

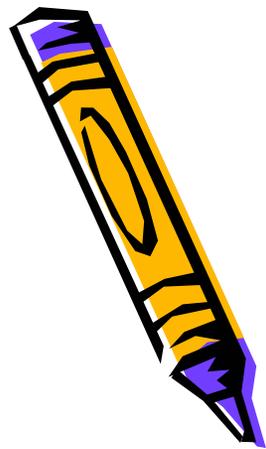


The doping-driven evolution of the superconducting state of a doped Mott insulator

[arXiv:0808.3948](https://arxiv.org/abs/0808.3948)

Marcello Civelli

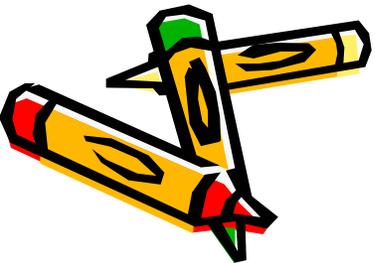
Plan de l'exposé



1) **Les supraconducteurs haute- T_c** :
électrons fortement corrélés
échec des méthodes perturbatives

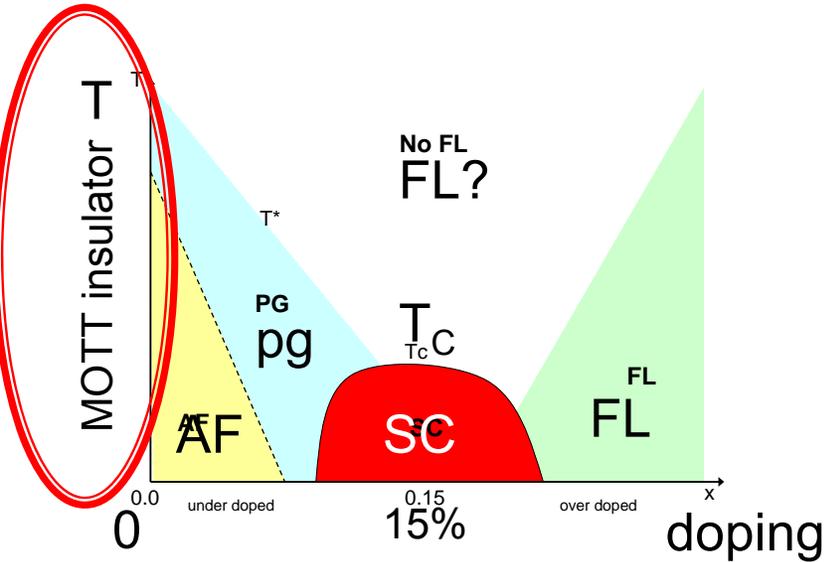
2) **Cellular Dynamical Mean Field Theory:**
extension cluster de la DMFT
une étude plaquette-CDMFT

3) **Etude de l'état supraconducteur d-wave**
Comparaison avec les expériences:
photoémission, Raman, tunneling,
magnéto-transport

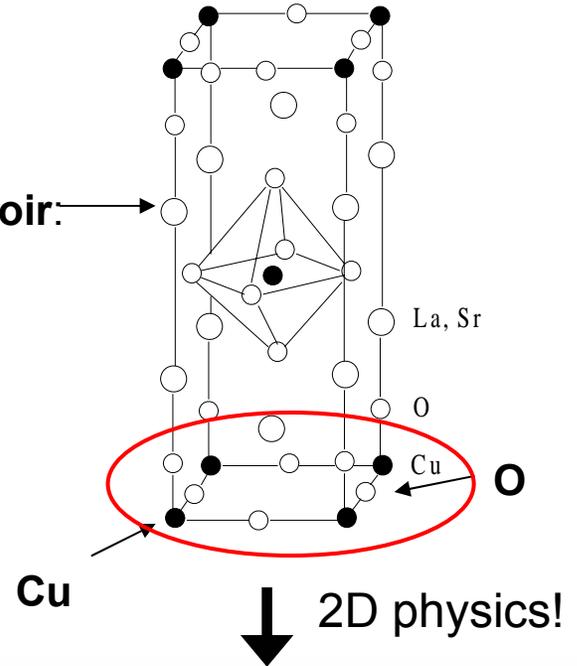


Les Supraconducteurs H-Tc

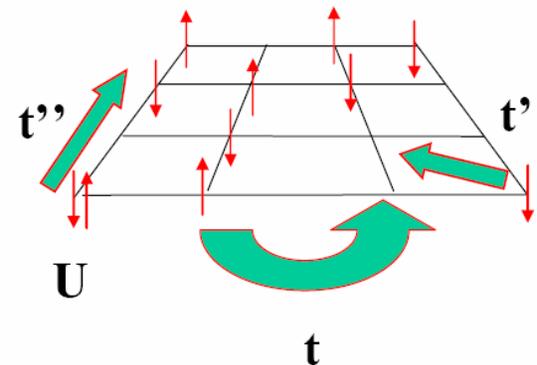
1986 Bednorz and Muller



Reservoir:
La, Sr

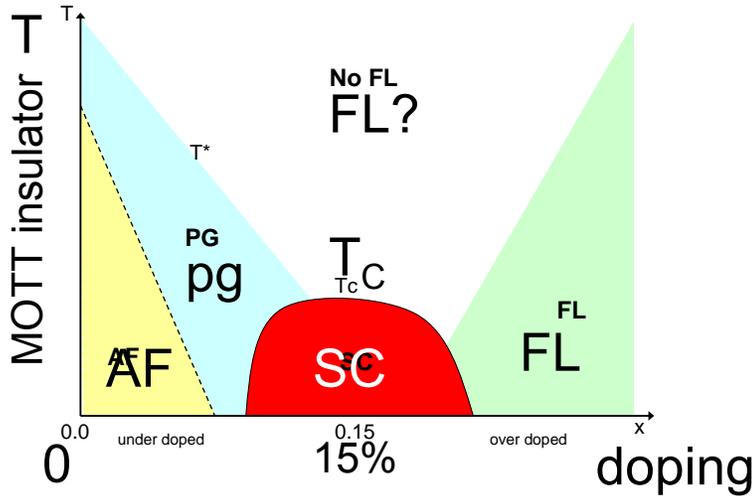


- FL → Fermi Liquid
- SC → superconducting
- pg → Pseudo-Gap
- AF → Antiferromagnetism

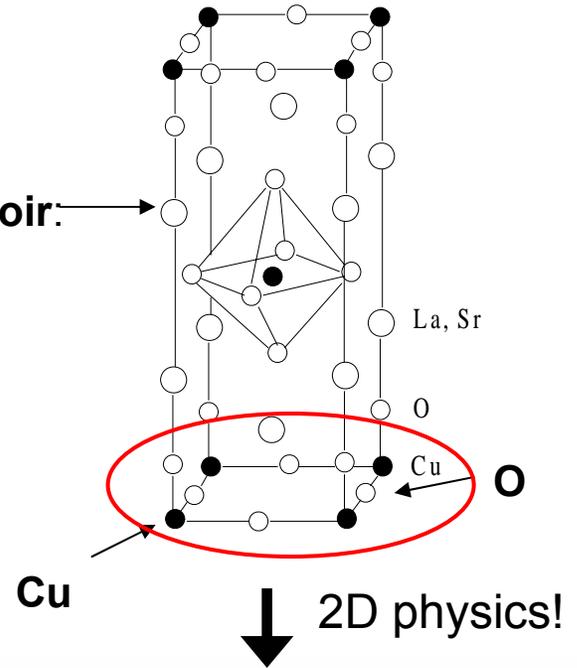


Les Supraconducteurs H-Tc

1986 Bednorz and Muller

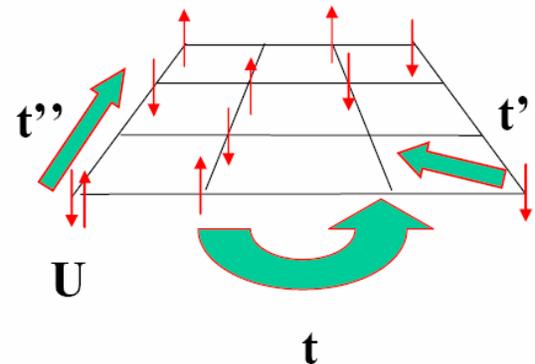


Reservoir:
La, Sr



échec des méthodes perturbatives

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

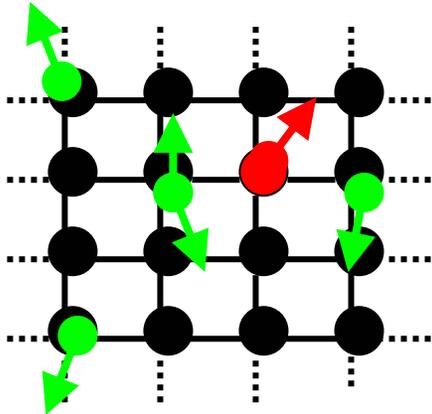


Une méthode puissante pour les systèmes fortement corrélés:

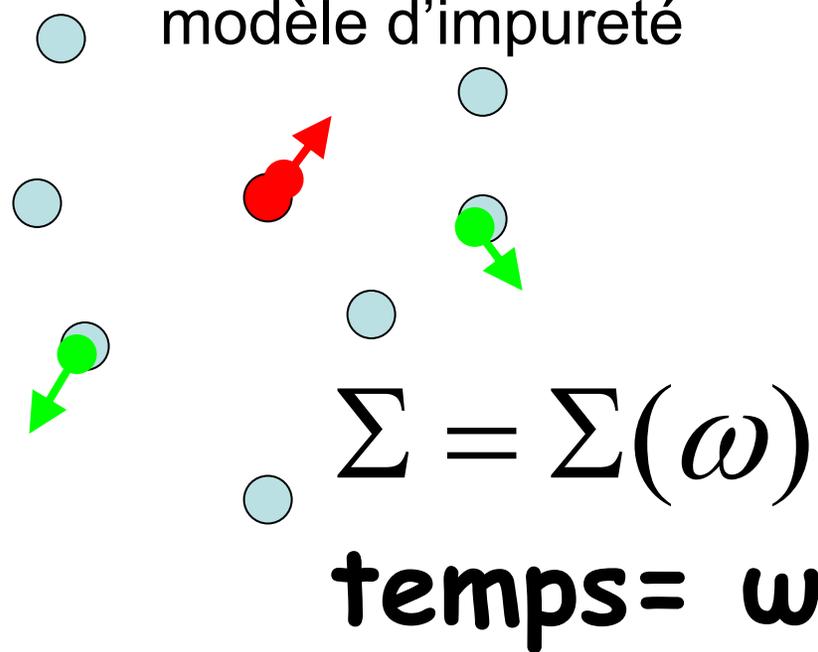
DMFT

A. Georges et al. Rev. Mod. Phys. 68, 13 1996

réseau



modèle d'impureté

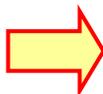


$$\Sigma = \Sigma(\omega)$$

temps = ω

Problème:

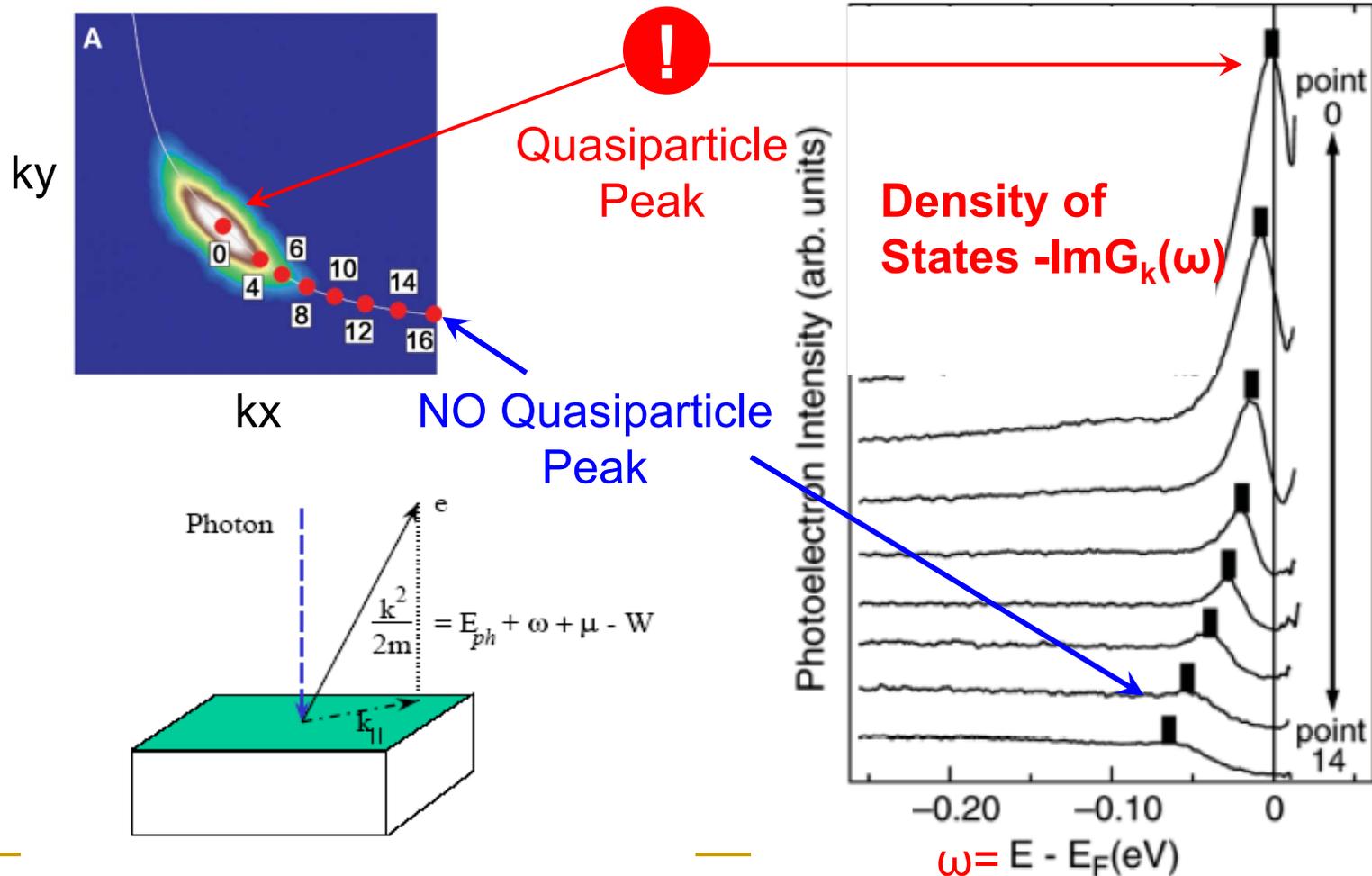
$$\Sigma \neq \Sigma(k) \text{ locale}$$



$$\frac{1}{\tau_k} = -\text{Im}\Sigma_k$$

Scattering properties

DICHOTOMIE NODALE/ANTINODALE: preuve expérimentale ARPES



Taken from Tanaka et al. Science 314, 1910 (2006)

