CPT study of the Fermi-surface reconstruction in the t-J model

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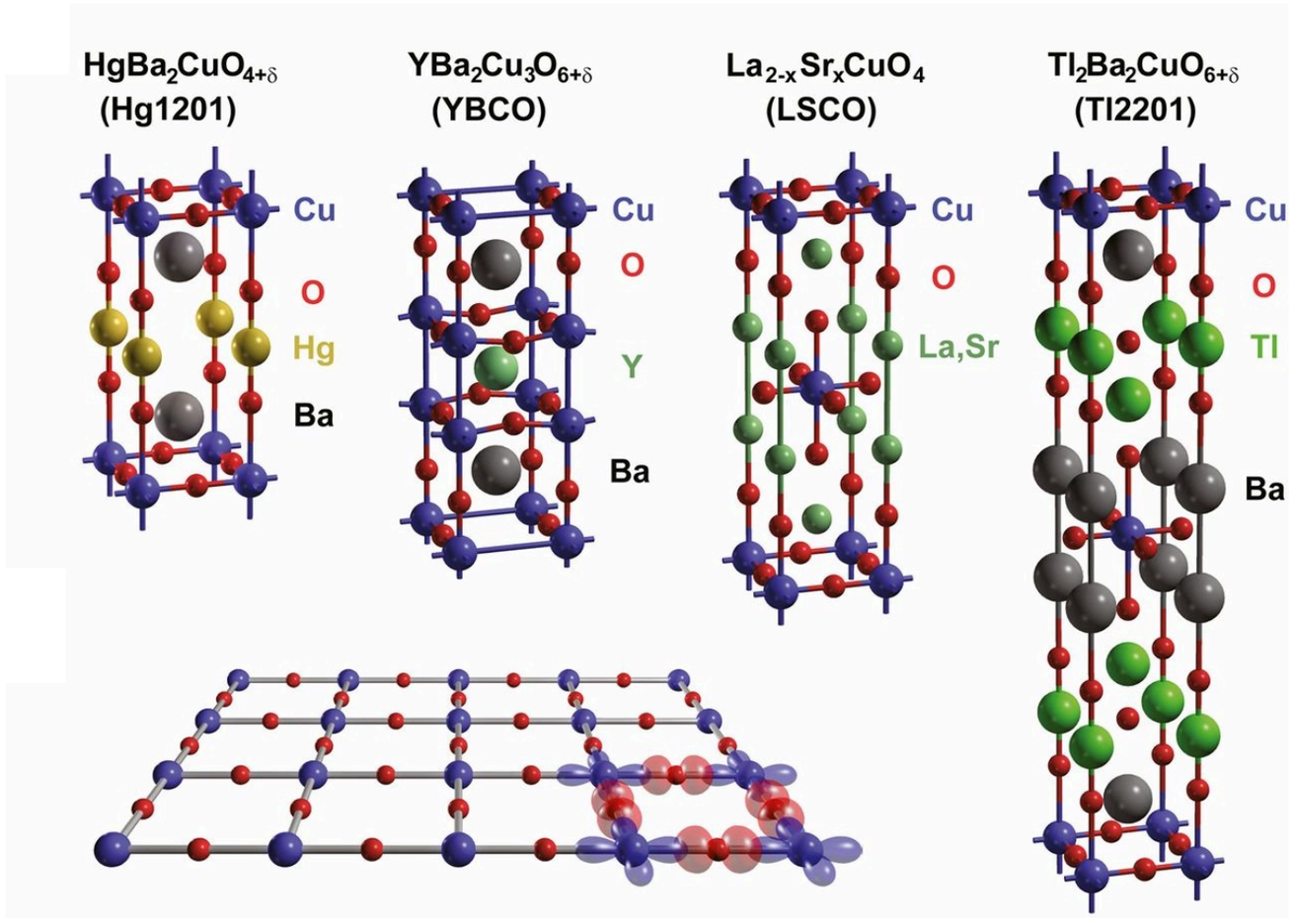
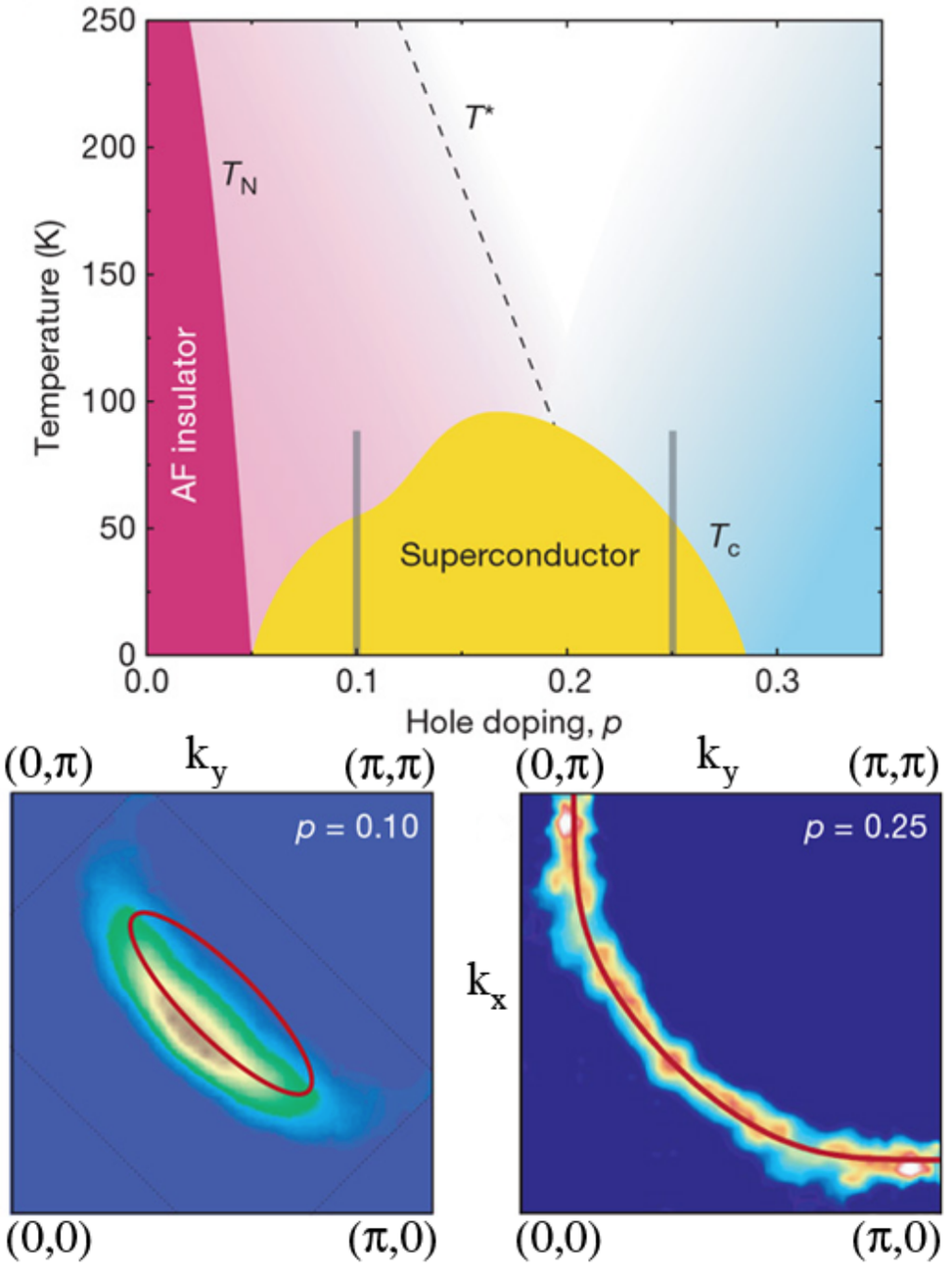
Cuprates

