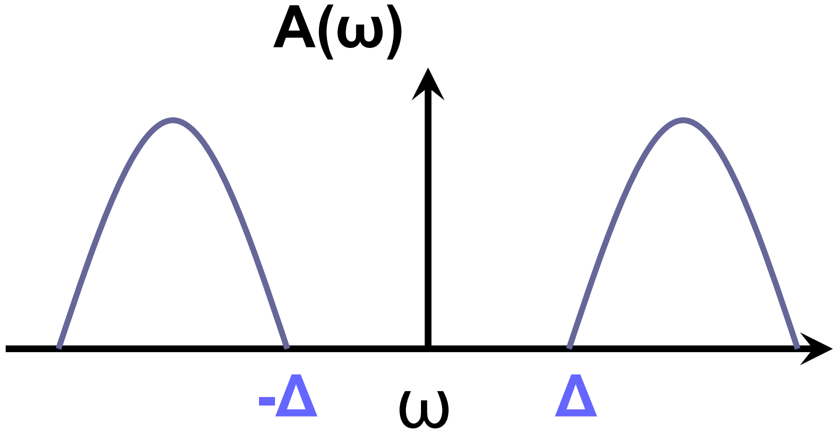

**Insulator**

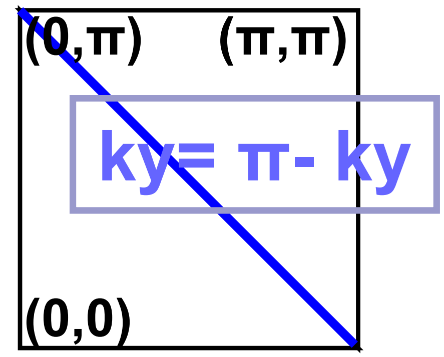


# Line of G(k,0+)=0 at halffilling

T.Stanescu et al. cond-mat/0602280



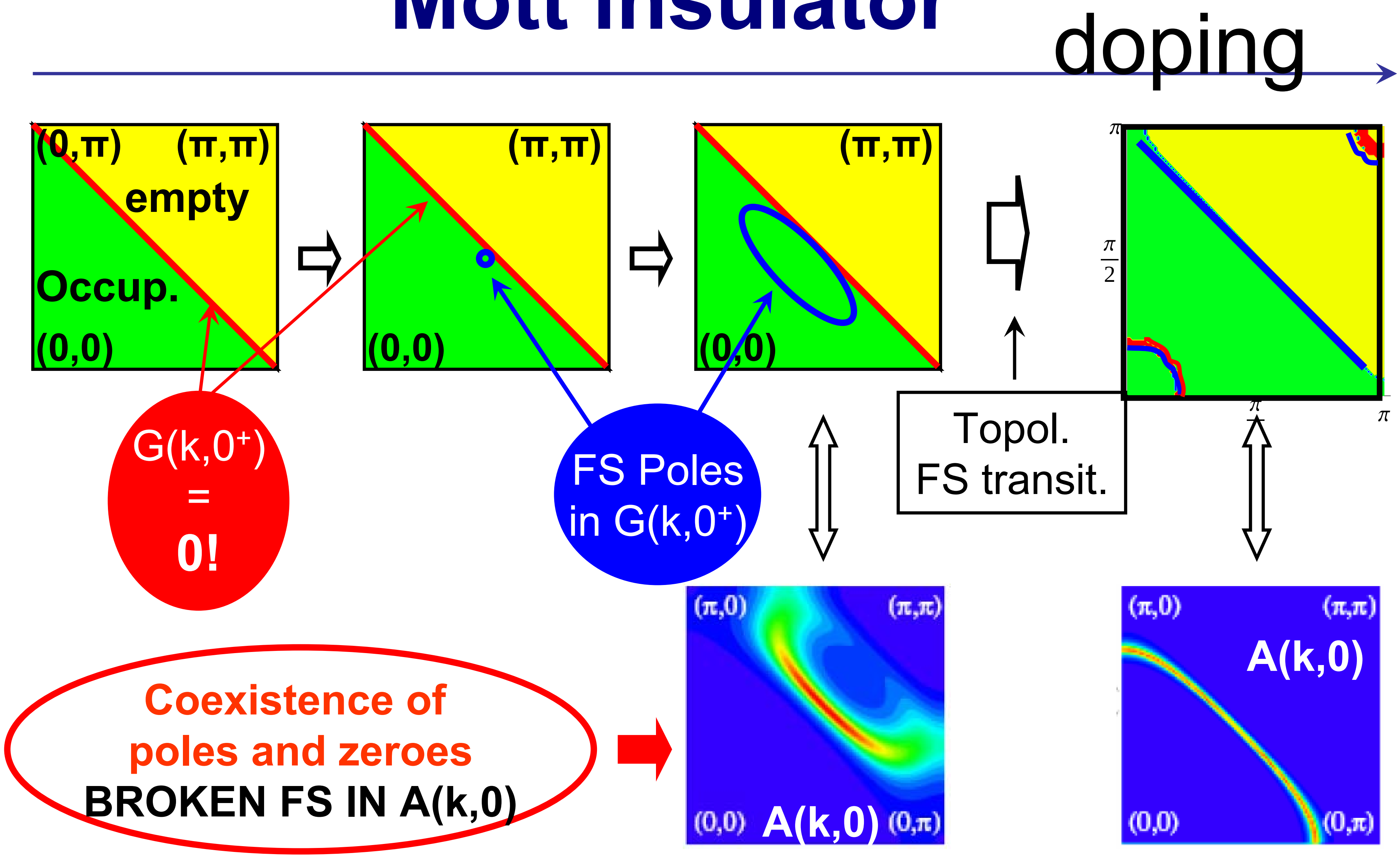

$$\mathrm{Re}G(\mathbf{k},0) = \frac{1}{\pi}\int_{-\infty}^{-\Delta}\frac{A(\mathbf{k},\omega)}{\omega}d\omega + \frac{1}{\pi}\int_{\Delta}^{\infty}\frac{A(\mathbf{k},\omega)}{\omega}d\omega$$

**ReG(k,0)=0** ⟷ **A(k,ω) is even**

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

**A(k,ω) = A(π-k,-ω)**

# Natural continuity into a doped Mott insulator



# OUTLINE

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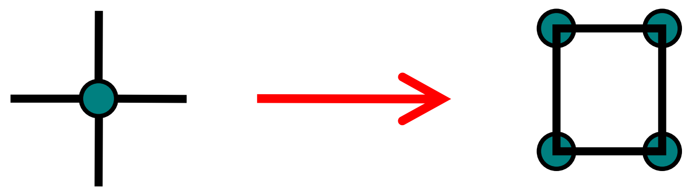
**Strongly correlated many-body physics** ⇨ **DMFT**

*fundamental* ***anisotropic properties*** *DMFT not enough !*

**DMFT**  **C**ellular –**DMFT**

## 2D Hubbard Model:

- **Normal component- Mott transition**
- **d-wave SC state**
- **nodal/antinodal dichotomy**
- **two nodal/antinodal energy-scales**