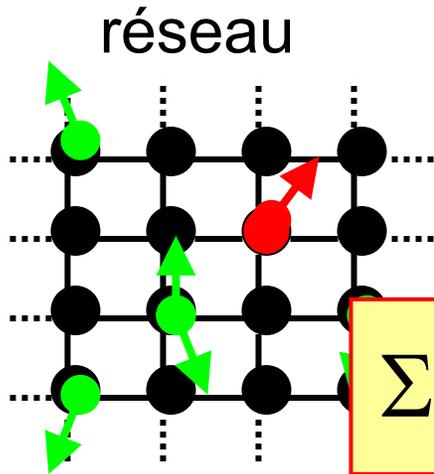
$$\frac{1}{\tau_k} = -\text{Im} \Sigma_k$$



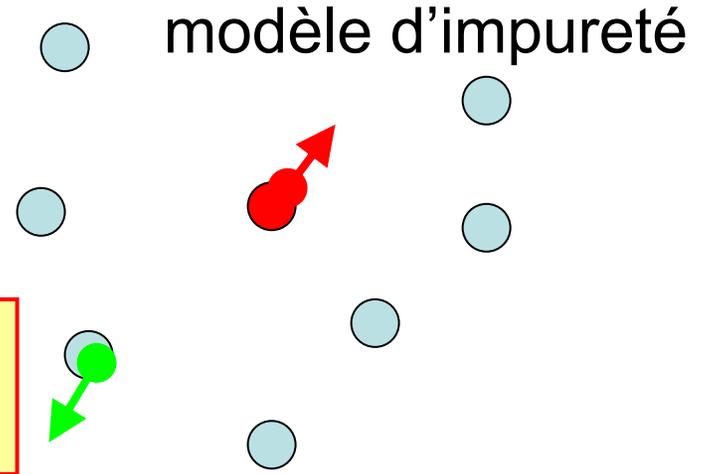
Il faut aller au delà de la
théorie locale (DMFT)?

DMFT

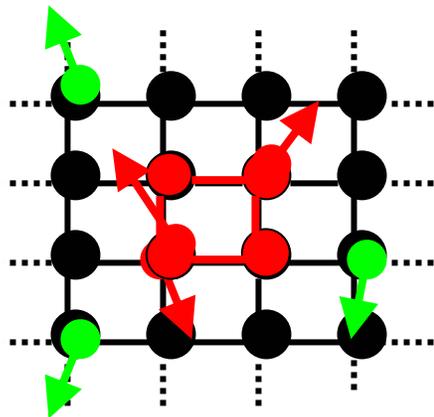
A. Georges et al. Rev. Mod. Phys. 68, 13 1996



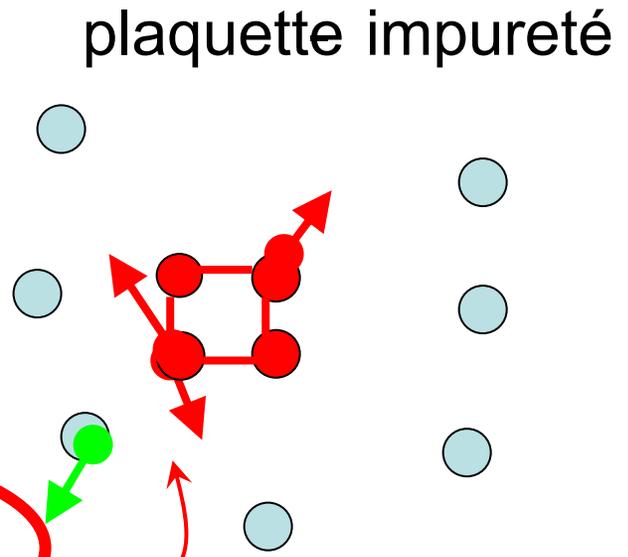
$\Sigma \neq \Sigma(k)$ locale



Cellular DMFT

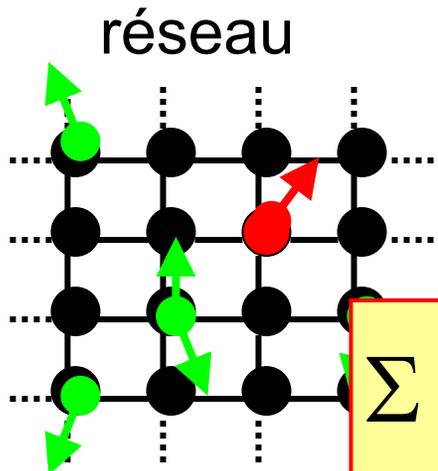


corrélations à courte portée

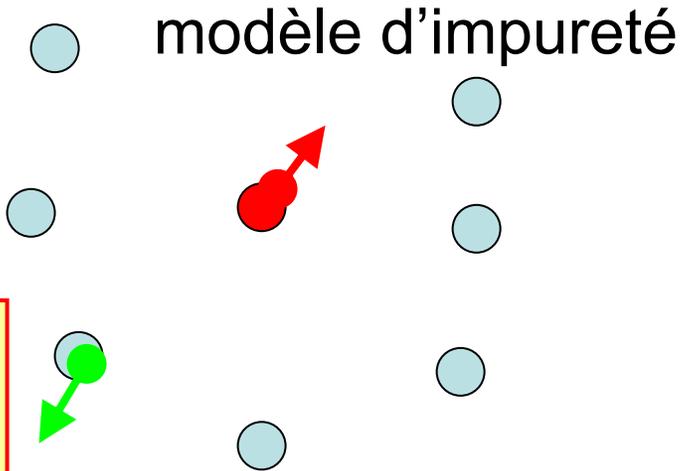


DMFT

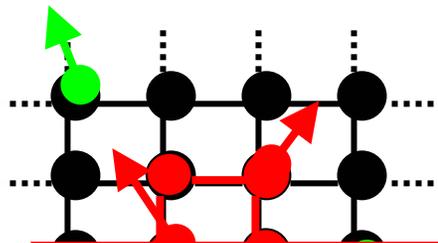
A. Georges et al. Rev. Mod. Phys. 68, 13 1996



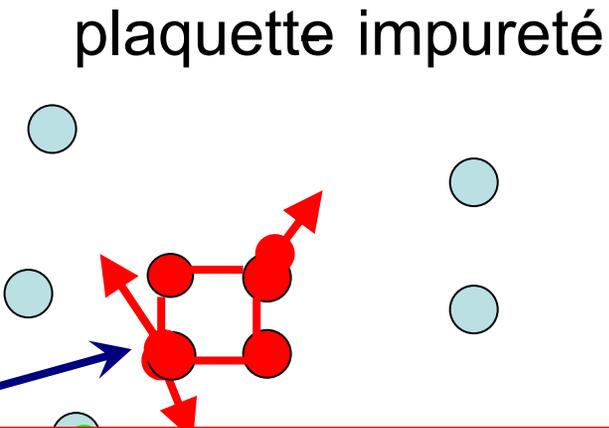
$$\Sigma \neq \Sigma(k) \text{ locale}$$



Cellular DMFT



$$\Sigma(k) \square \Sigma_{11} + \frac{1}{2} \Sigma_{12} (\cos k_x + \cos k_y) + \frac{1}{4} \Sigma_{13} \cos k_x \cos k_y$$



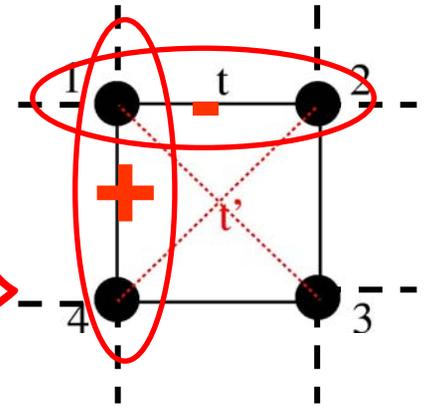
Etude CDMFT sur une plaquette

→ Préserve la symétrie carrée du réseau

→ Avec CMFT on sort peu de paramètres:
self-énergie du cluster

$$\Sigma_{11}, \Sigma_{12}, \Sigma_{13} \rightarrow \langle c_{1\uparrow}^\dagger c_{2\uparrow} \rangle$$

Fonction de paires $\Sigma_{ano} \rightarrow \langle c_{1\uparrow} c_{2\downarrow} \rangle$



→ Configuration minimale qui permet d'étudier l'état supra

Toutes les infos sont dérivées par la fonction de Green

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

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

Comment on sort la dépendance en k?

Par exemple Σ_k

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

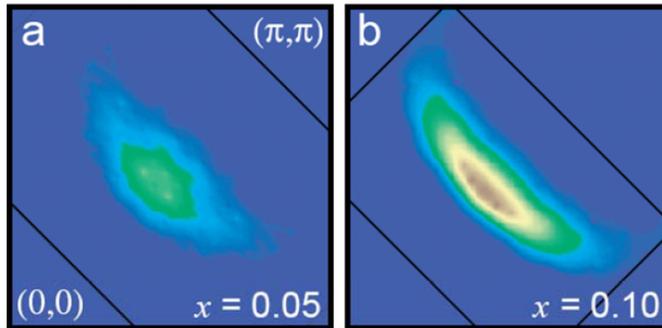
Transition de Mott dans l'Etat Normal: hot/cold Spots

Civelli et al., PRL 95, 106402 ('05)

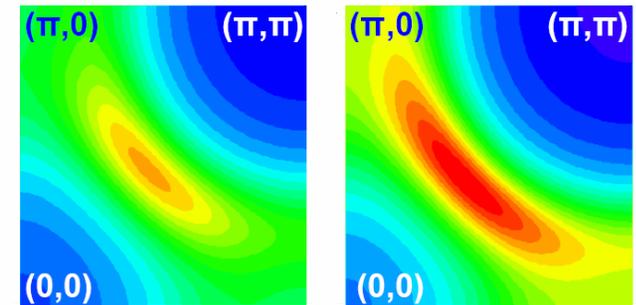
$$A(\omega) = -\frac{1}{\pi} \text{Im} G_{\sigma}(k, \omega)$$

Expériences en fonction
du dopage x

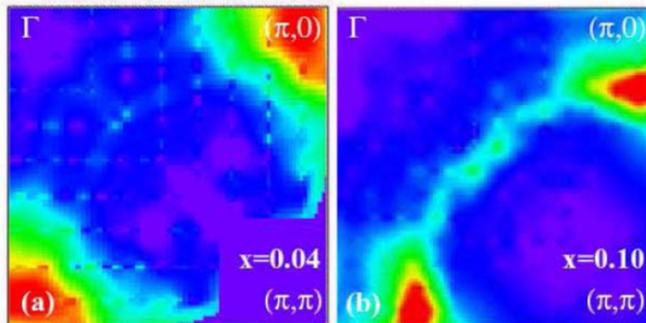
hole doped



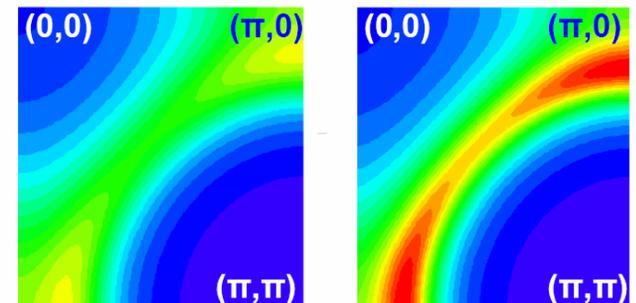
hole doped



e- doped

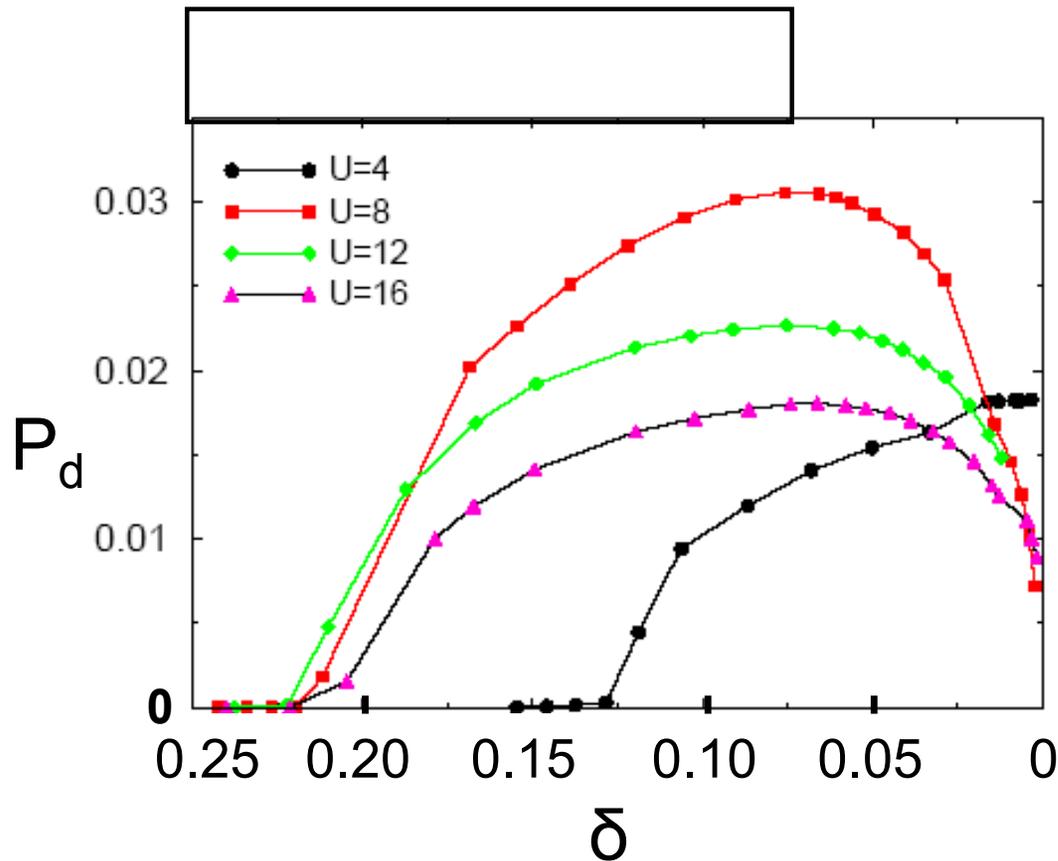


e- doped



Etat supra d-wave !