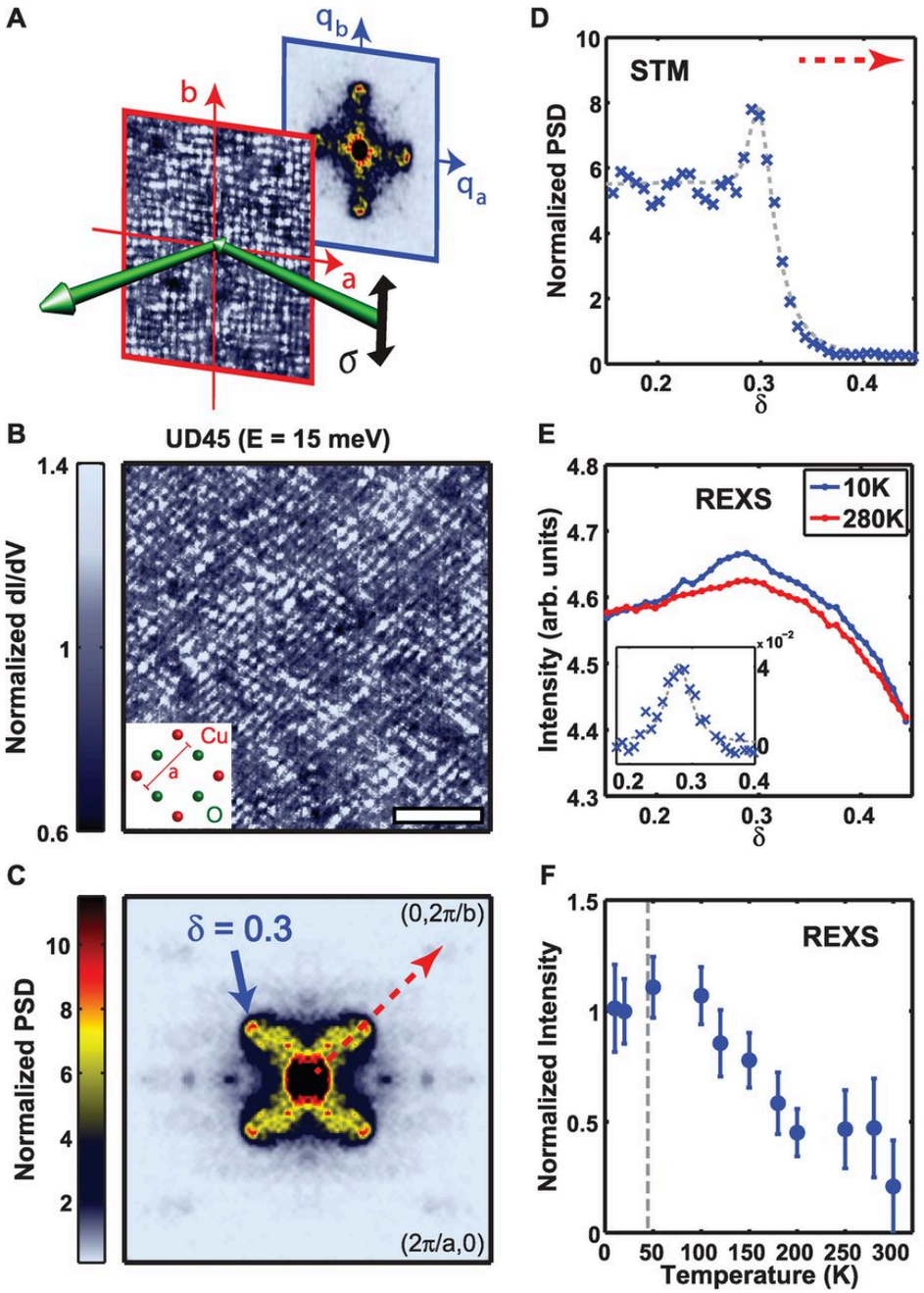


N. Barišić et al., Proc. Natl. Acad. Sci. 110, 12235 (2013)