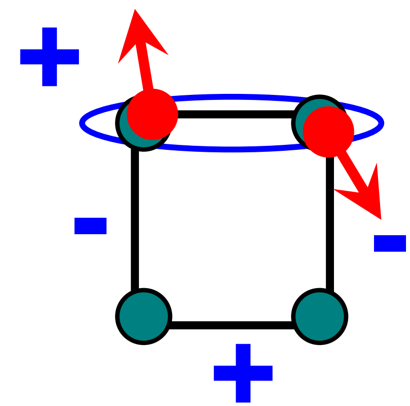
# d-wave SC with CDMFT

**Kancharla et al. cond-mat/0508205**

## AIM with d-wave SC bath

$$
\begin{aligned}
H_{\rm imp} \;=\; & \sum_{\mu\nu\sigma} E_{\mu\nu\sigma} c^\dagger_{\mu\sigma} c_{\nu\sigma} + \sum_{m\sigma} \epsilon^\alpha_{m\sigma} a^{\dagger\alpha}_{m\sigma} a^\alpha_{m\sigma} \\
& + \sum_{m\mu\sigma} V^\alpha_{m\mu\sigma} a^{\dagger\alpha}_{m\sigma} (c_{\mu\sigma} + \text{h.c.}) + U \sum_\mu n_{\mu\uparrow} n_{\mu\downarrow} \\
& + \sum_\alpha \Delta^\alpha (a^\alpha_{1\uparrow} a^\alpha_{2\downarrow} - a^\alpha_{2\uparrow} a^\alpha_{3\downarrow} + a^\alpha_{3\uparrow} a^\alpha_{4\downarrow} - a^\alpha_{4\uparrow} a^\alpha_{1\downarrow} \\
& + a^\alpha_{2\uparrow} a^\alpha_{1\downarrow} - a^\alpha_{3\uparrow} a^\alpha_{2\downarrow} + a^\alpha_{4\uparrow} a^\alpha_{3\downarrow} - a^\alpha_{1\uparrow} a^\alpha_{4\downarrow} + h.c.).
\end{aligned}
$$

SC

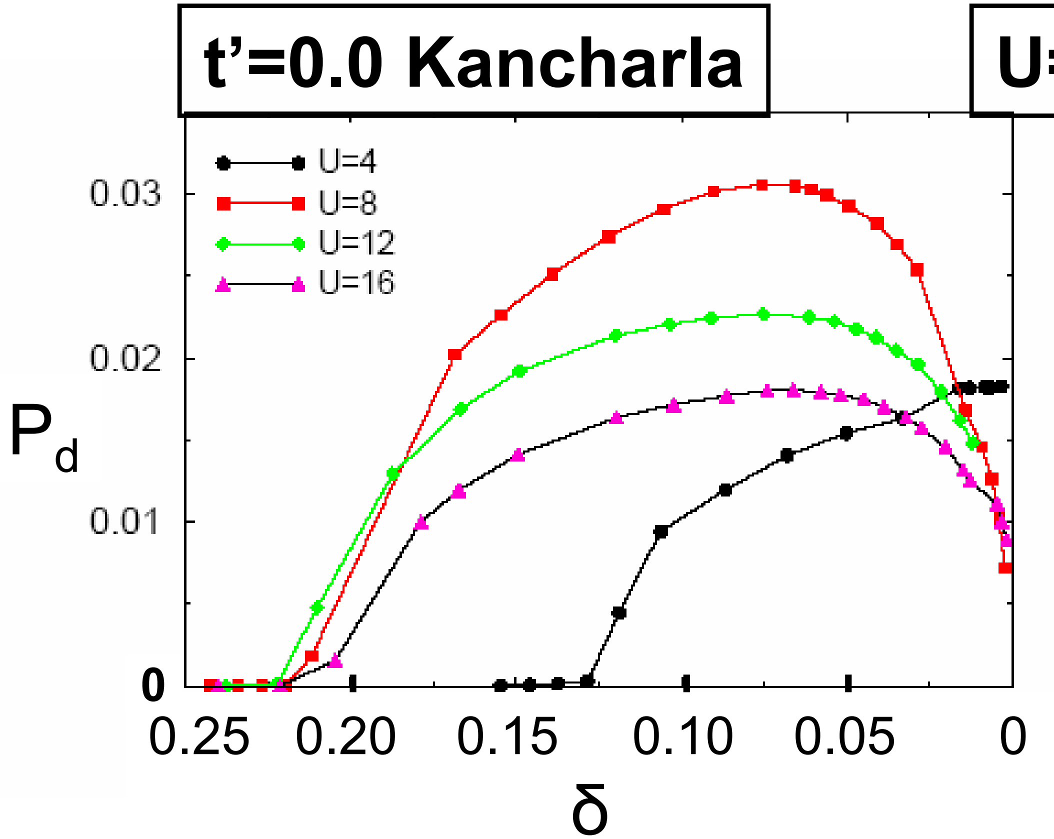


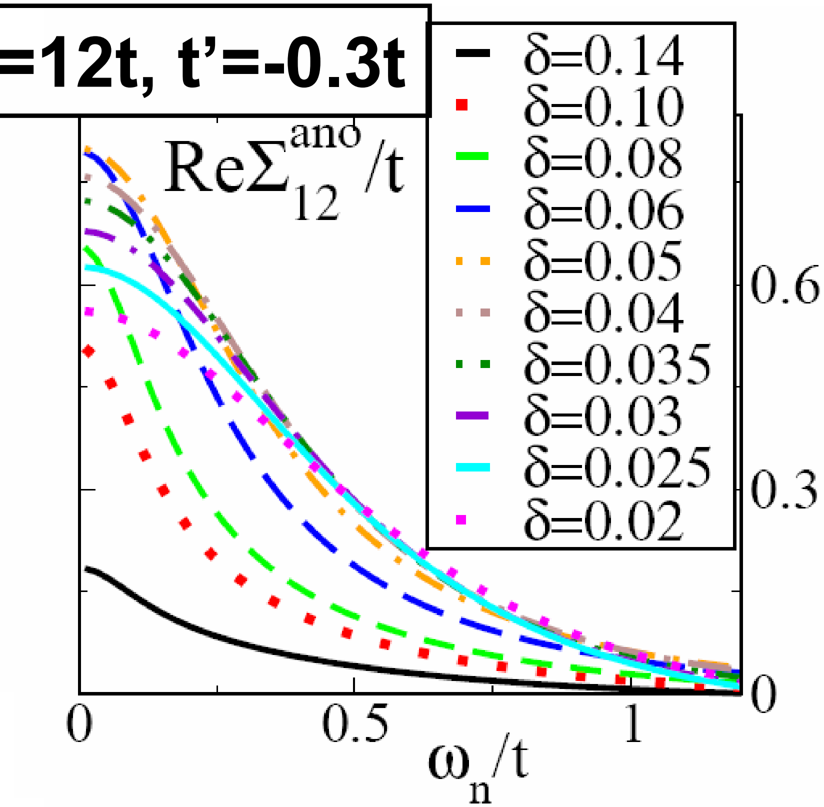

$$F_{\mu\nu} \equiv -T \langle c_{\mu\downarrow}(\tau) c_{\nu\uparrow}(0) \rangle$$

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 !




dSc non-zero $P_d=\langle c_\uparrow c_\downarrow \rangle$ in the 2D Hubbard Model