parametre d'ordre $P_d = \langle c_{\uparrow} c_{\downarrow} \rangle$ dans le modele de Hubbard

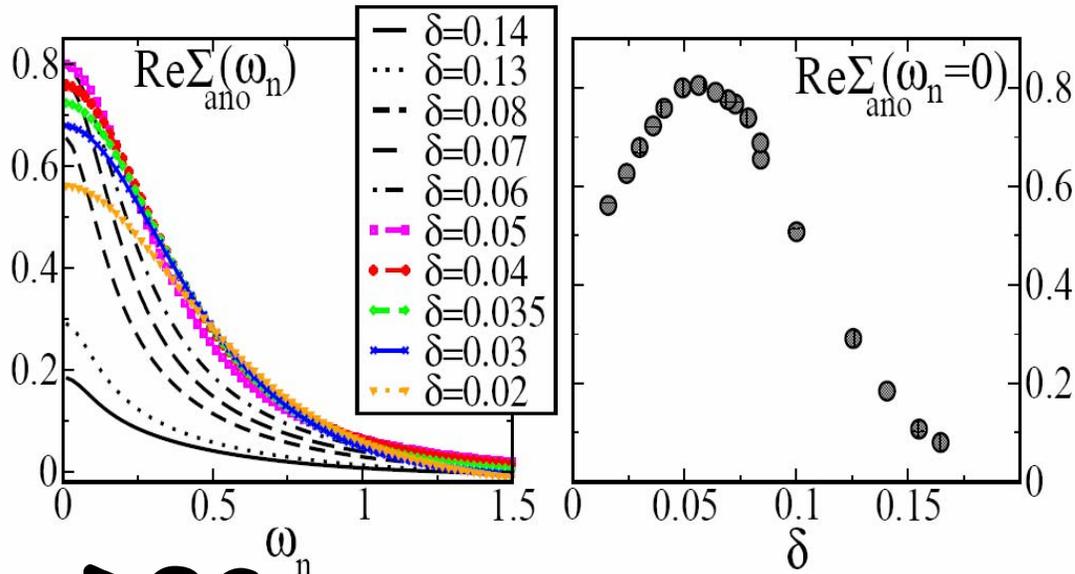


S.S Kancharla et al, PRB '08

M. Civelli et al. [PRL '08](#)

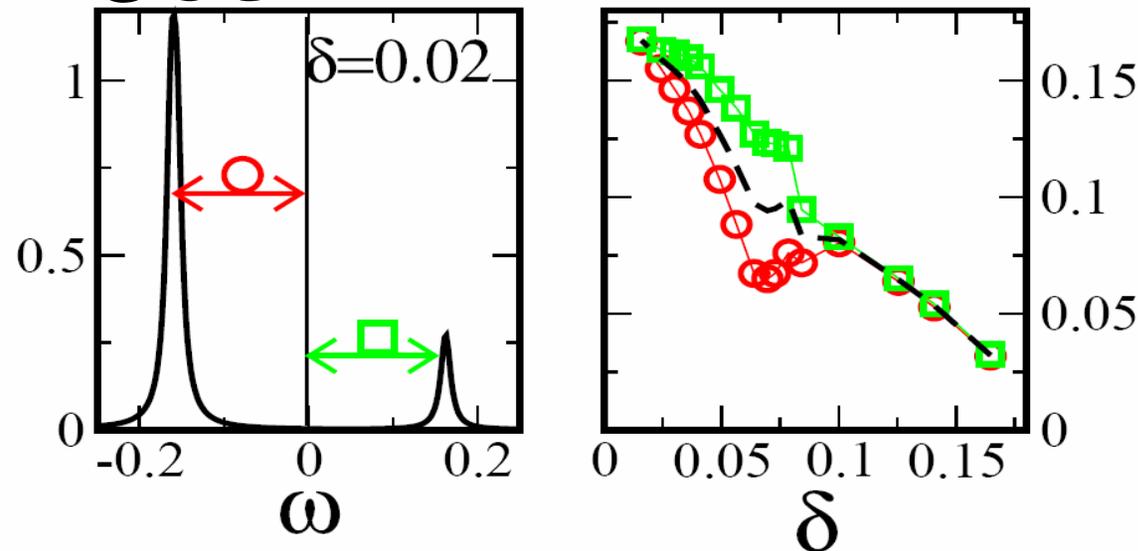
Résultats cluster: deux échelles d'énergie

$$U=12t \quad t'=-0.3t$$



**Non-monotone
avec le dopage δ !**

DOS



**Monotone avec
le dopage δ !**

Objectif: lien avec les expériences

cluster

$$\Sigma_{\mu\nu}$$

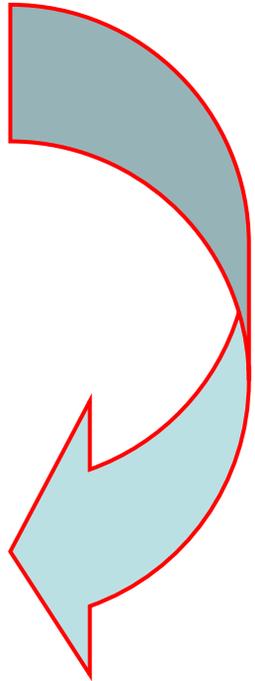
?

réseau

$$\Sigma(k)$$



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



Fonction de Green dans l'état SUPRA

$$\hat{G}_{k\sigma}^{-1}(\omega) = \begin{pmatrix} \omega - t_k - \underline{\Sigma_{\sigma}^{\text{nor}}(k, \omega)} & -\underline{\Sigma^{\text{ano}}(k, \omega)} \\ -\Sigma^{\text{ano}}(k, \omega) & \omega + t_k + \Sigma_{\sigma}^{\text{nor}}(k, -\omega)^* \end{pmatrix}$$

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

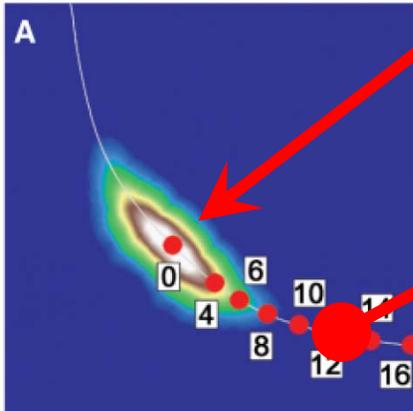
1ere hypothèse: forme d-wave pour la fonction d'appariement de Cooper

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

2eme hypothèse: Dichotomie nodale/antinodale

métal

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



Isolant: cumulant

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

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

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

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

TEST: état isolant en 2D

Σ
 M

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

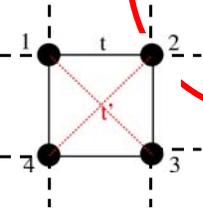
periodize

$G_k(\omega)$

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

K-space

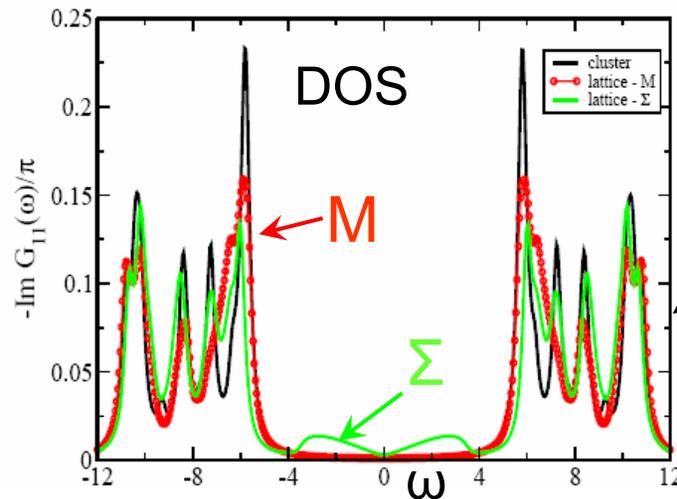
cluster



local

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

Σ
états
dans le gap
De Mott

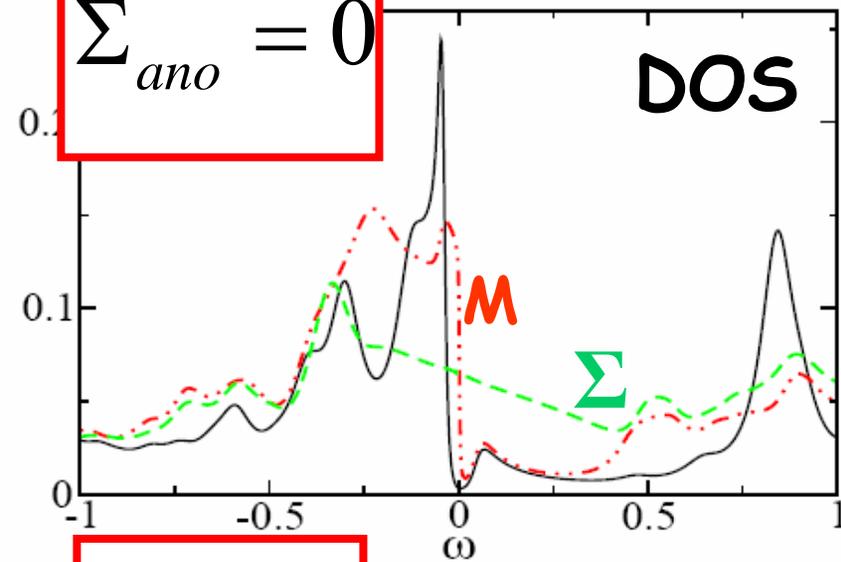


INSULATOR

5% doping

Test auto-consistent

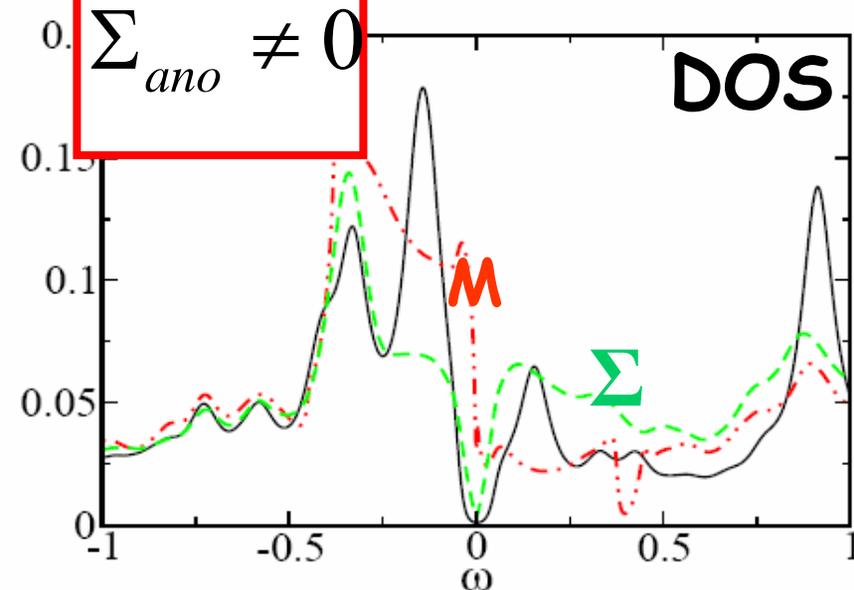
$$\Sigma_{ano} = 0$$



- Cluster DOS
- - - Self-energy Σ
- . - . cumulant M

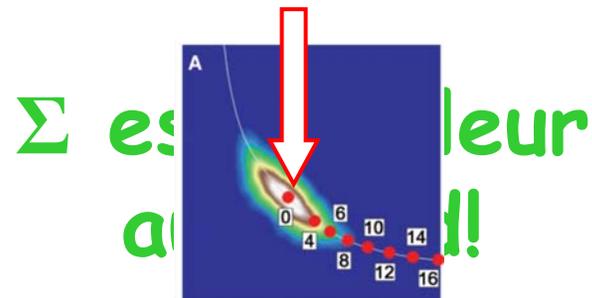
M décrit mieux le pseudo gap !

$$\Sigma_{ano} \neq 0$$



$$N(\omega) = -\frac{1}{\pi} \sum_k \text{Im} G_{\sigma}^{11}(k, \omega) \sim \frac{1}{\pi} \frac{Z_{nod}}{U_{nod} U_{\Delta}} \omega$$

Sélection du noeud!