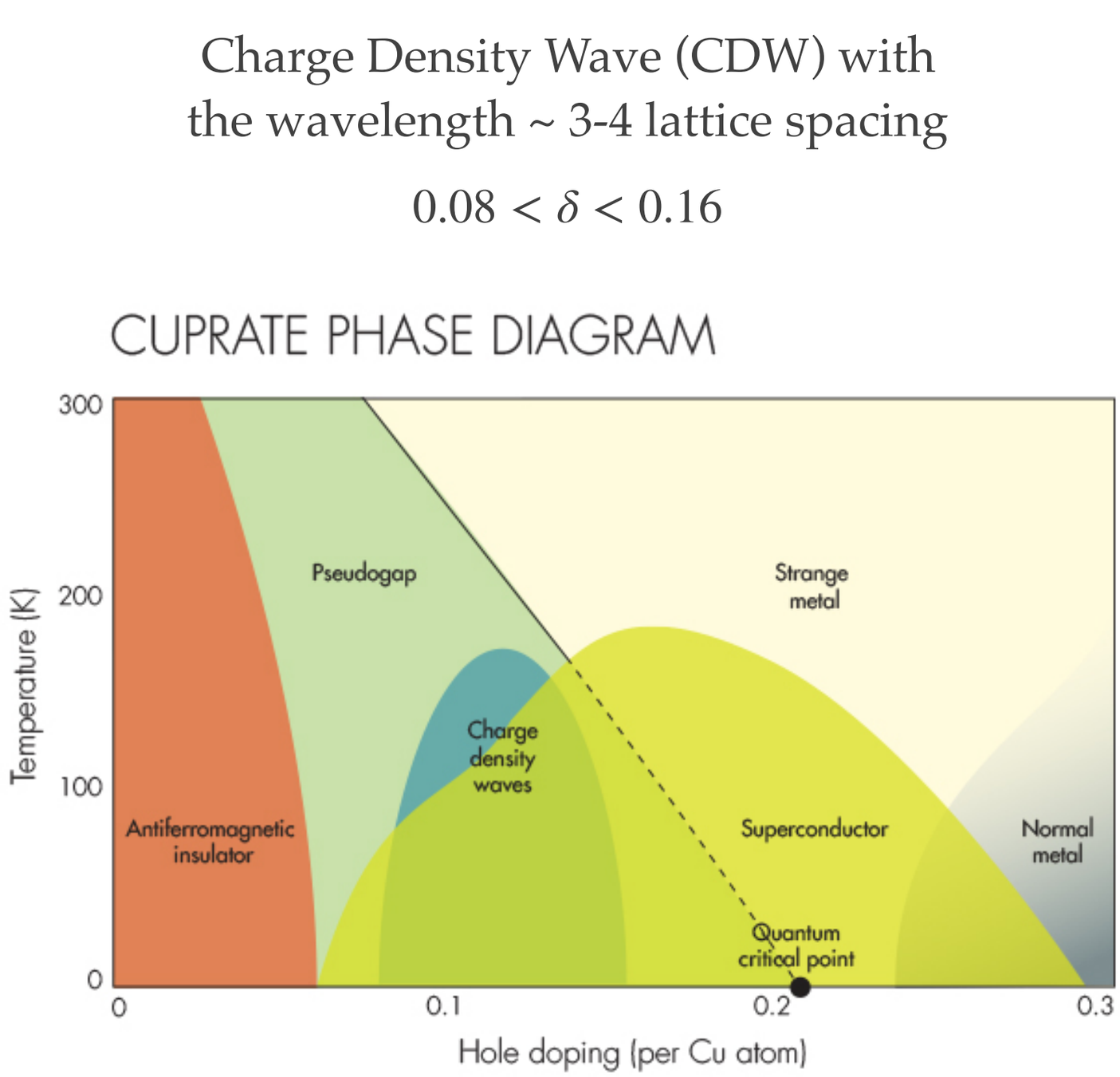
N. Doiron-Leyraud et al, Nature 447, 565 (2007)