Anomalous $\Sigma_{ano} \neq 0$, low energy non-momotonic in doping δ

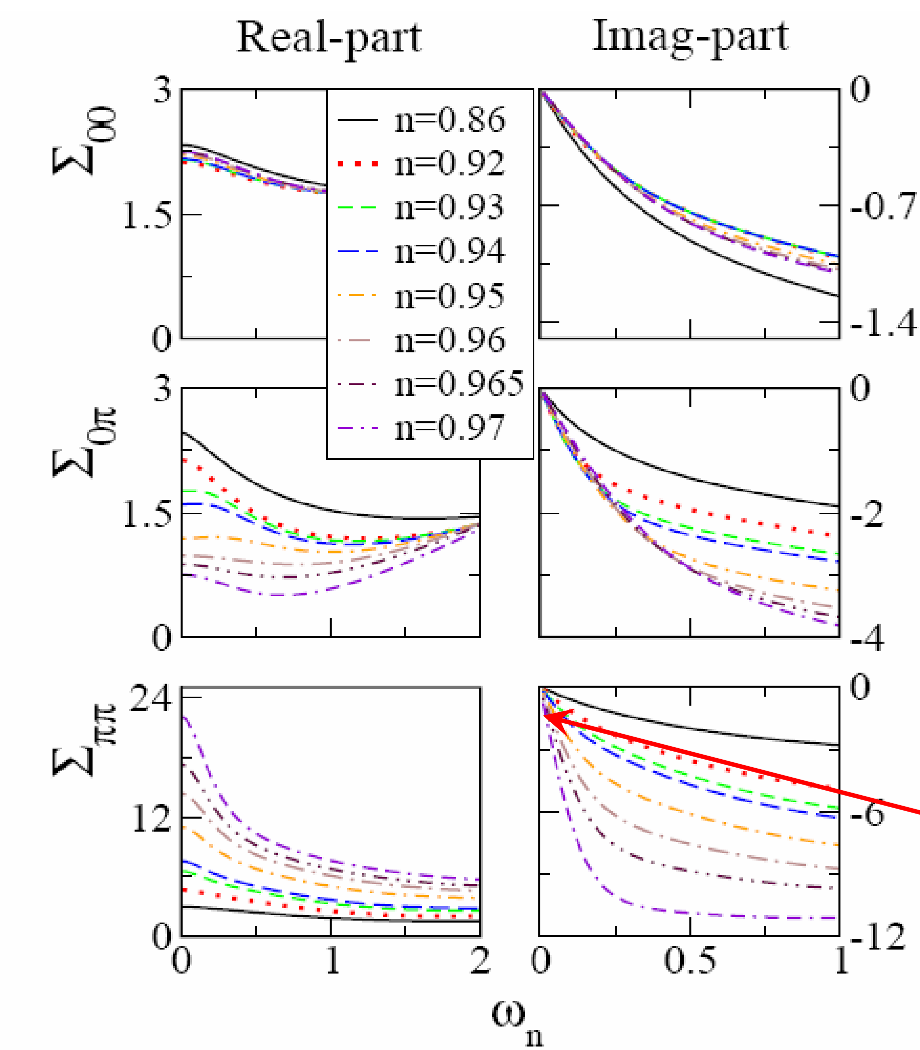
S.S Kancharla et al, cond-mat/0508205
M. Civelli et al. cond-mat/0704.1486v1

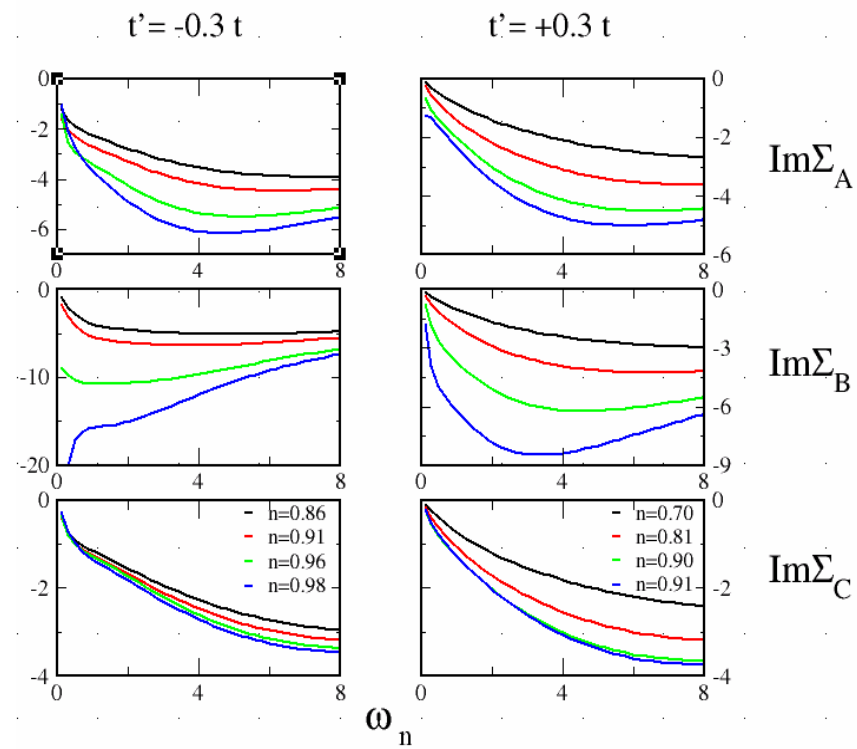
Very important!

# Σ cluster-Eigenvalues

superconducting

normal




Im Σ→0

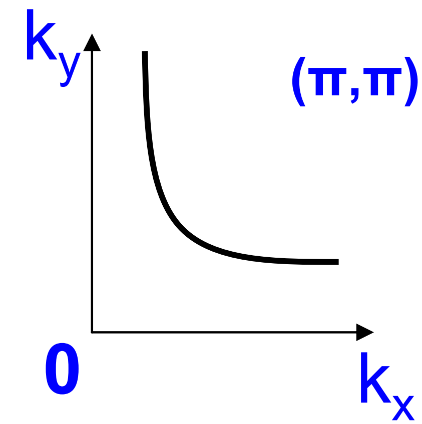
Fermi Liquid

# Superconducting Green's function
## Nambu's notation

$$G^{-1}_{k\sigma}(\omega) = \begin{pmatrix} \omega - \varepsilon_k - \Sigma^{\rm nor}_\sigma(k,\omega) & -\Sigma^{\rm ano}(k,\omega) \\ -\Sigma^{\rm ano}(k,\omega) & \omega + \varepsilon_k + \Sigma^{\rm nor}_\sigma(k,-\omega)^* \end{pmatrix}$$