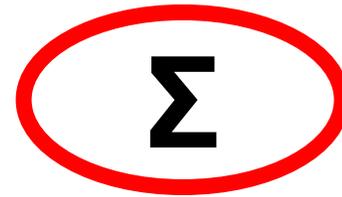


Le message pour aller dans l'espace k

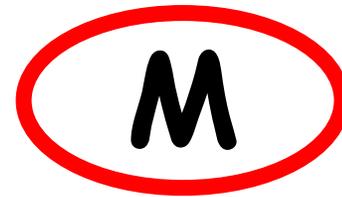
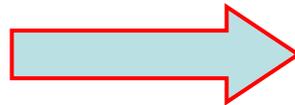
d-wave
pairing

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

Liquide de Fermi
Nœud

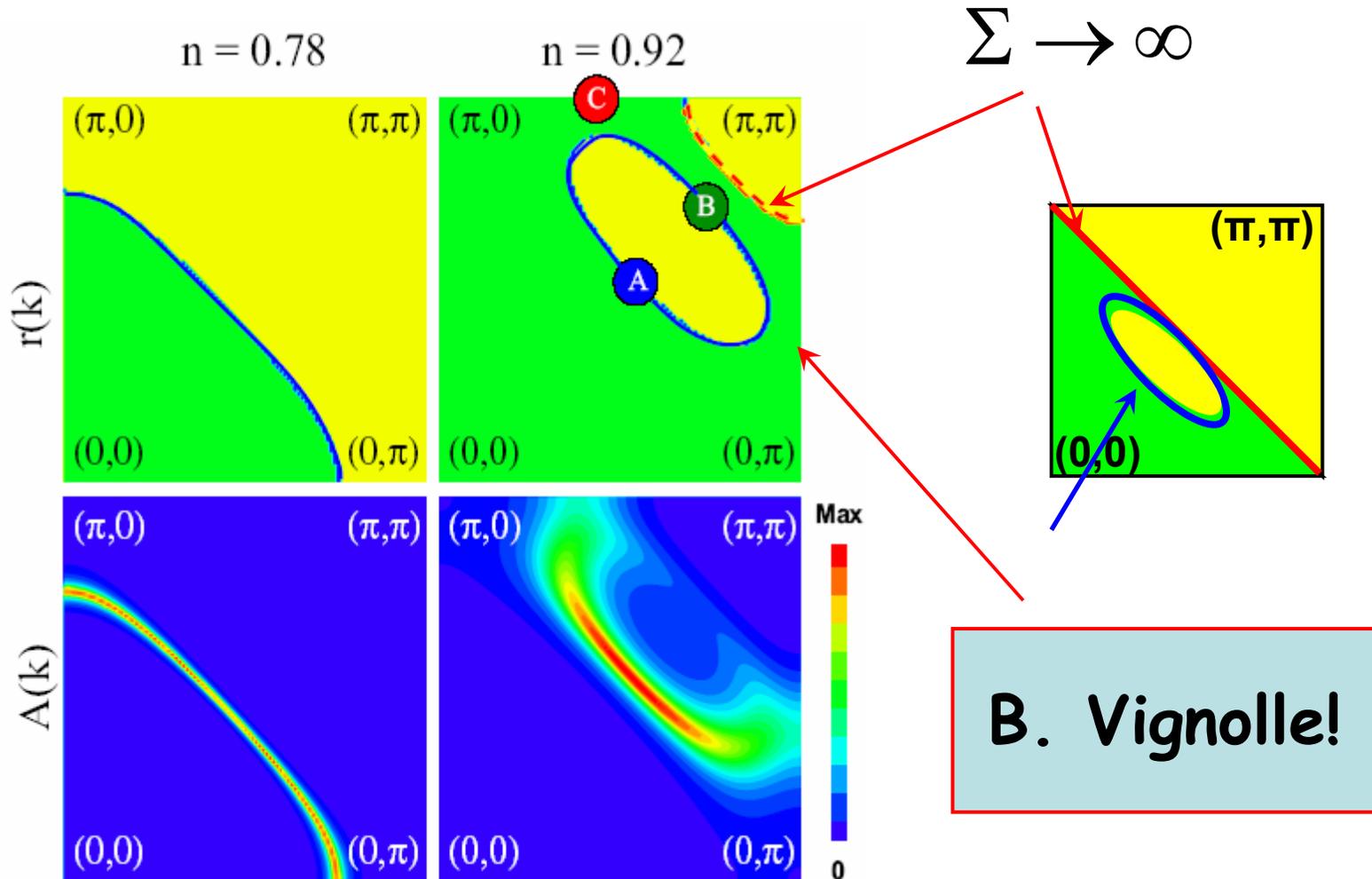


Isolant
Anti-nœud



La description donnée par M

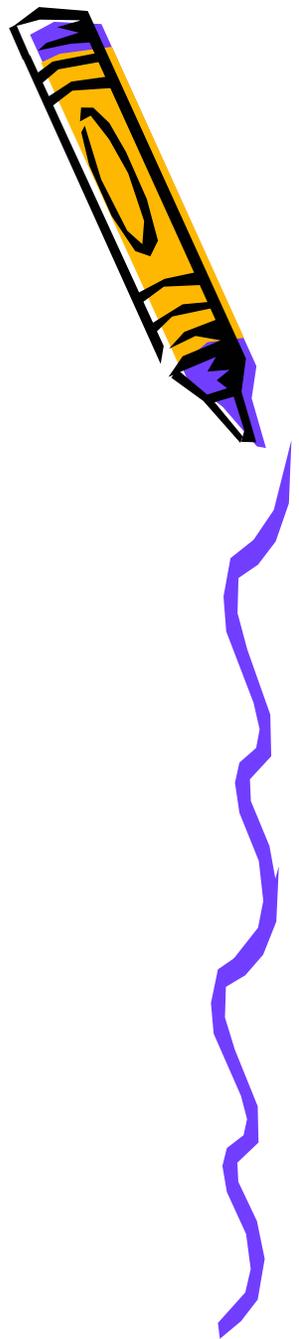
T. Stanescu et al. PRB, 74 06



Propriétés aux

nœud et

anti-nœud



Nœud:

on fait un développement à bas $\omega \rightarrow 0$

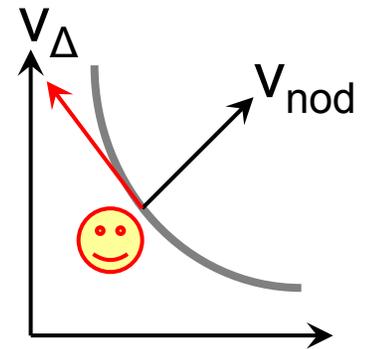
$$G_{k\sigma}^{-1}(\omega) = \begin{pmatrix} \omega - \varepsilon_k - \Sigma_{\sigma}^{\text{nor}}(k, \omega) & -\Sigma^{\text{ano}}(k, \omega) \\ -\Sigma^{\text{ano}}(k, \omega) & \omega + \varepsilon_k + \Sigma_{\sigma}^{\text{nor}}(k, -\omega)^* \end{pmatrix}$$

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

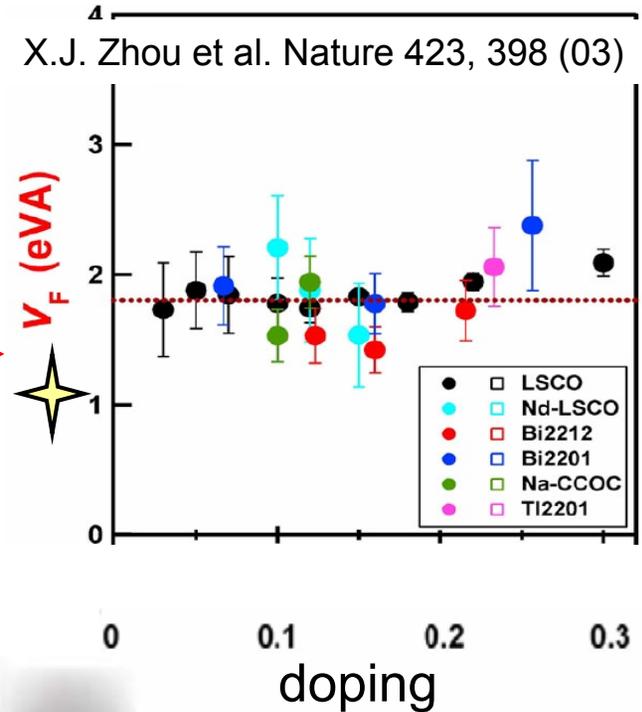
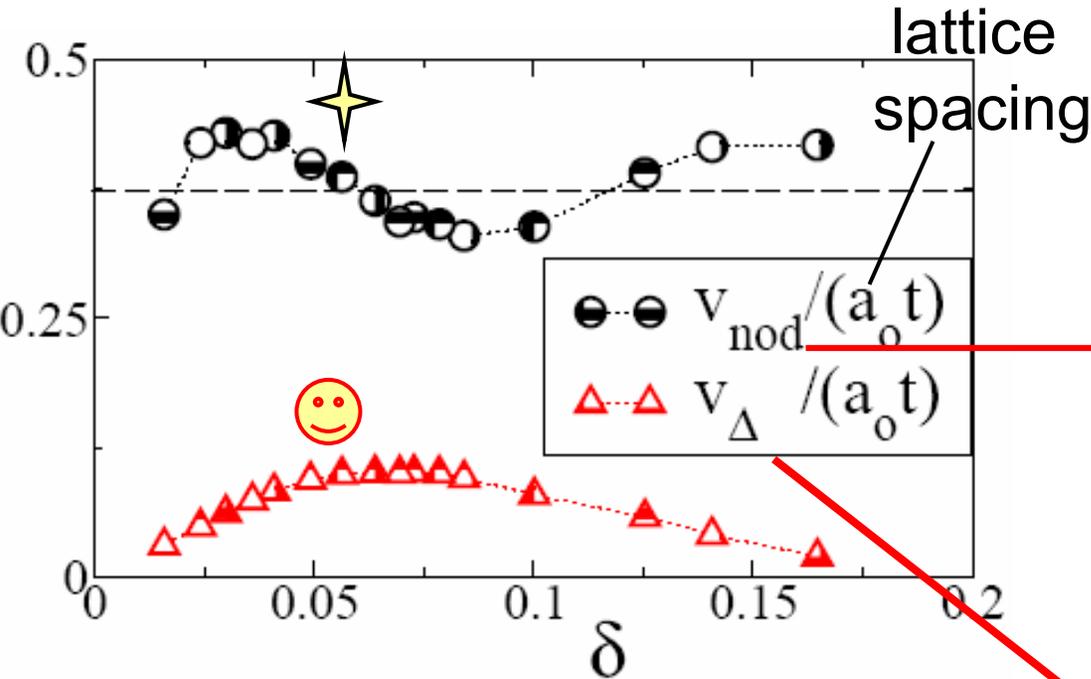
$$\mathcal{Z}_{\text{nod}} = (1 - \partial_{\omega} \text{Re}\Sigma_k(\omega))^{-1} \Big|_{\omega=0}$$

$$v_{\text{nod}} = \mathcal{Z}_{\text{nod}} |\nabla_k \xi_k^0|$$

$$v_{\Delta} = \mathcal{Z}_{\text{nod}} |\nabla_k \Sigma^{\text{ano}}(k)|$$



Vélocités au nœud Analyse de liquide de Fermi

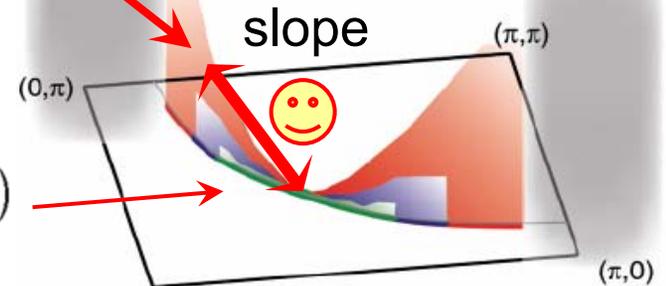


$$\xi_k^0 \equiv \varepsilon_k + \text{Re}\Sigma^{nor}(k, 0)$$

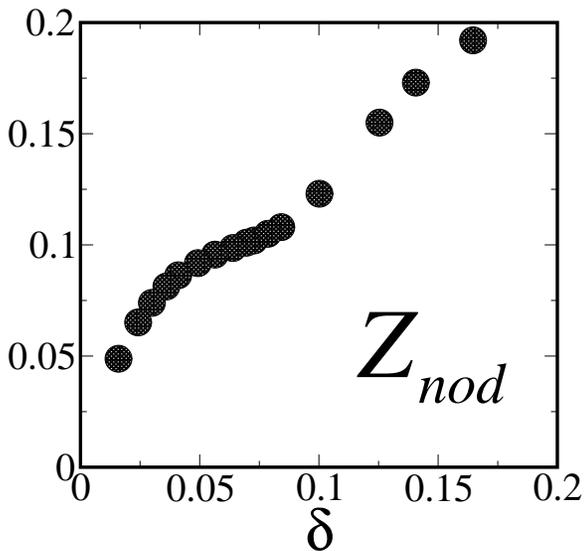
$$Z_{nod} = (1 - \partial_{\omega} \text{Re}\Sigma_k(\omega))^{-1} \Big|_{\omega=0}$$

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

$$v_{\Delta} = Z_{nod} |\nabla_k \Sigma^{ano}(k)| \sim \underline{Z_{nod} \Sigma_{12}^{ano}(\omega \rightarrow 0)}$$



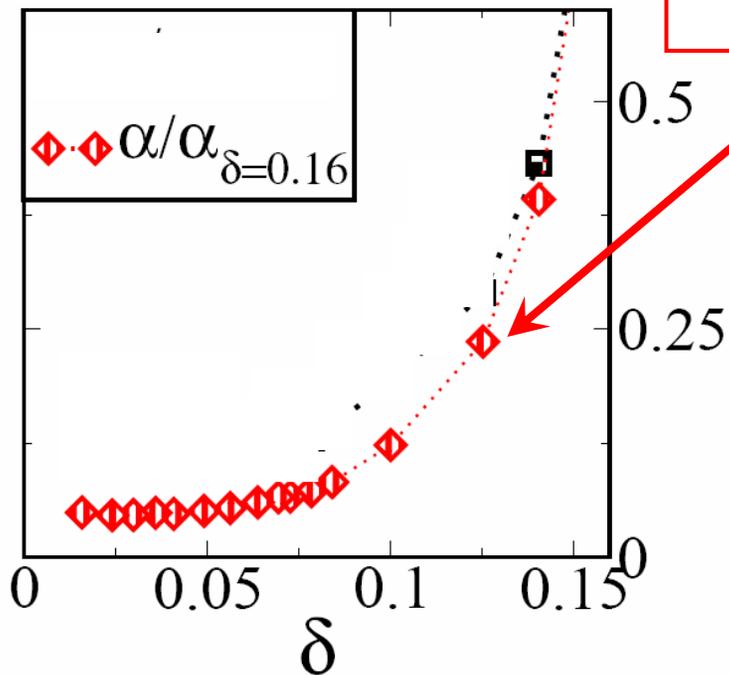
Quantités qu'on peut extraire au nœud $\omega \rightarrow 0$