Charge ordering

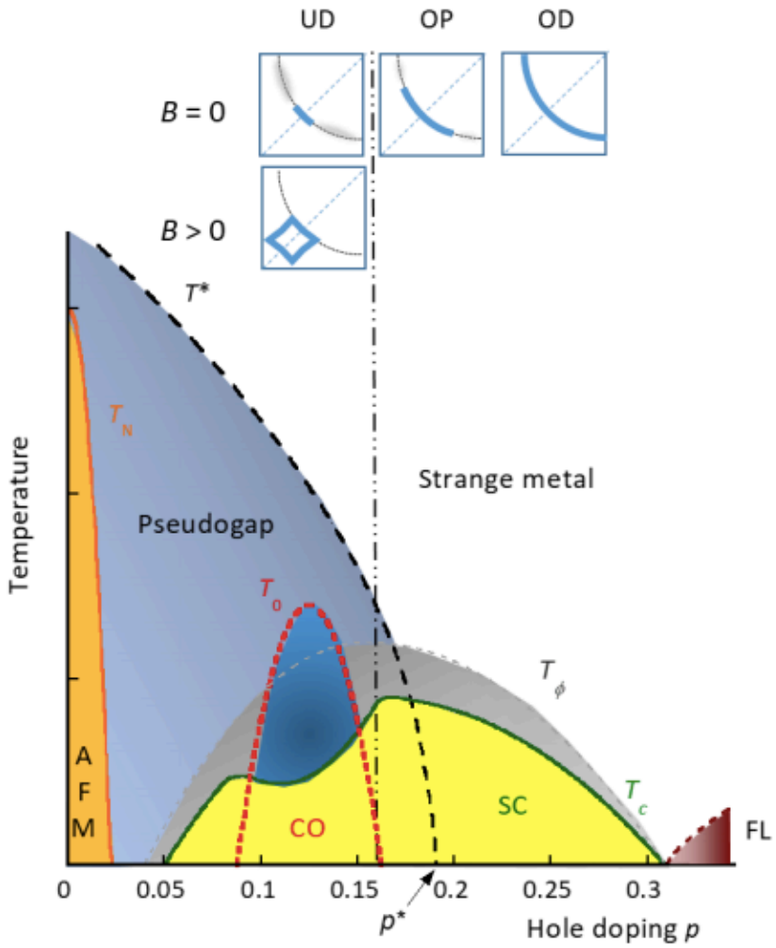


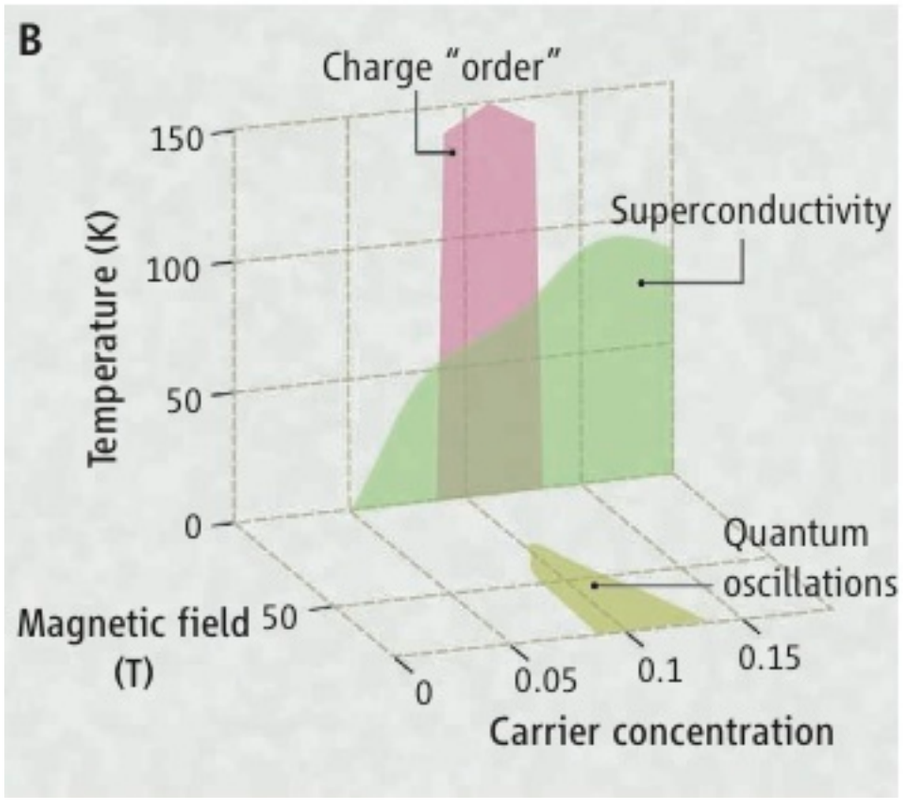
Charge Density Wave (CDW) with the wavelength ~ 3-4 lattice spacing

$0.08 < \delta < 0.16$



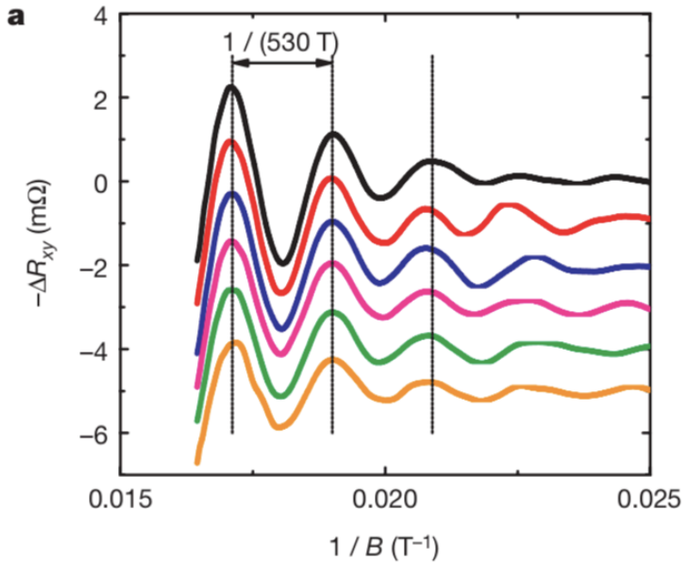
Quantum oscillation



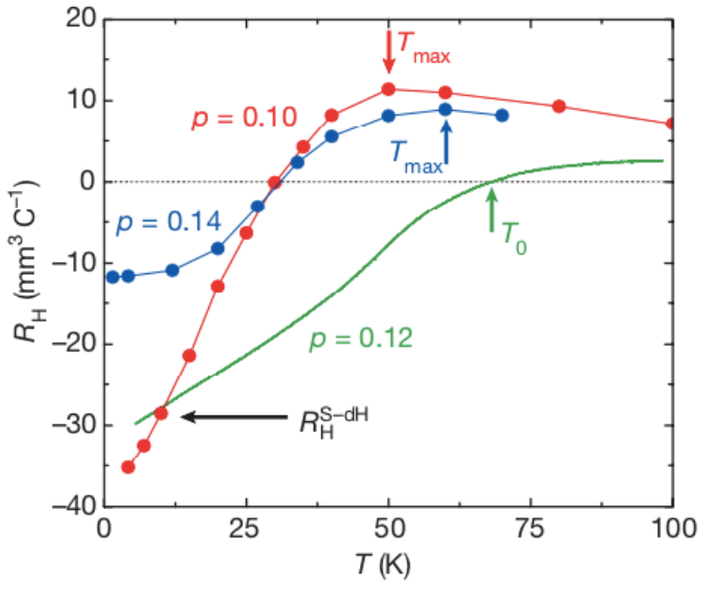


Contradiction!
Quantum oscillations imply a closed Fermi surface.