<u>quasi-particle particle band</u>

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

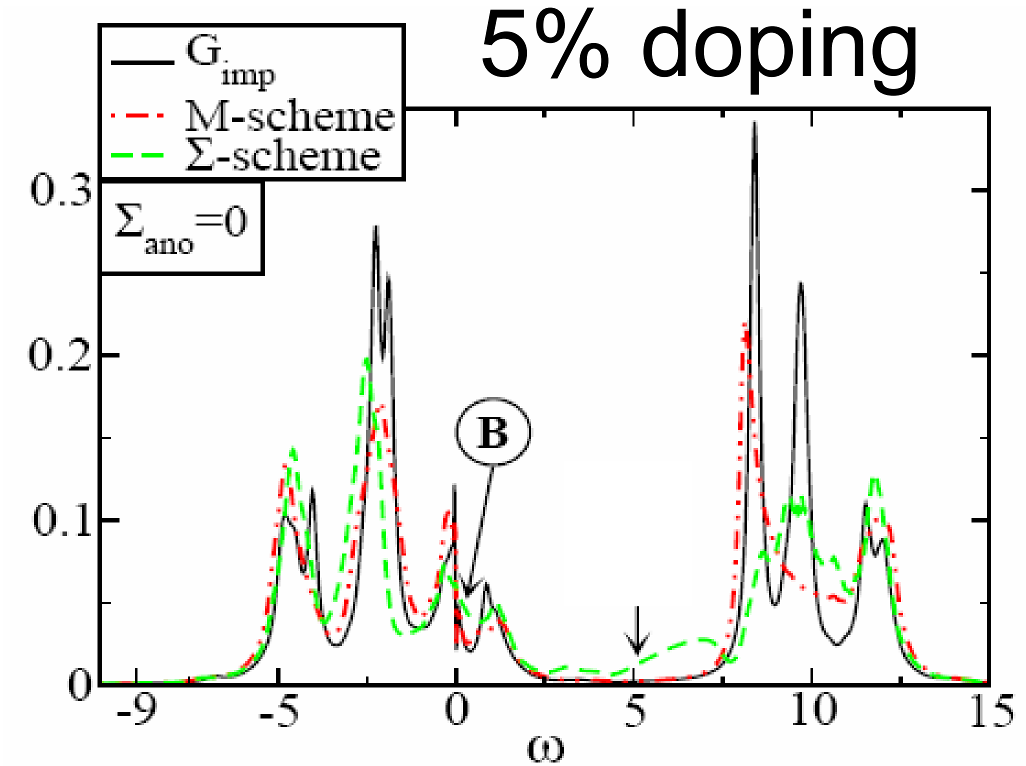


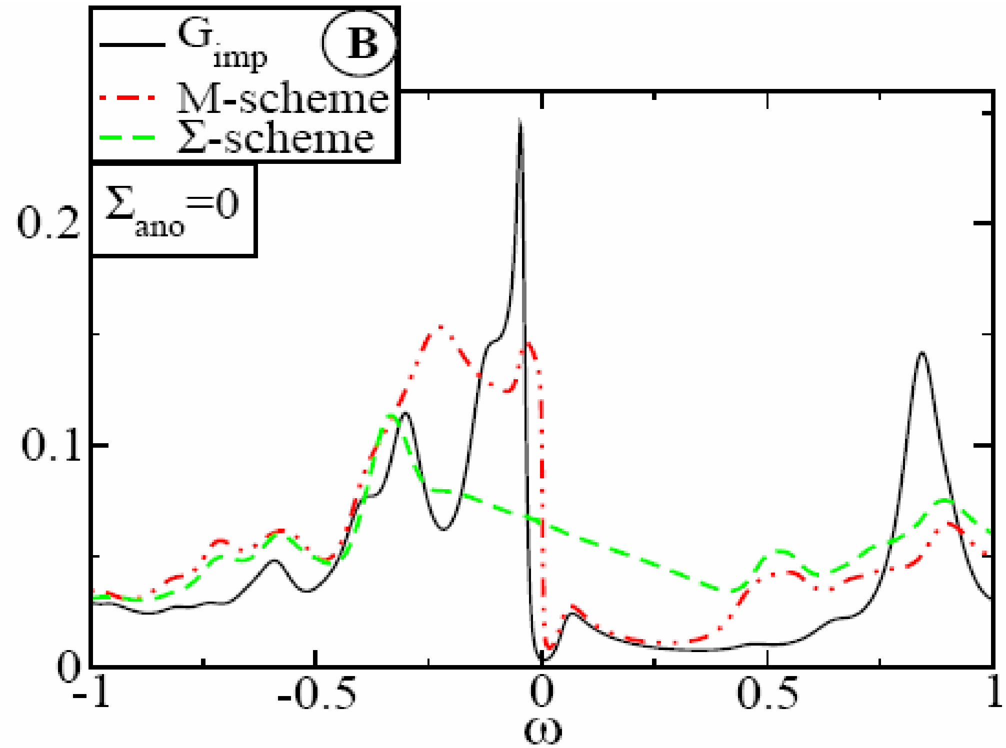
# Periodization procedure

## Normal component set $\Sigma_{ano}=0$

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

5% doping




Better M

# Periodization procedure2 $\Sigma_{ano}\neq 0$ superconducting component

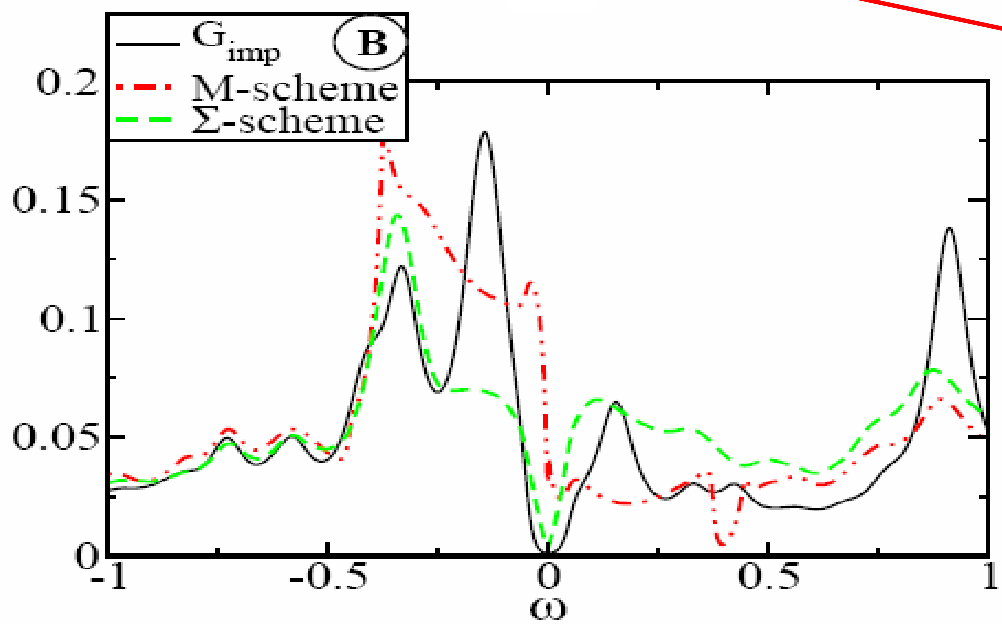
$$\mathrm{Im}G^{11}_{\sigma}(k,\omega) \simeq Z_{nod}\,\delta\left(\omega - \sqrt{v^2_{nod}k^2_{\perp} + v^2_{\Delta}k^2_{\parallel}}\right)$$

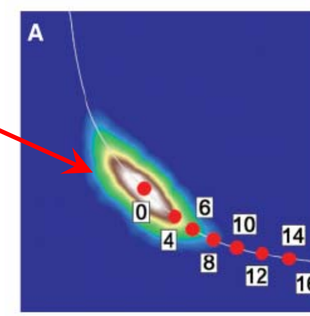
Only the nodal point is gapless

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

Spectrum Linearized!

Sum selects Nodal area only




Better Σ!

# Periodizing recipe:

- Nodal point→ periodize Σ

⇨ In particular d-wave gap

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

- Anti-nodal point → periodize M

as in the normal state case

# EXPERIMENTS: ARPES SPECTRA

Tanaka et al. Science 314, 1910 (2006)