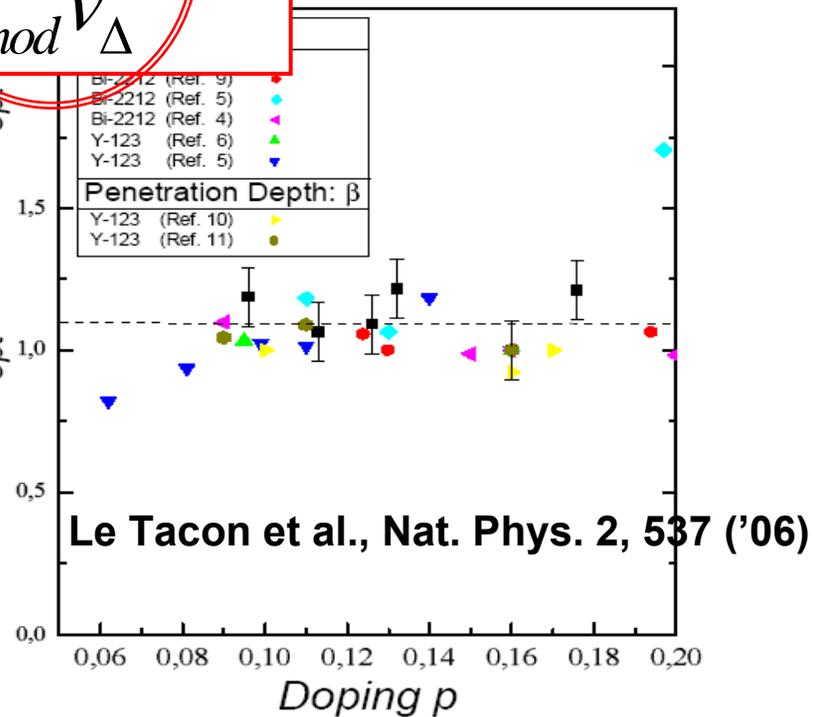
Raman response - superfluid density

$$\chi_{B_{2g}} \propto \frac{Z_{nod}^2}{v_{nod} v_{\Delta}} \omega$$

$$\rho_s(T) - \rho_s(0) \propto \alpha T$$

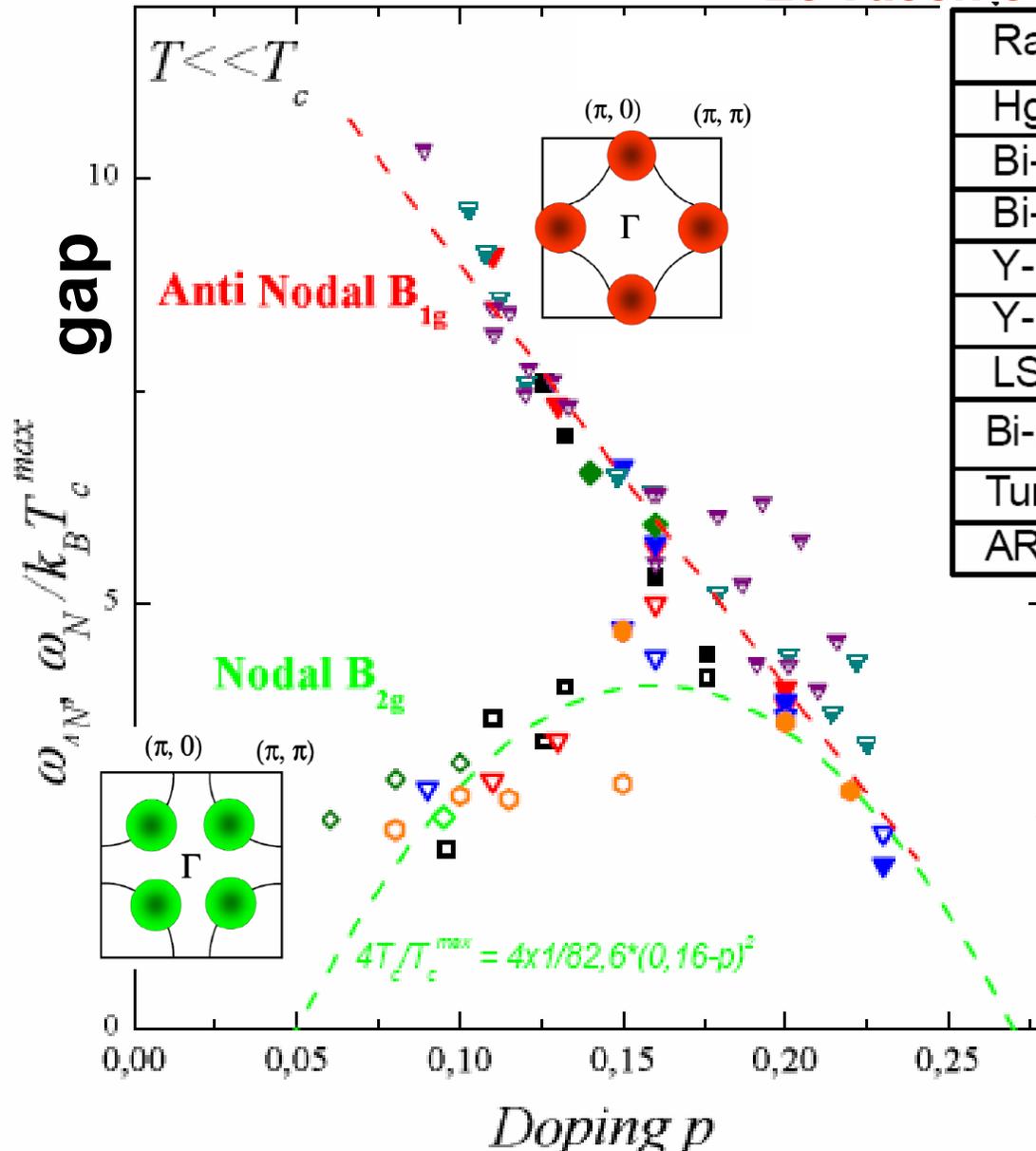


α



Résultats de spectroscopie Raman

Le Tacon et al. Nat. Phys.2 (2006)



Raman	B_{1g}	B_{2g}
Hg-1201 (This work)	■	□
Bi-2212 (Ref. xx)	▼	▽
Bi-2212 (Ref. xx)	▼	▽
Y-123 (Ref xx)	◆	◇
Y-123 (Ref. xx)	◆	◇
LSCO (Ref. xx)	●	○
Bi-2212 Δ_{max} form other techniques		
Tunneling (Ref. xx)		▽
ARPES (Ref. xx, xx, xx)		▽

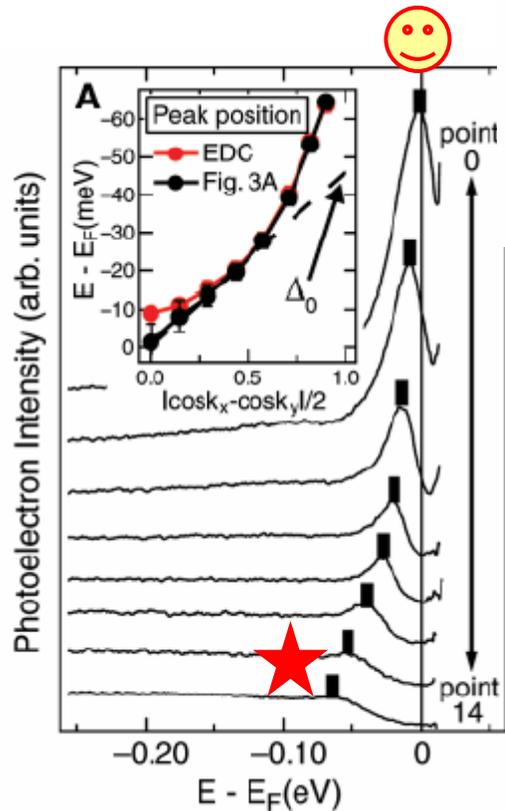
deux échelles
d'énergie
Différentes!

Anti-Nœud: ARPES SPECTRA

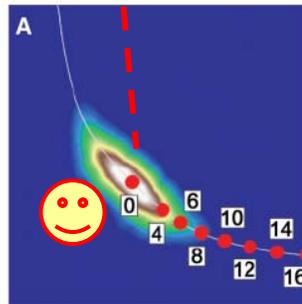
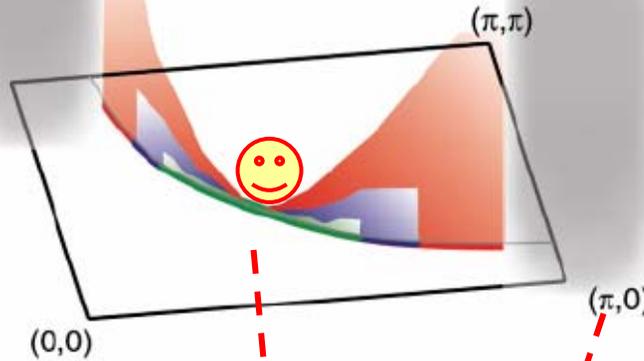
Tanaka et al. Science 314, 1910 (2006)

spectres

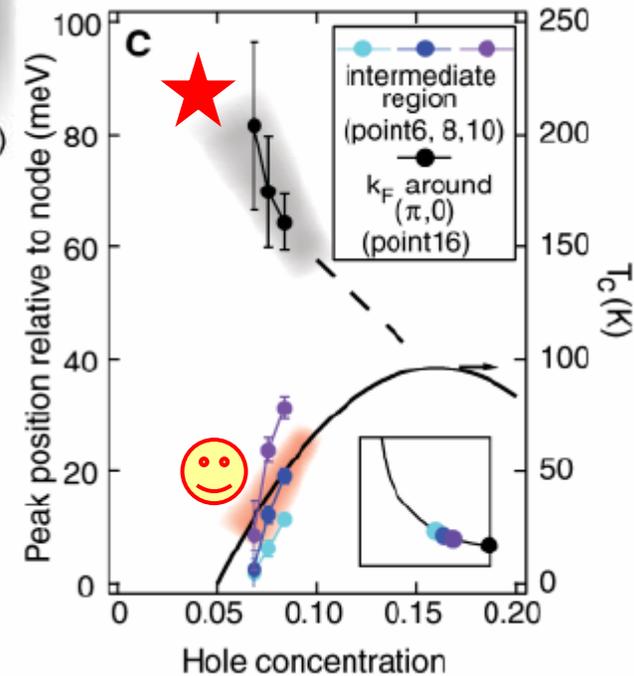
$$A(\omega) = -\frac{1}{\pi} \text{Im} G_{\sigma}^{11}(k, \omega)$$



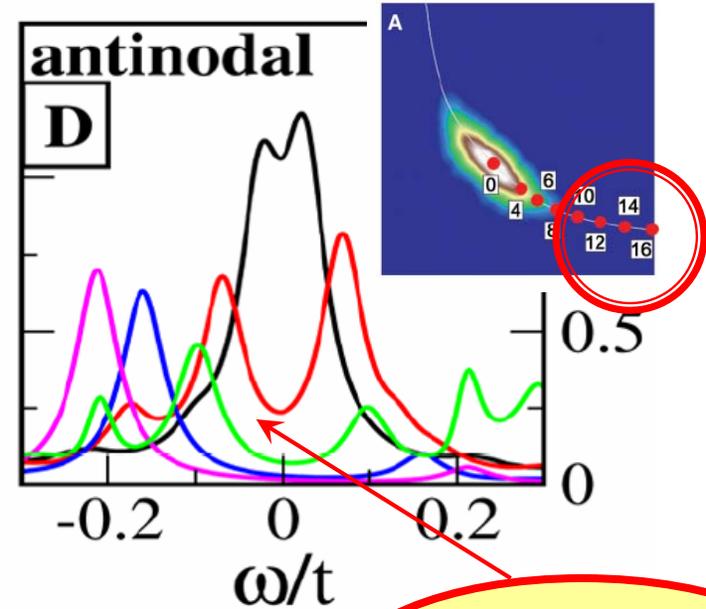
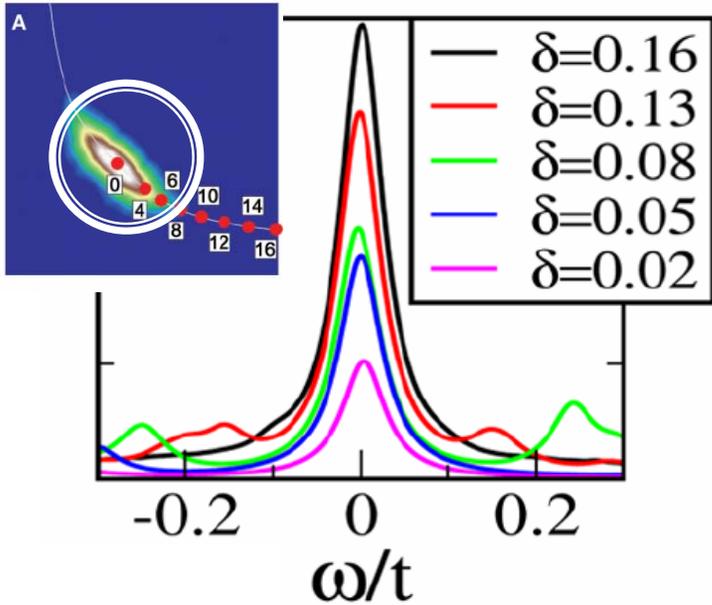
gaps