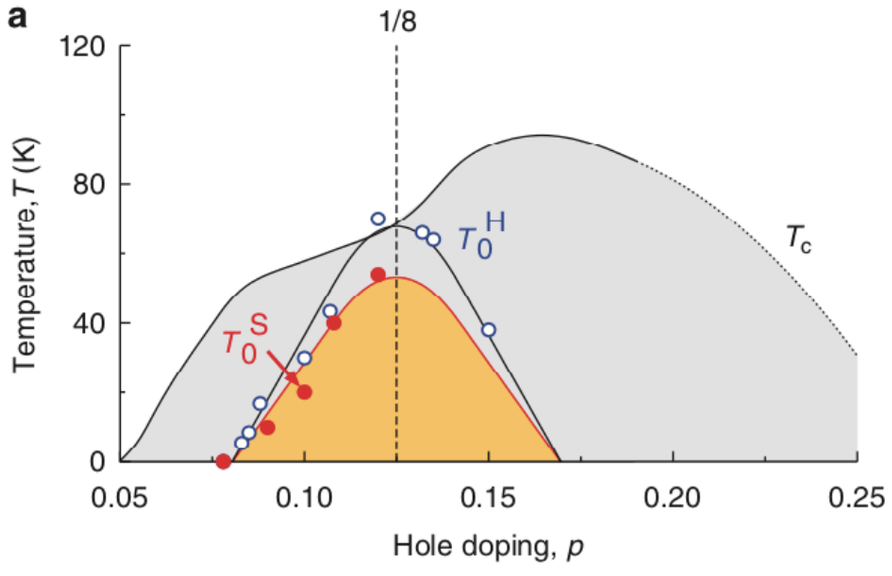
Quantum oscillation

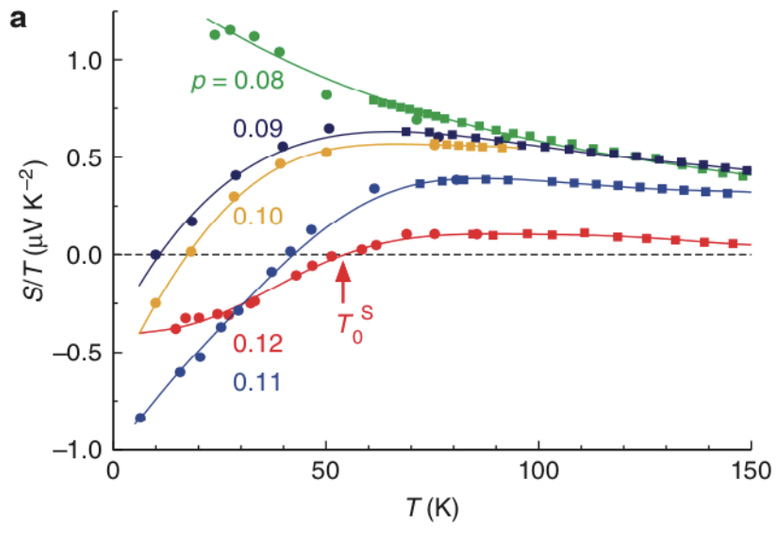


N. Doiron-Leyraud et al, Nature 447, 565 (2007)



D. LeBoeuf et al, Nature 450, 533 (2007).





F. Laliberte et al, Nat. Commun. 2, 432 (2011).

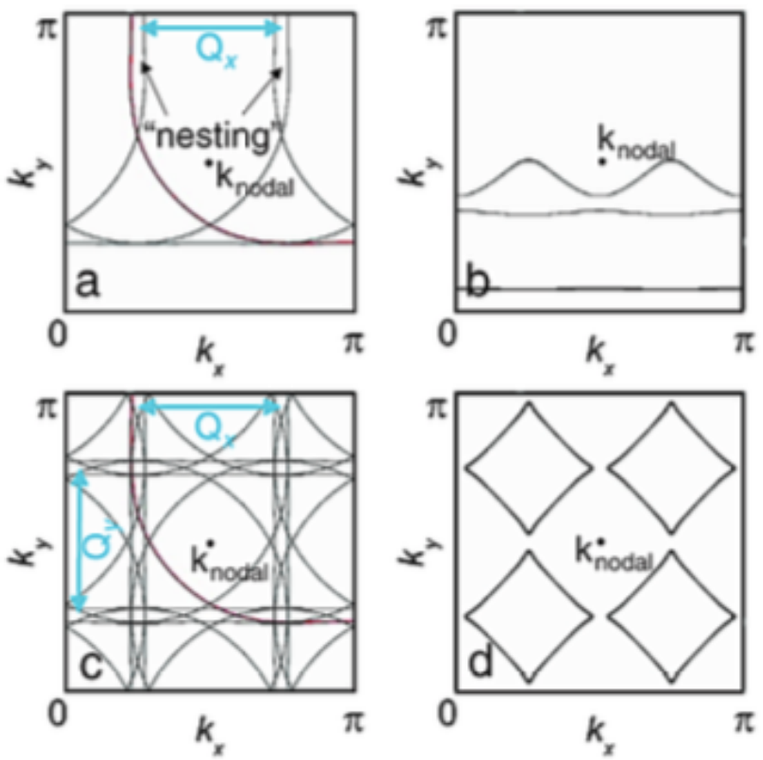
Phenomenology

Tight-binding model:

$$H = \sum_{ij\sigma} (t_{ij} - \mu\delta_{ij}) c^{\dagger}_{i\sigma} c_{j\sigma}$$