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

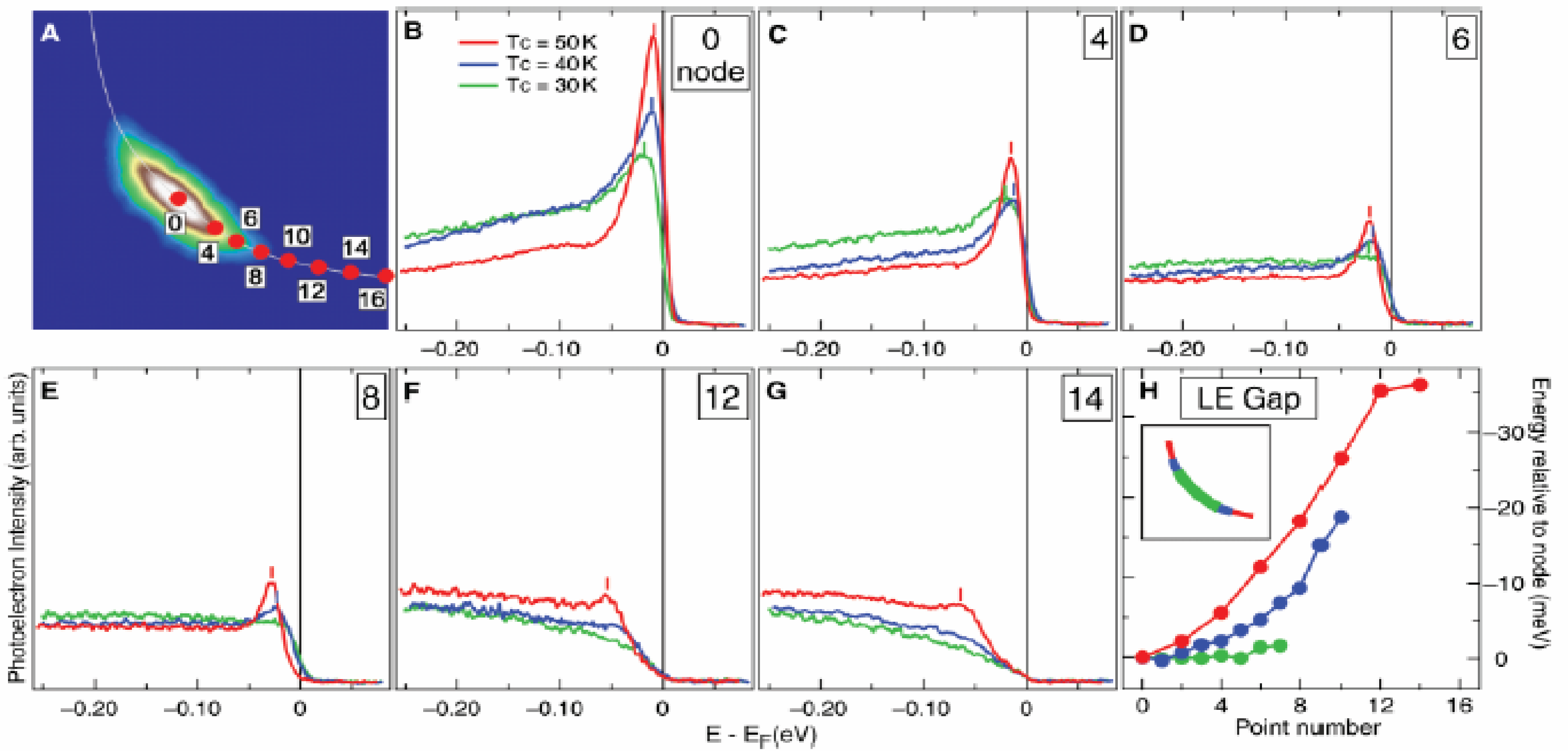
Optimal doping

Tc = 50 K

Tc = 40 K

Tc = 30 K

doping



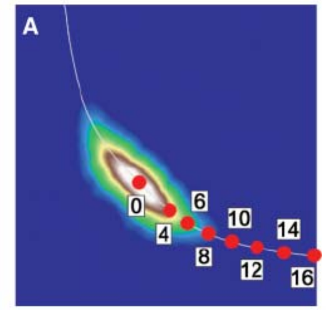
# Question: one or two energy-gaps?

e.g.

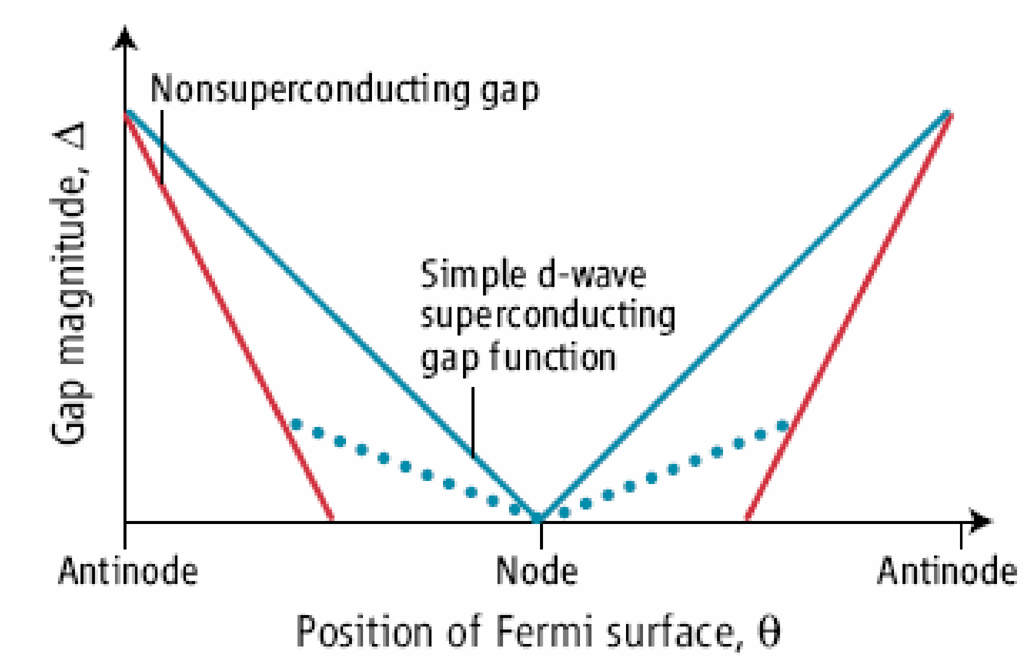
e.g.

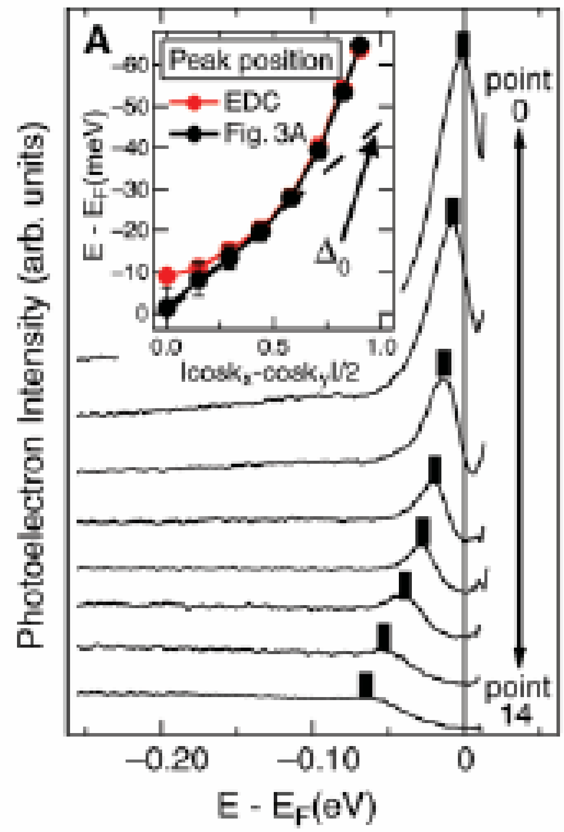
T. Valla et al. Science 314, 1914 (2006)

Tanaka et al. Science 314, 1910 (2006)