gaps

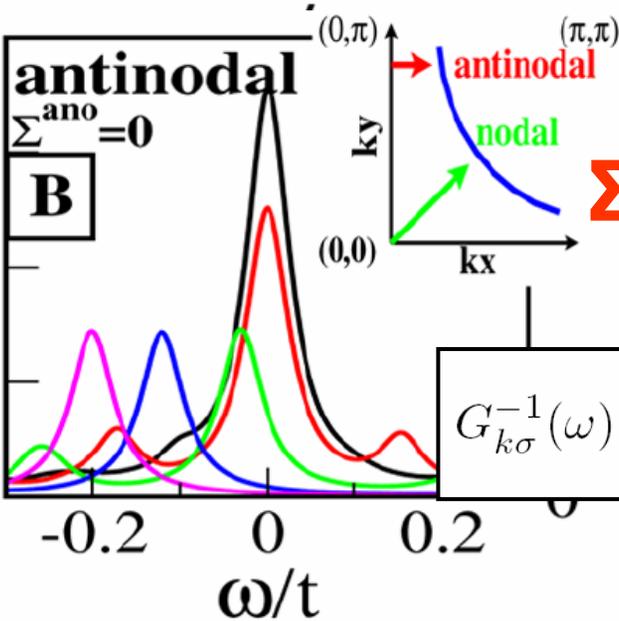
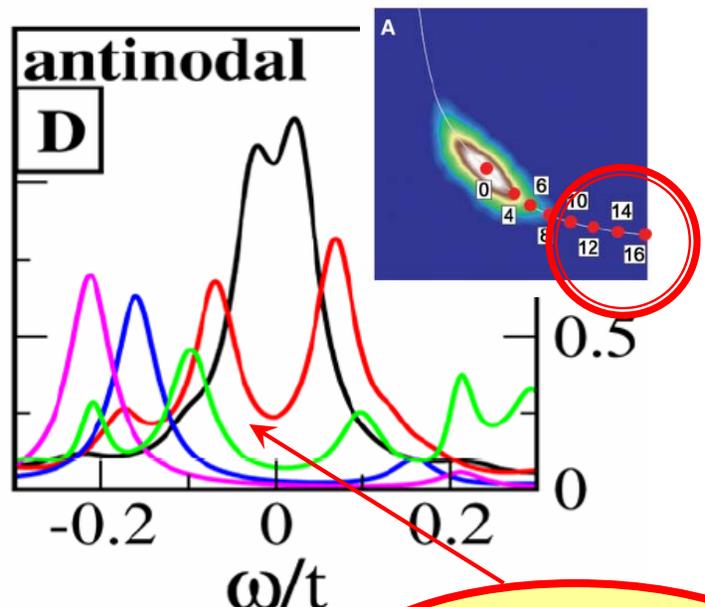
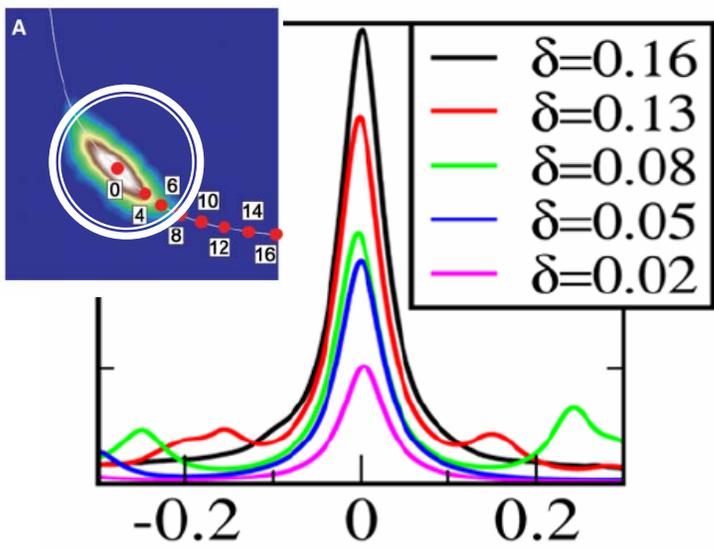


Spectre de quasiparticules CDMFT



asymmetry

Spectre de quasiparticules CDMFT

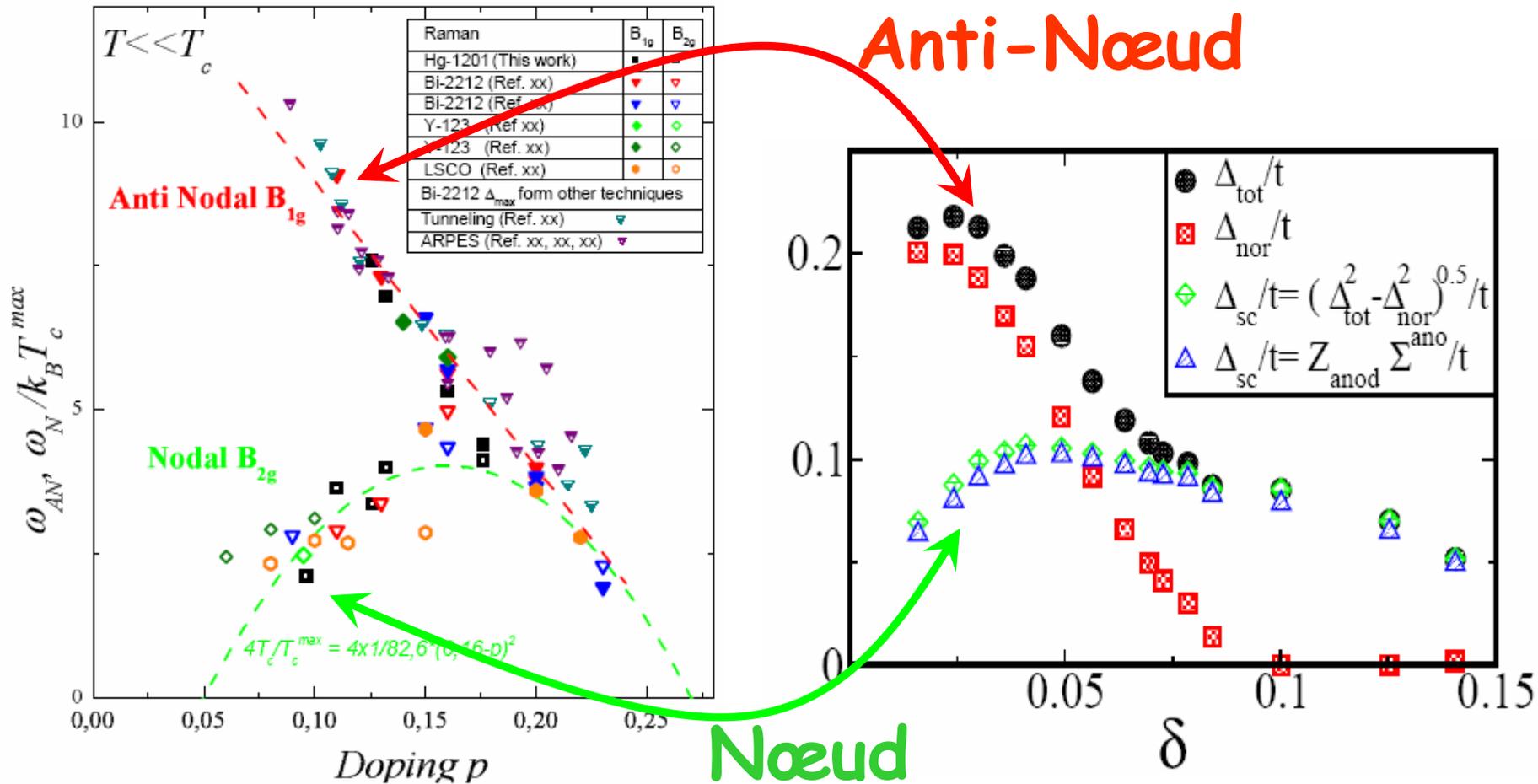


$\Sigma_{\text{ano}} = 0$

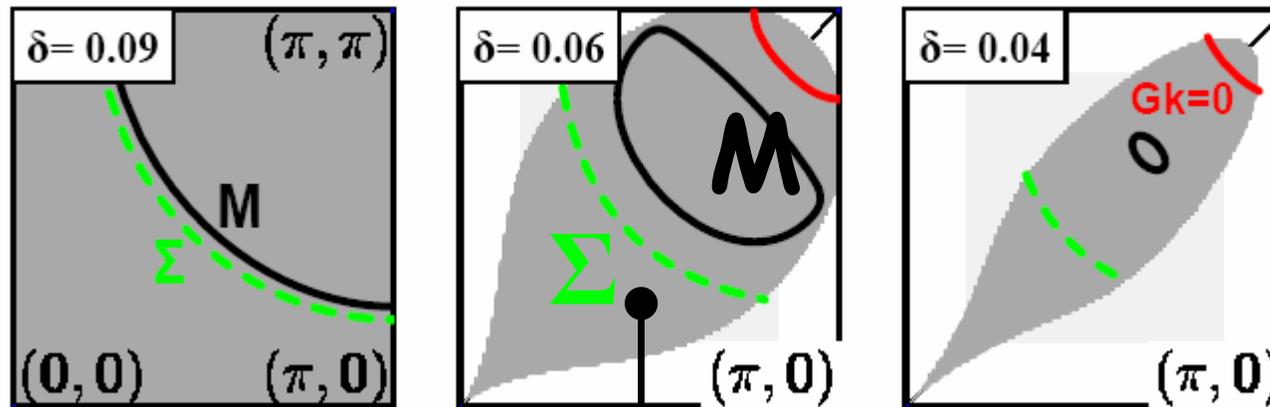
asymétrie

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

Deux gaps avec comportements différents selon le dopage



Extension à tout l'espace k



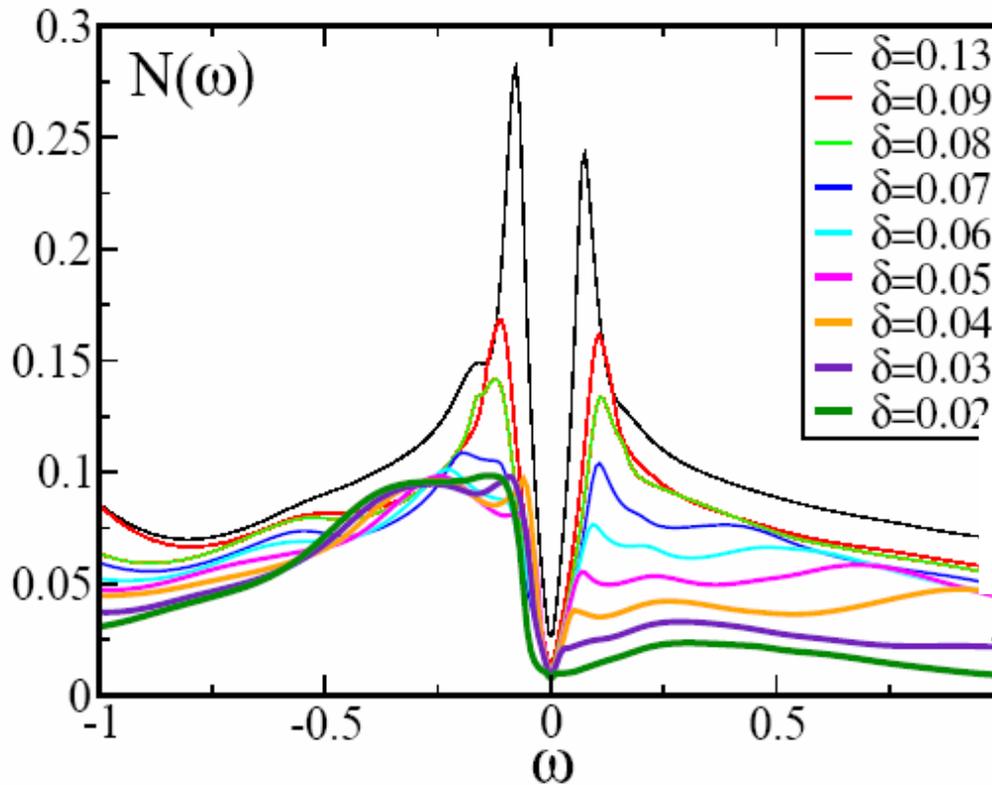
$\Phi(k)$ patch

Perali et al. EPJ B 24, 487 (2002)

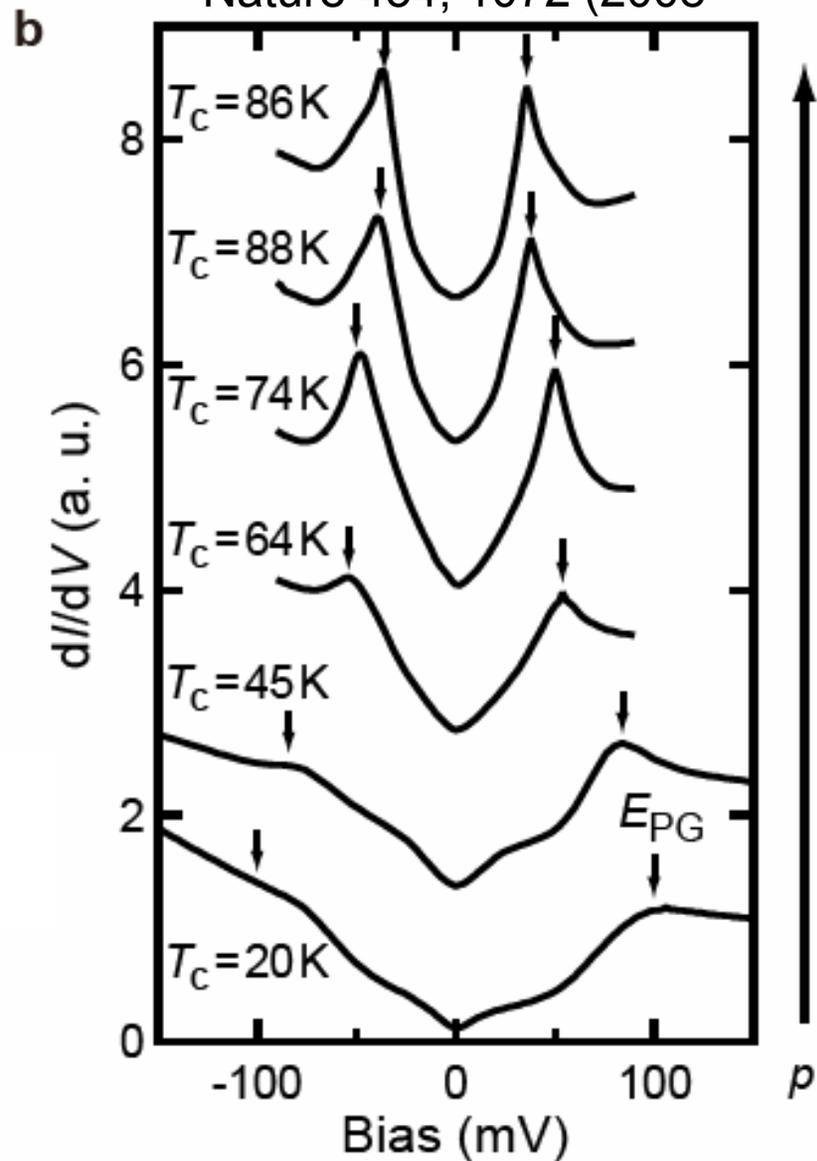
$$\Sigma_k(\omega) = \Phi(k, \omega) \Sigma_k(\omega) [\hat{\Sigma}] + [1 - \Phi(k, \omega)] \Sigma_k(\omega) [\hat{\mathcal{M}}]$$