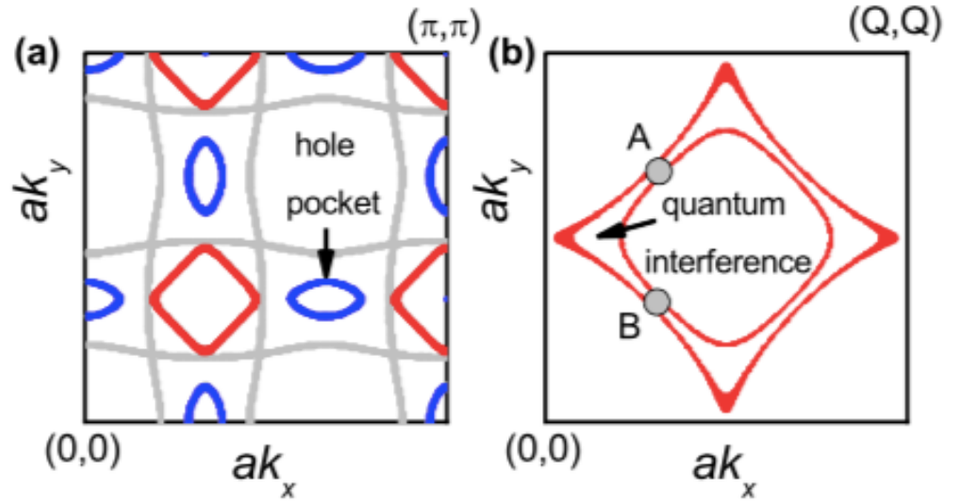
Long-range ordering term:

$$H_{CDW} = \sum_{ij\sigma} P_{ij} c^{\dagger}_{i\sigma} c_{j\sigma}$$

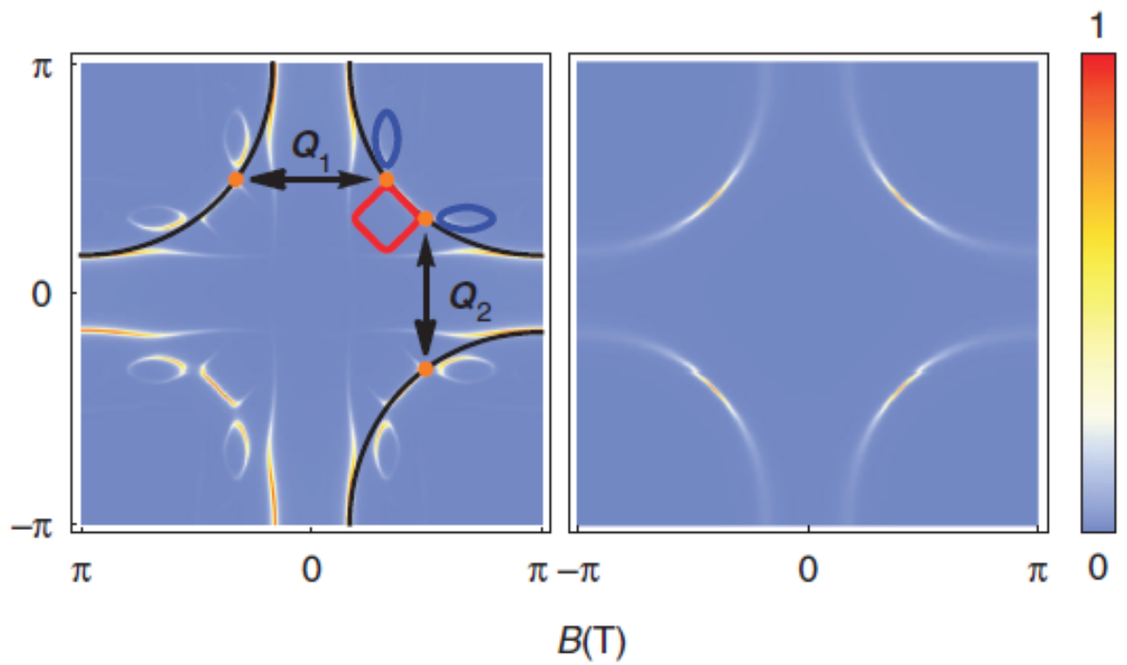


N. Harrison and S.E. Sebastian, PRL 106, 226402 (2011)

e vs *e*+2*h*



N. Harrison and S.E. Sebastian, PRB **92**, 224505 (2015)



A. Allais, D. Chowdhury, S. Sachdev, Nat. Commun. 5, 5771 (2014)

Model

Superlattice Hamiltonian:

$$H = \sum_{fg} H_{fg}^{\text{int}} + \sum_{f} H_{f}^{0}$$

Intercluster interaction:

$$H_{fg}^{\text{int}} = \sum_{ab\sigma} t_{ab}^{fg} c_{fa\sigma}^{\dagger} c_{gb\sigma}$$

Intracluster interaction:

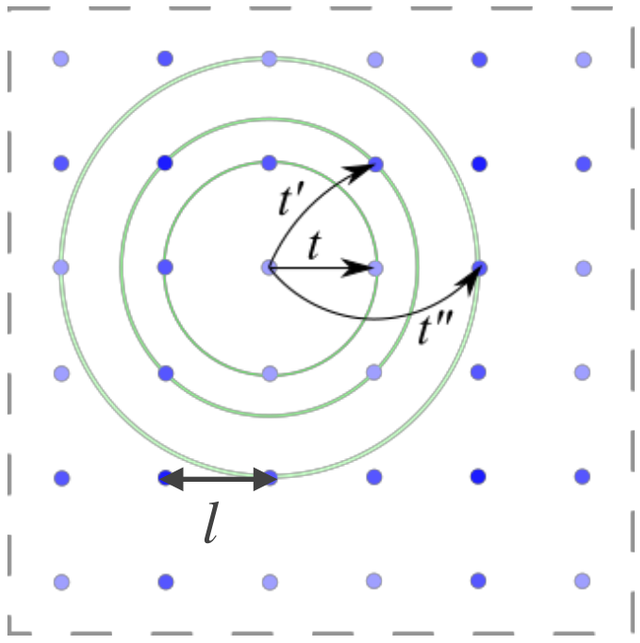
$$H_{f}^{0} = H_{ff}^{\text{int}} + U \sum_{a} n_{a\uparrow} n_{a\downarrow}$$