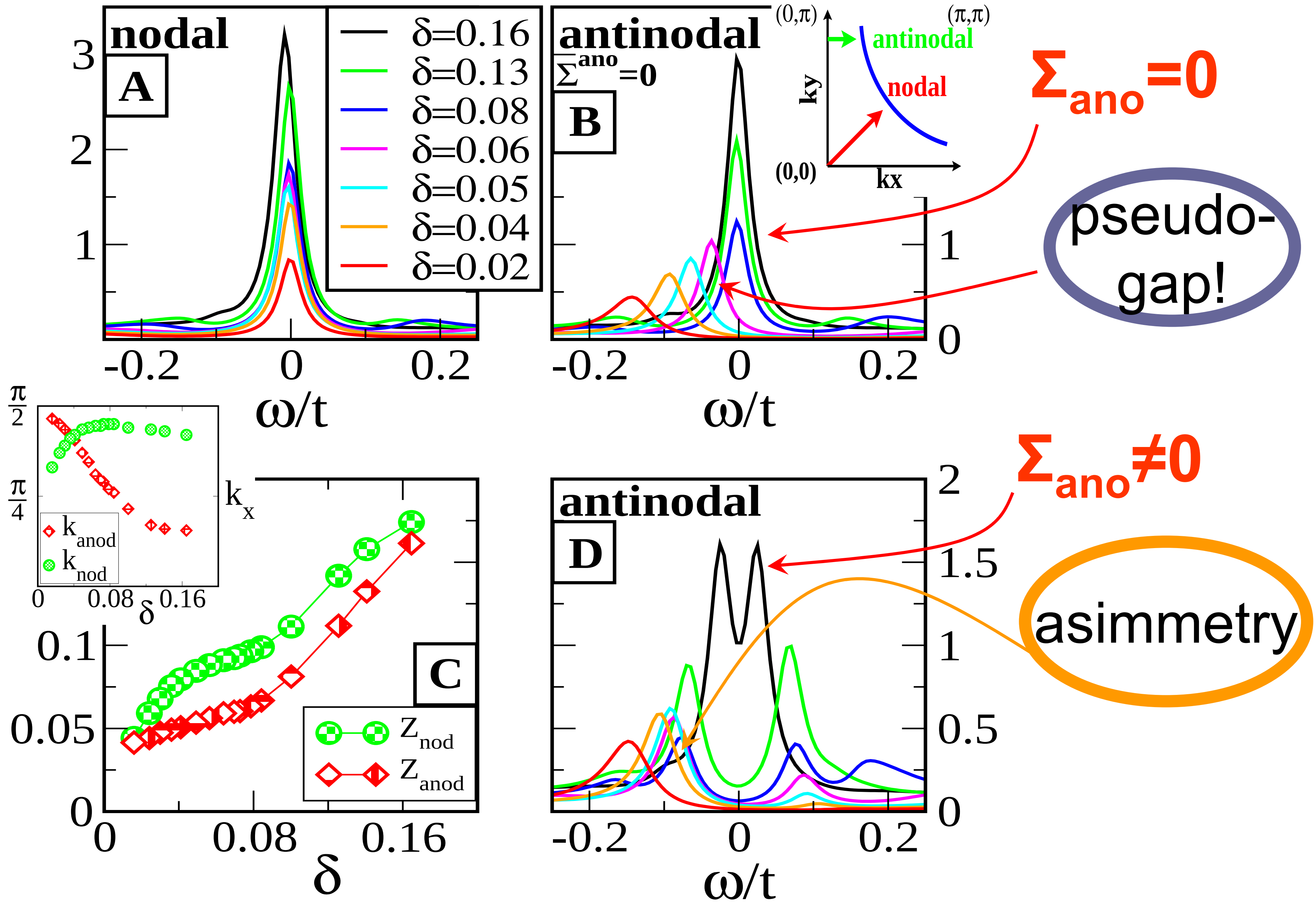



See e.g. discussion Science Dec 2006
A. J. Millis, Science 314, 1888 (2006).



# Quasi-particle Spectra CDMFT



# At the node I have a quasiparticle

$$G_{k\sigma}^{-1}(\omega) = \begin{pmatrix} \omega - \varepsilon_k - \Sigma_\sigma^{\mathrm{nor}}(k,\omega) & -\Sigma^{\mathrm{ano}}(k,\omega) \\ -\Sigma^{\mathrm{ano}}(k,\omega) & \omega + \varepsilon_k + \Sigma_\sigma^{\mathrm{nor}}(k,-\omega)^* \end{pmatrix}$$

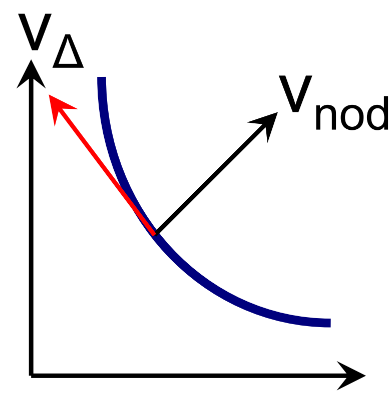
We can attempt a standard Fermi-Liquid Expansion at low energy

$$\xi_k^0 \equiv \varepsilon_k + \mathrm{Re}\Sigma^{nor}(k,0)$$

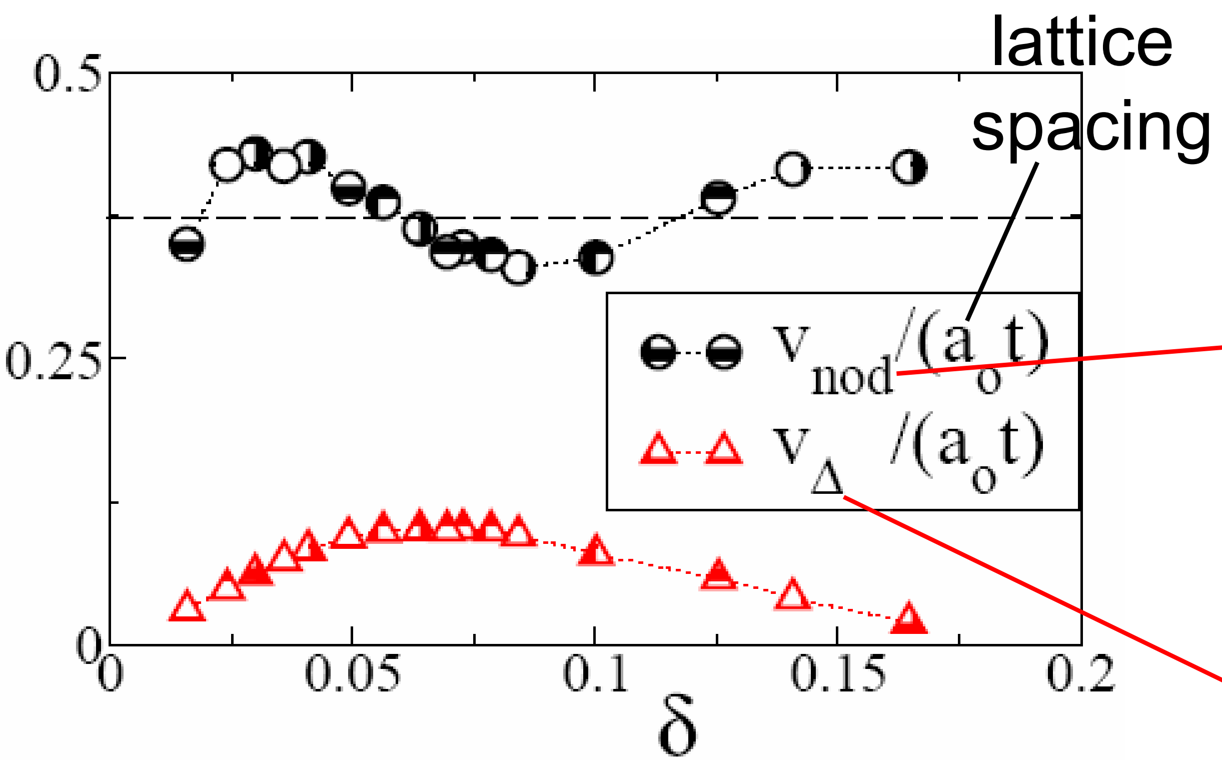
$$Z_{nod} = \left.(1 - \partial_\omega \mathrm{Re}\Sigma_k(\omega))^{-1}\right|_{\omega=0}$$