Scanning tunnelling

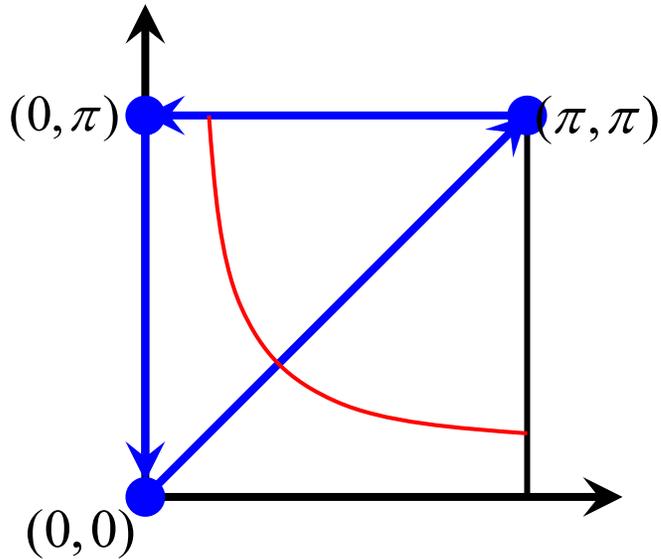
$$G_{11}(\omega) = \sum_k G(k, \omega)$$



e.g. Y. Kohsaka et al.
Nature 454, 1072 (2008)