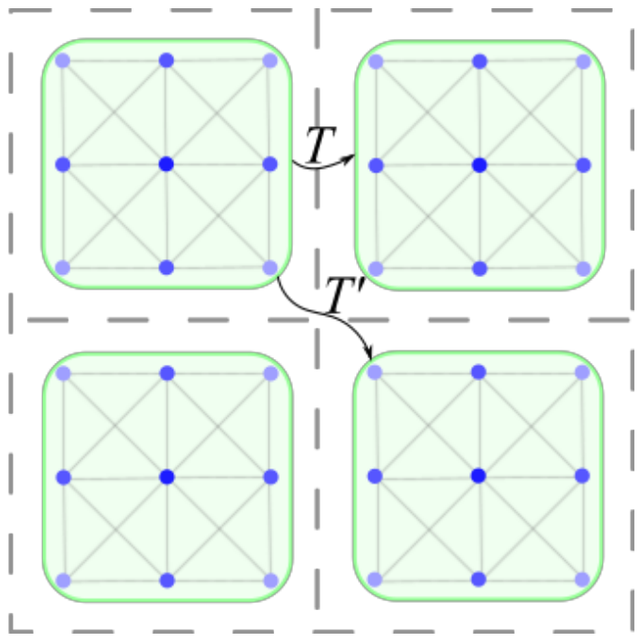
Model parameters:

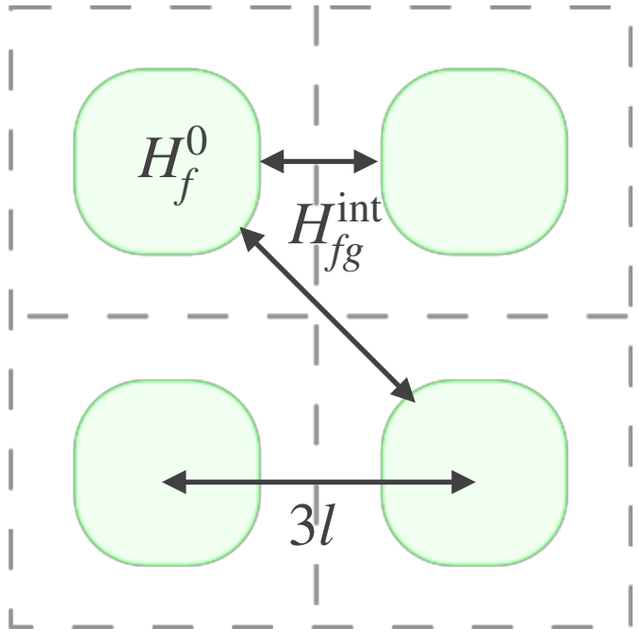
$$t = -1, t' = 0.27, t'' = -0.2$$
$$J = 0.5 \quad (U = 8)$$

t-J model:

$$H_{f}^{0} = \sum_{ab\sigma} (t_{ab}^{ff} - \mu\delta_{ab}) \tilde{c}_{fa\sigma}^{\dagger} \tilde{c}_{fb\sigma} + J \sum_{ab} \mathbf{S}_{fa} \cdot \mathbf{S}_{fb}$$







Cluster Perturbation Theory (CPT)

1) Exact diagonalization of the intracluster Hamiltonian:

$$H_f^0 = \sum_{ab\sigma} (t_{ab}^{ff} - \mu\delta_{ab})\tilde{c}_{fa\sigma}^{\dagger}\tilde{c}_{fb\sigma} + J\sum_{ab}\mathbf{S}_{fa}\cdot\mathbf{S}_{fb}$$

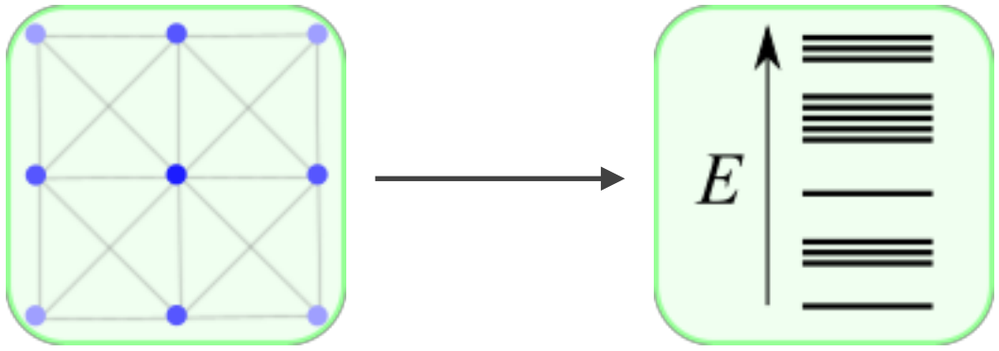
$$X^{pq} = |p\rangle\langle q|$$

where $|p\rangle$ are the eigenstates of cluster.