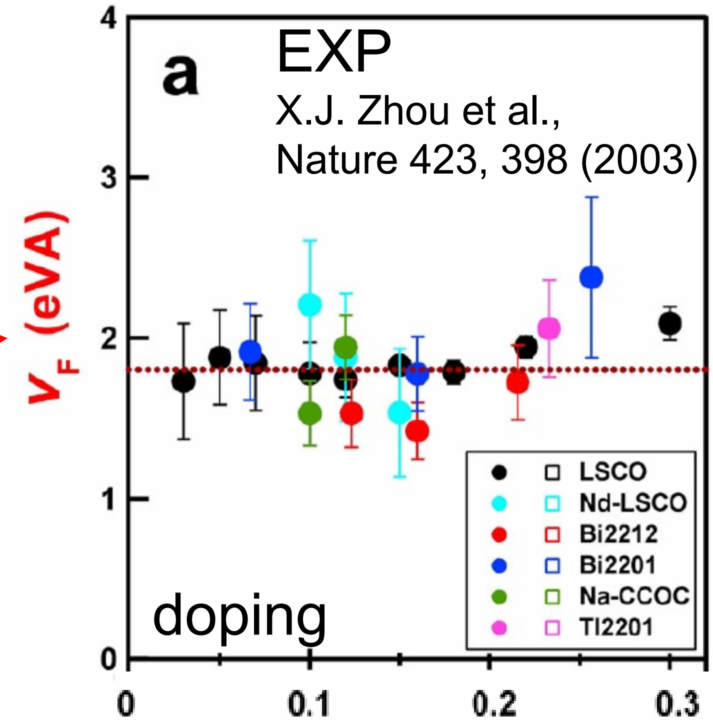
$$v_{nod} = Z_{nod}|\nabla_k \xi_k^0|$$

$$v_\Delta = Z_{nod}|\nabla_k \Sigma^{ano}(k)|$$



# Nodal velocities- standard Fermi Liquid Analysis



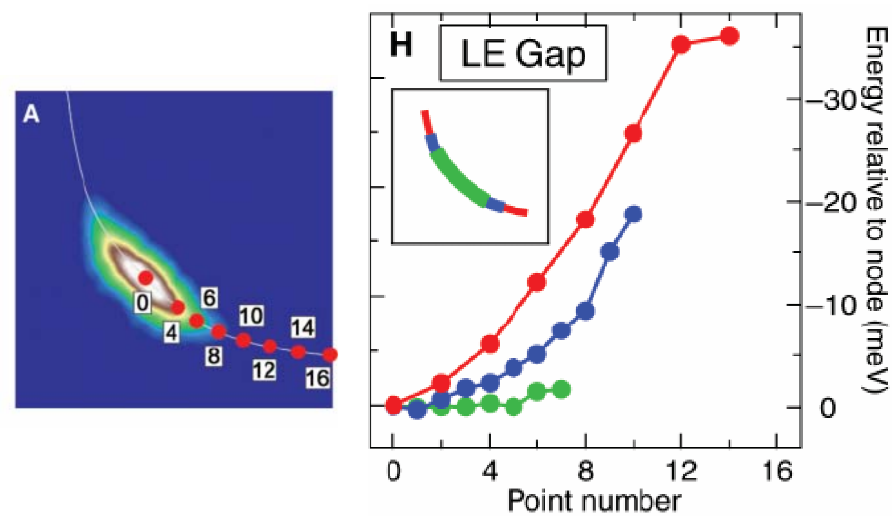




$$\xi_k^0 \equiv \varepsilon_k + \mathrm{Re}\Sigma^{nor}(k,0)$$

$$Z_{nod} = \left.(1 - \partial_\omega \mathrm{Re}\Sigma_k(\omega))^{-1}\right|_{\omega=0}$$

$$v_{nod} = Z_{nod}|\nabla_k \xi_k^0|$$

$$v_\Delta = Z_{nod}|\nabla_k \Sigma^{ano}(k)|$$

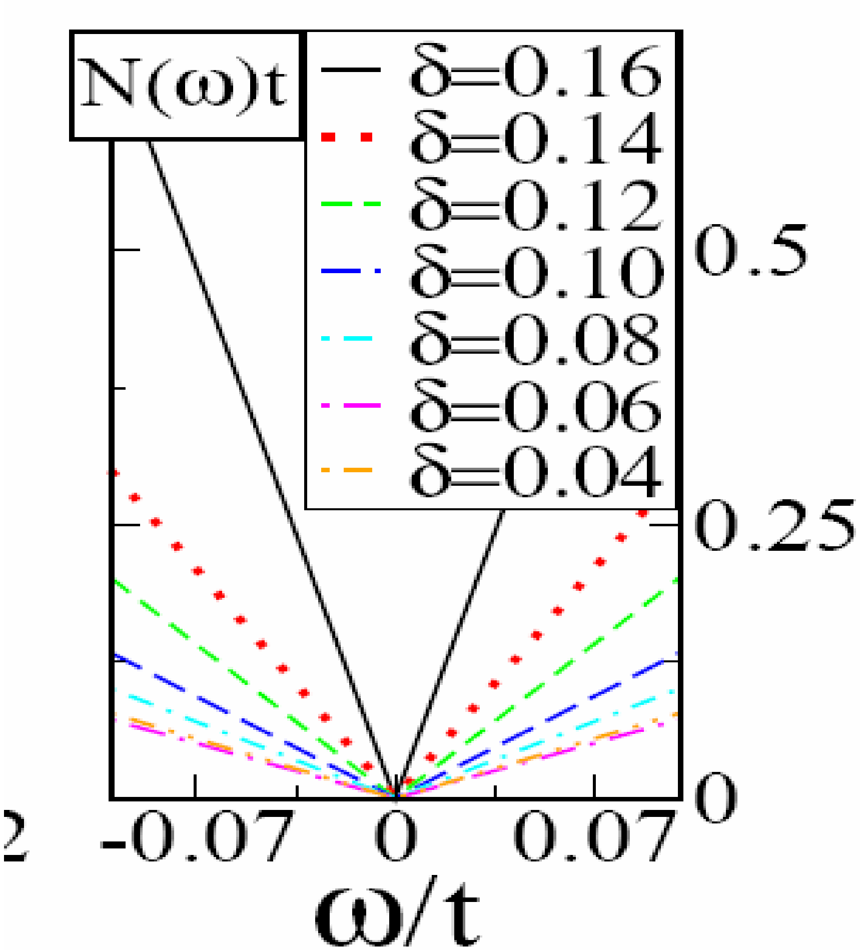


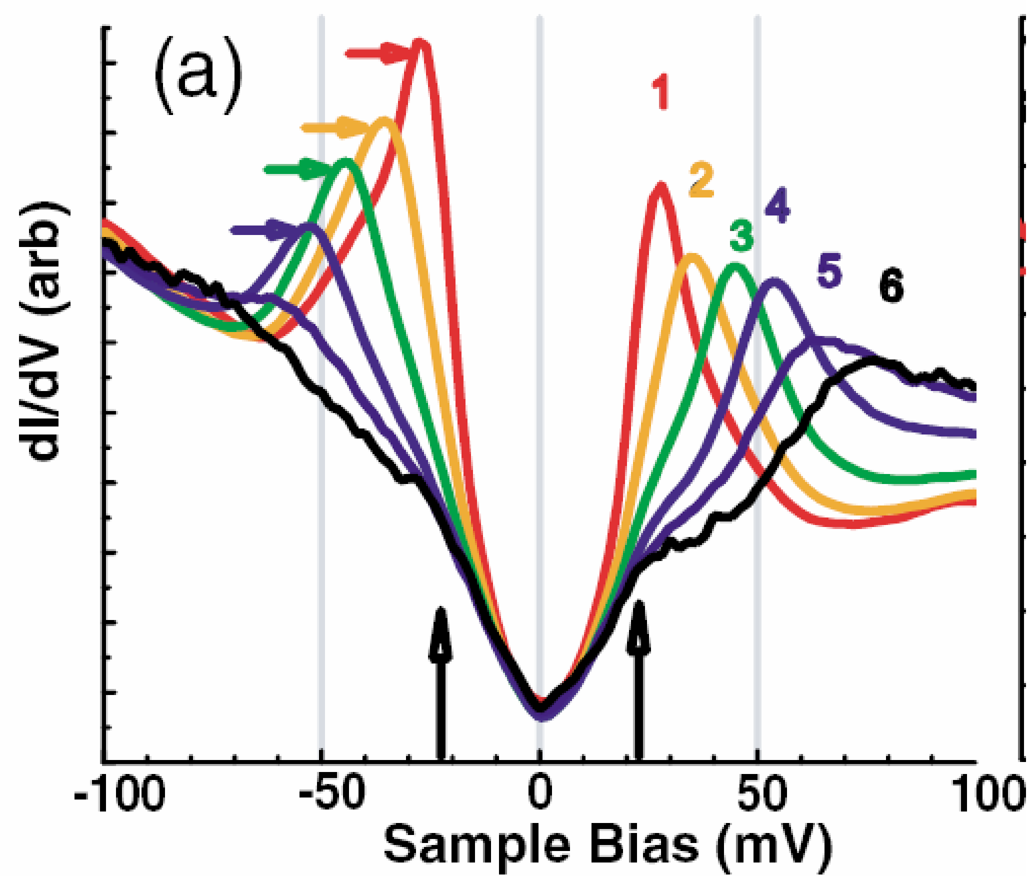

Tanaka et al. Science 314, 1910 (2006)