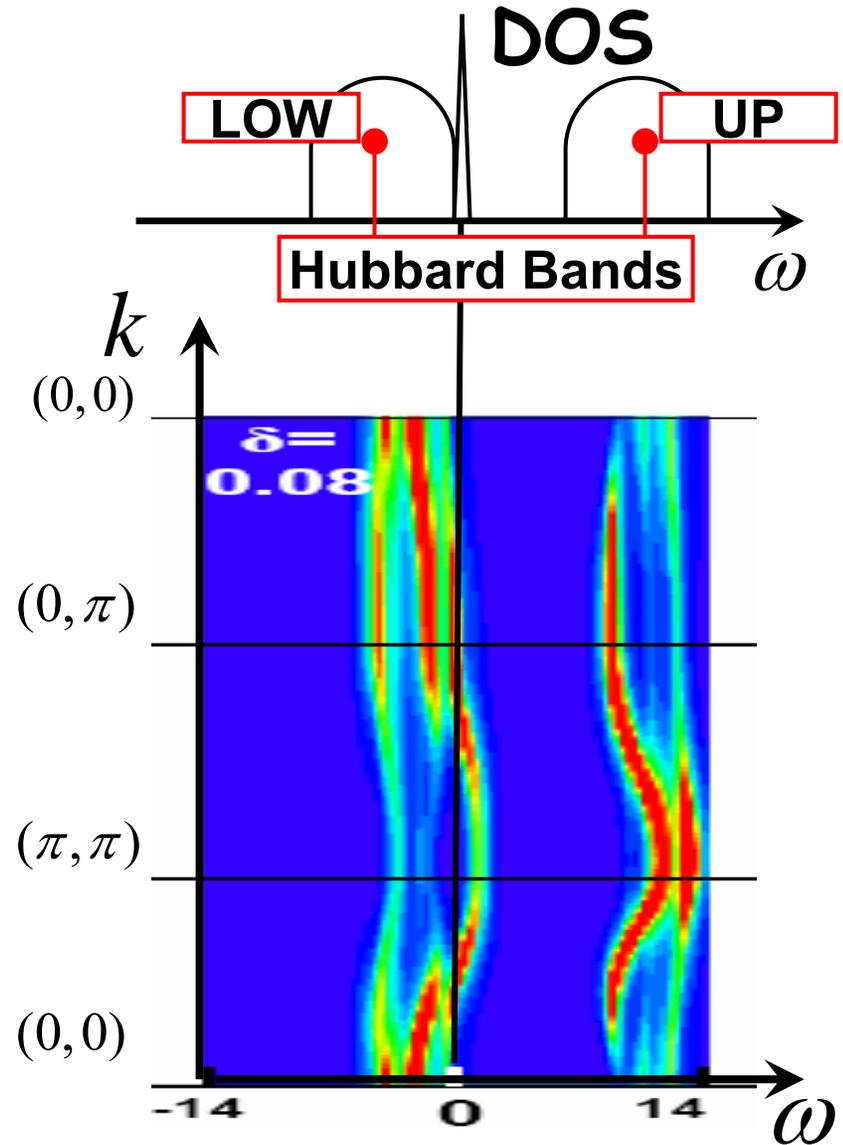
Photoémission-ARPES



On regarde les spectres

$$-\frac{1}{\pi} \text{Im} G(k, \omega)$$

Dans l'espace $k-\omega$

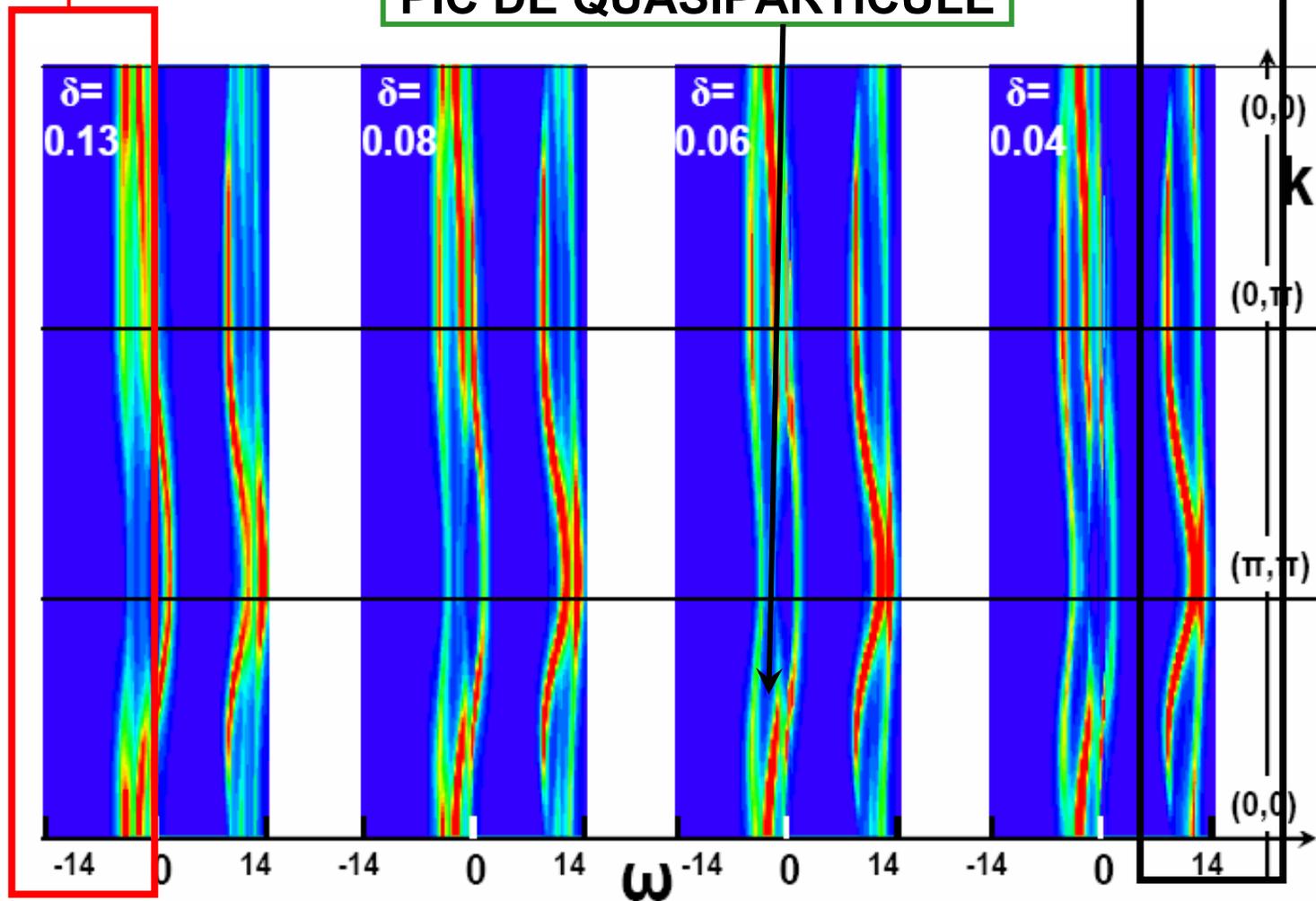


Evolution des spectres

LOWER HUBBARD BAND

UPPER HUBBARD BAND

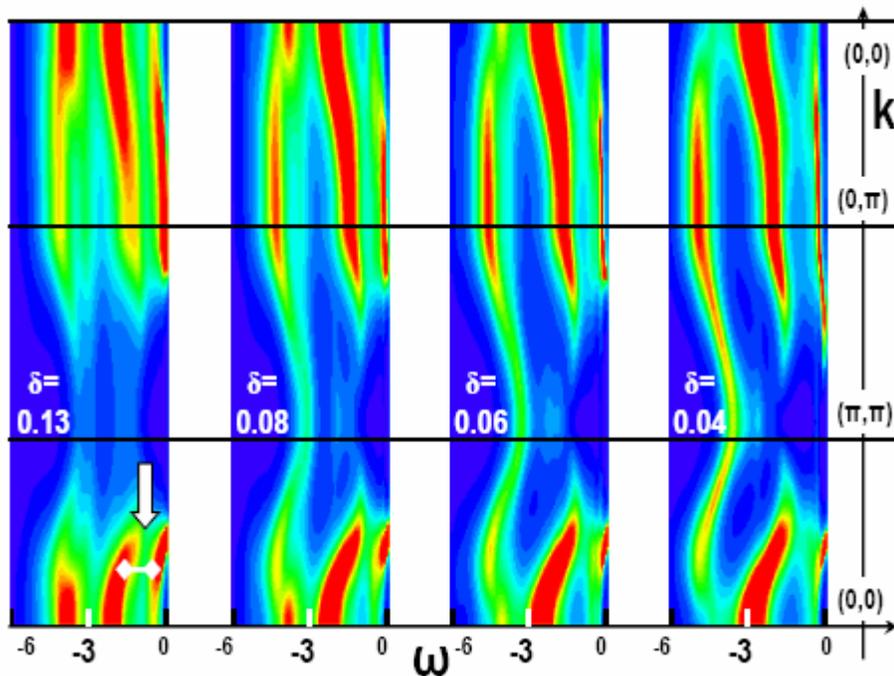
PIC DE QUASIPARTICULE



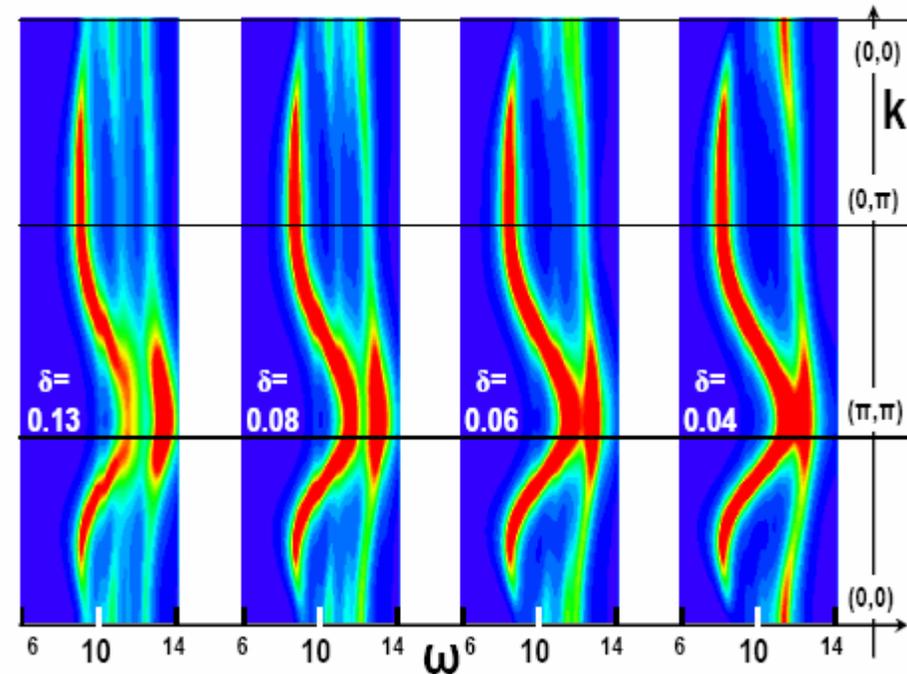
Evolution des bandes de Hubbard

Le poids spectral des bandes de Hubbard augmente lorsqu'on réduit le dopage δ

LOWER HUBBARD BAND

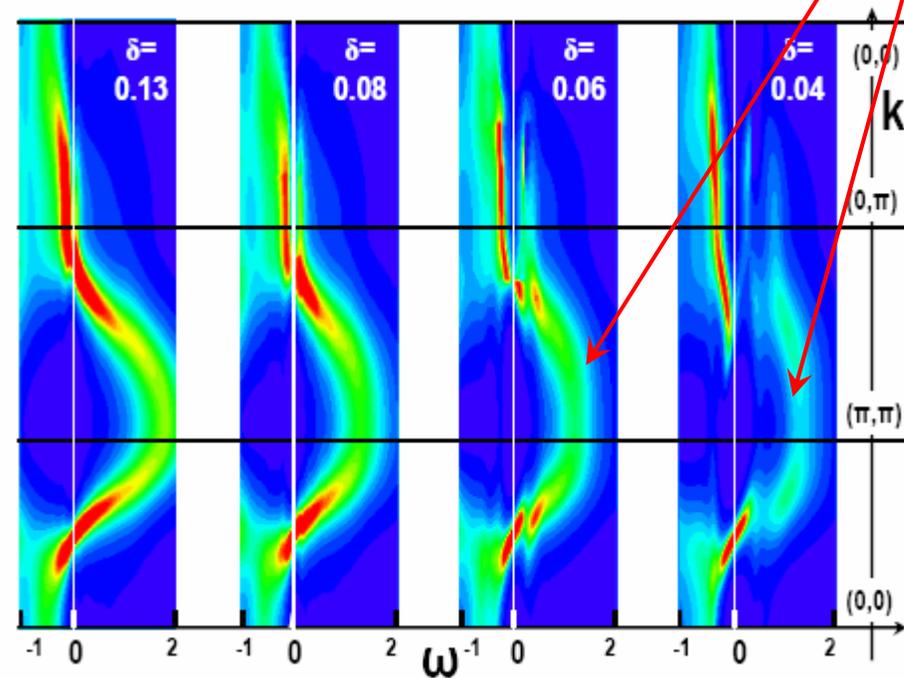


UPPER HUBBARD BAND



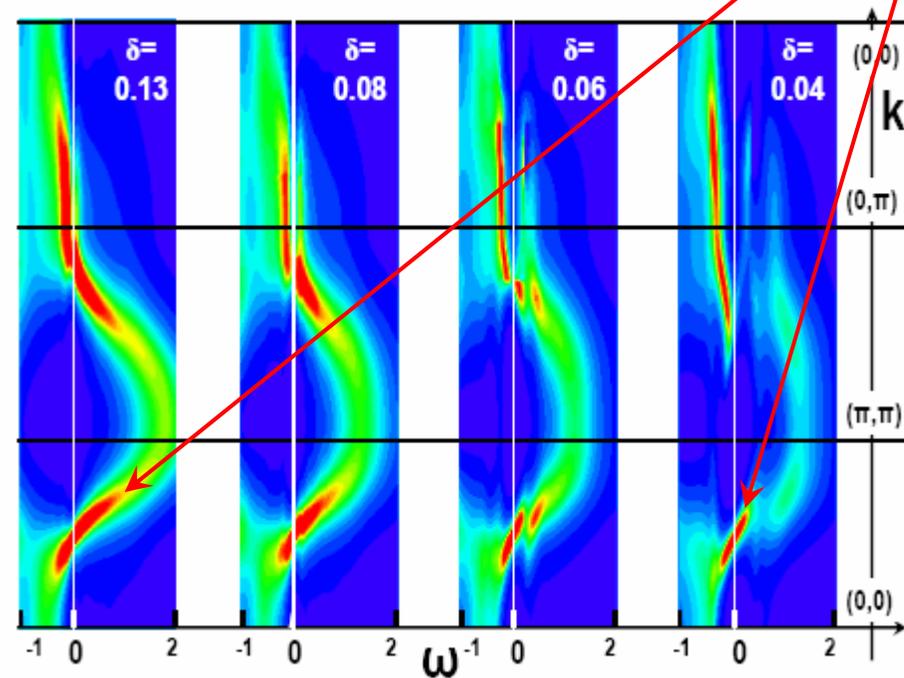
Evolution du pic à basse énergie

diminution du poids spectral



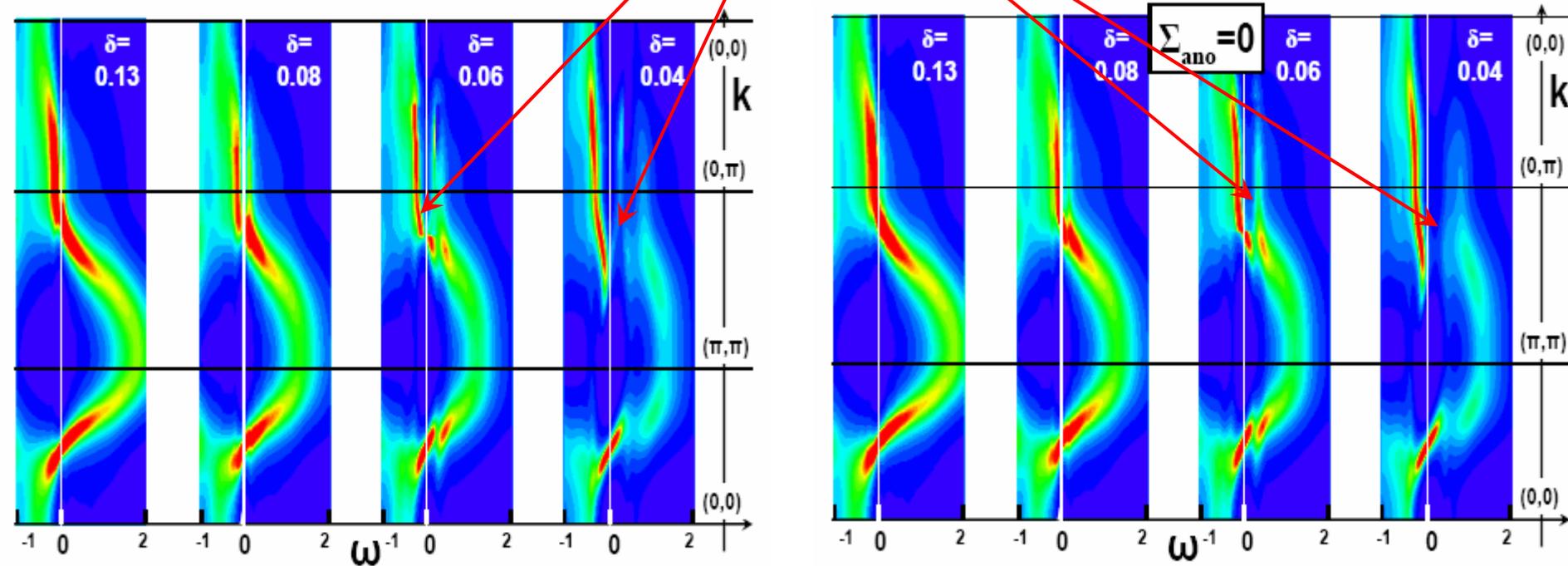
Evolution du pic à basse énergie

Dispersion typique de quasi particule au nœud



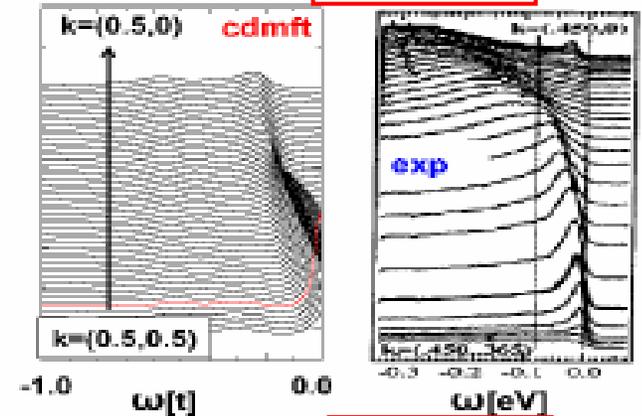
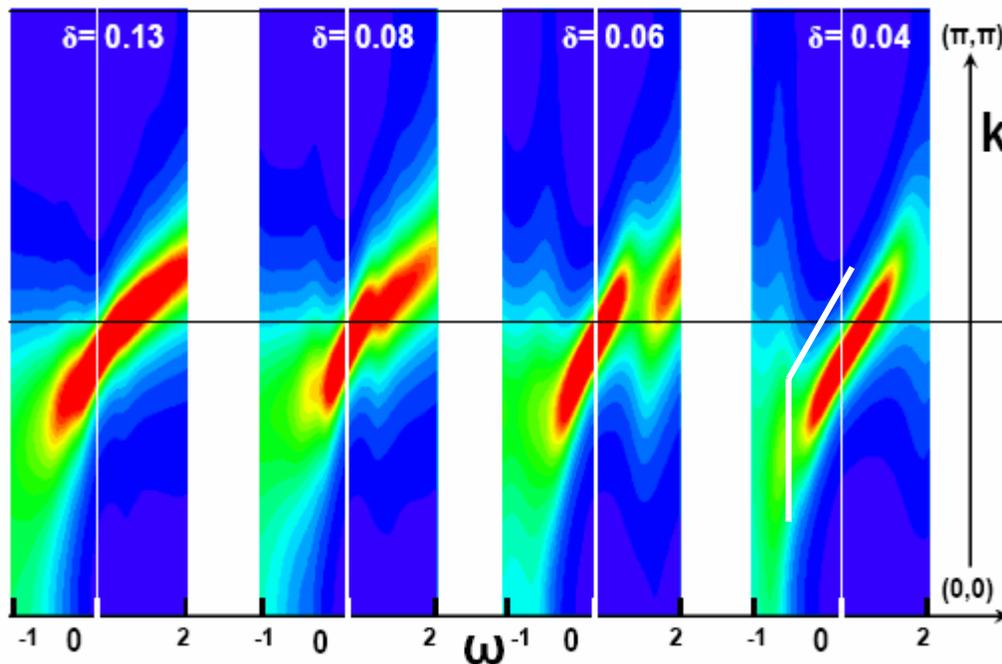
Evolution du pic à basse énergie

Gap déjà présent dans la partie normale autour de $k=(0,\pi)$: PSEUDOGAP

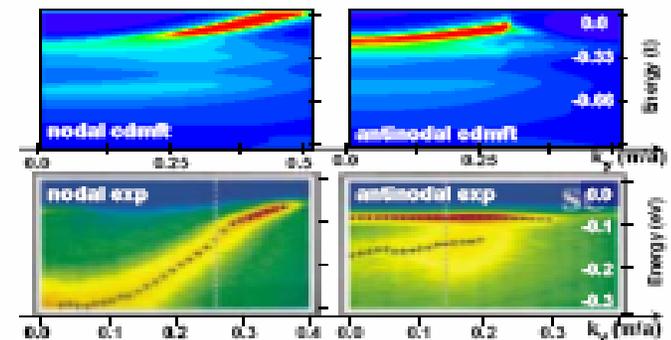
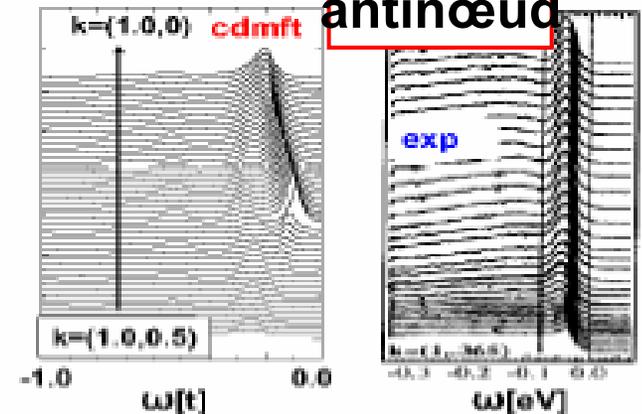


« KINKS » dans les spectres

nœud



antinœud



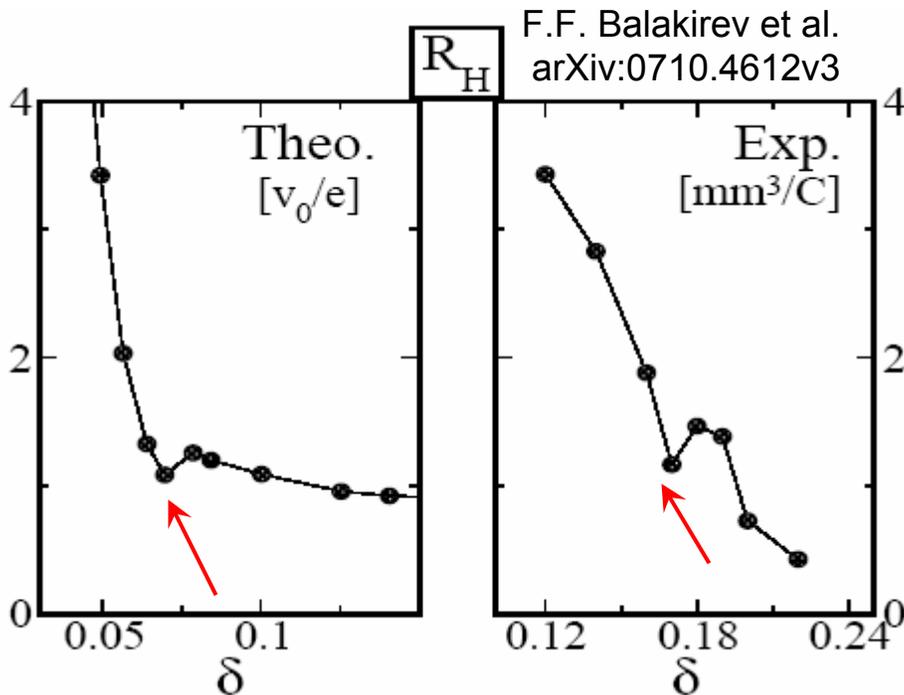
Résistance de Hall

Théorie de Boltzmann

$$\sigma_{xx} = -2e^2\tau \sum_k (v_k^x)^2 \frac{\partial f(Z_k \zeta_k)}{\partial \zeta_k} \quad (41)$$

$$\sigma_{xy} = \frac{2e^3 H \tau^2}{\hbar c} \sum_k v_k^x [v_k^y \partial_{k_x} v_k^y - v_k^x \partial_{k_y} v_k^y] \frac{\partial f(Z_k \zeta_k)}{\partial \zeta_k}$$

$$R_H = - \frac{\sigma_{xy}}{\sigma_{xx}^2 - \sigma_{xy}^2} \frac{1}{H}$$



$$G(k, \omega_n) = \frac{1}{i \frac{(2n-1)\pi}{Z_k \beta} - \zeta_k}$$

$$\zeta_k = [\xi_k + \underline{\text{Re}\Sigma_k(0)}]$$

bande renormalisée

CONCLUSION

- ❑ Développement de la 2x2 plaquette-**CDMFT** pour l'étude des **supraconducteurs H-Tc**
 - ❑ Le concept de dichotomie **nodale-antinodale** permet de relier les résultats du cluster aux **expériences**:
 - ❑ Photoémission (Raman, ARPES)
 - ❑ Tunneling (STM)
 - ❑ Résistivité de Hall
- Scénario auto consistant **théorie/expériences**

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