# Local density of states

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

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

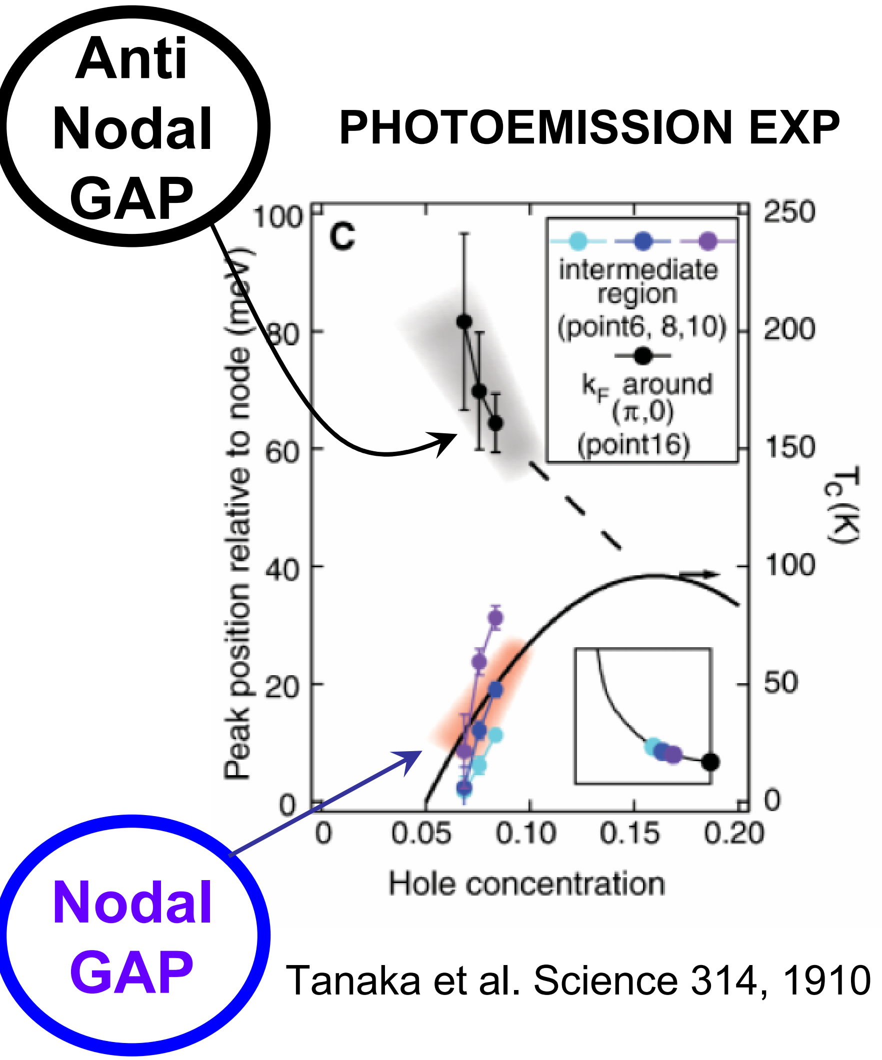


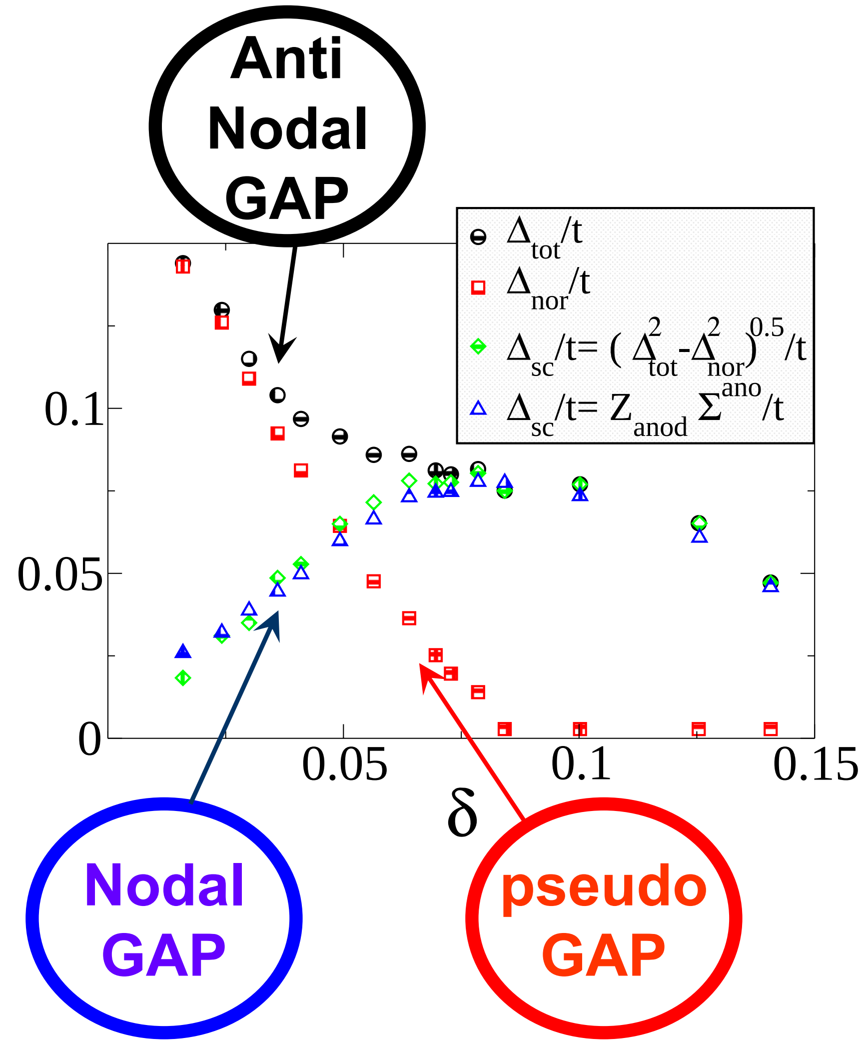

K. McElroy et al., Phys. Rev. Lett. 94, 197005 (2005).

# 2 ENERGY GAPS !

From quasi-particle spectra
we measure gaps!




Tanaka et al. Science 314, 1910 (2006)



# 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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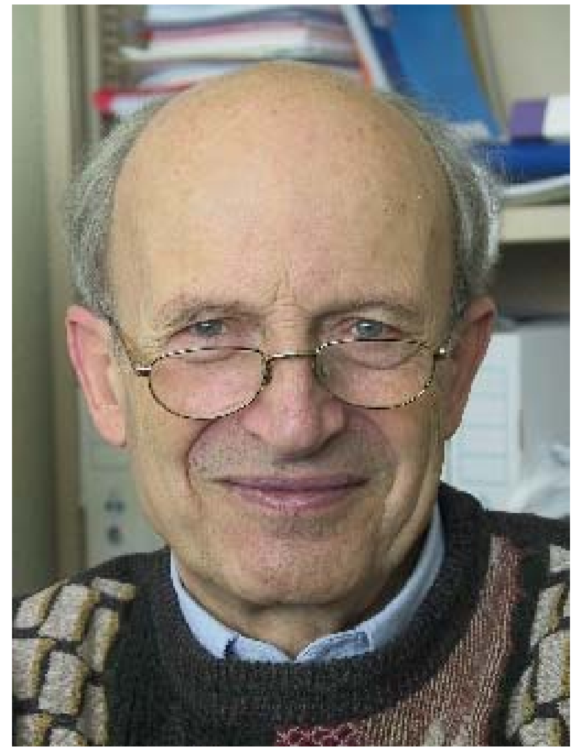
# SPECIAL THANKS TO:

E. KATS



P. NOZIÈRES