3 states per site in t-J model ($|0\rangle, |\uparrow\rangle, |\downarrow\rangle$)

$3^9 = 19683$ states per cluster

[19683 x 19683] matrix



2) Transition to the new basis

$$H_f^0 = \sum_p \varepsilon_p X_f^{pp} \qquad c_{fa\sigma} = \sum_{pq}\gamma_{a\sigma}^{pq}X_f^{pq} \qquad H_{fg}^{\text{int}} = \sum_{ab\sigma} t_{ab}^{fg}c_{fa\sigma}^{\dagger}c_{gb\sigma} \longrightarrow \sum_{pqrs} T_{qs}^{pr}(f,g)X_f^{pq}X_g^{rs}$$

In the **k**-space the Hamiltonian takes the form:

$$H = \sum_p\sum_{\mathbf{k}} \varepsilon_p(\mathbf{k})X_{\mathbf{k}}^{pp} + \sum_{pqrs}\sum_{\mathbf{k}} T_{qs}^{pr}(\mathbf{k})X_{\mathbf{k}}^{pq}X_{\mathbf{k}}^{rs}$$

Cluster Perturbation Theory (CPT)

3) Dyson equation

$$(\hat{D}(\mathbf{k},\omega))^{-1} = (\hat{D}_0(\mathbf{k}))^{-1} - T(\mathbf{k})$$

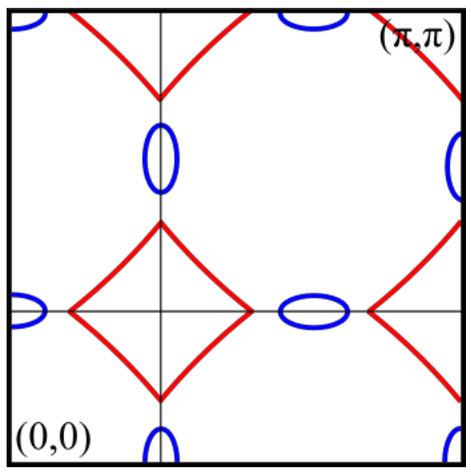
$$(D_0)^{pq}_{rs}(\omega) = \delta_{ps}\delta_{rq}\frac{\langle X^{pp} + X^{qq}\rangle}{\omega + \varepsilon_p - \varepsilon_q - \mu}$$

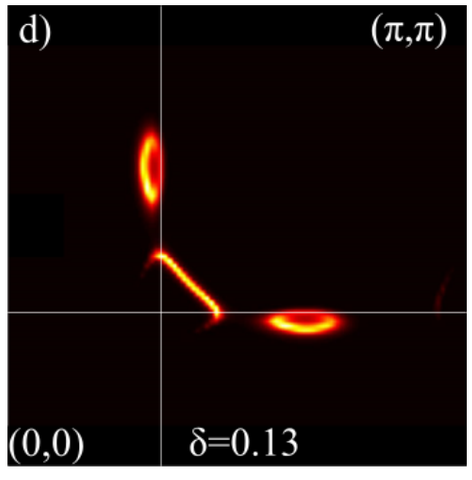
$$D^{pq}_{rs}(f,t;g,t') = \langle\langle X^{pq}_f(t) \,|\, X^{rs}_g(t')\rangle\rangle$$

$$G_{\sigma\sigma'}(af,t;bg,t') = \langle\langle c^{\dagger}_{fa\sigma}(t) \,|\, c_{gb\sigma}(t')\rangle\rangle$$

restored electron Green function: $$G_\sigma(\mathbf{k},\omega) = \sum_{ab}\sum_{pqrs}\gamma^{pq}_{a\sigma}\gamma^{rs}_{b\sigma}e^{-i\mathbf{k}(\mathbf{r_i}-\mathbf{r_j})}D^{pq}_{rs}(\mathbf{k},\omega)$$

spectral function: $$A(\mathbf{k},\omega) = -\frac{1}{\pi}\lim_{\eta\to 0^+}(\mathrm{Im}G(\mathbf{k},\omega+\mu+i\eta))$$





	GB RAM	Calculation time:
3x3 cluster:	**~28**	**2-20** hours
4x4 cluster:	**~138 060 762**	at least **1000** years

Charge density wave

$$\langle n\rangle(\vec{r}) \approx \langle n\rangle_0 + A_n(\cos(Q_x x) + \cos(Q_y y))$$

$$Q_x = 2\pi(Q,0)$$

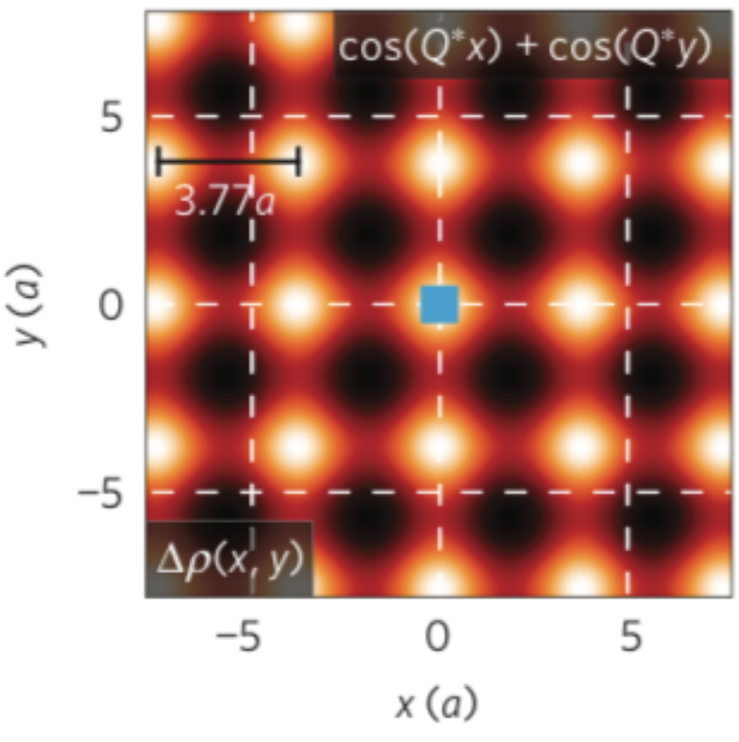
$$Q_y = 2\pi(0,Q)$$

$$Q = \frac{1}{L} = \frac{1}{3}$$

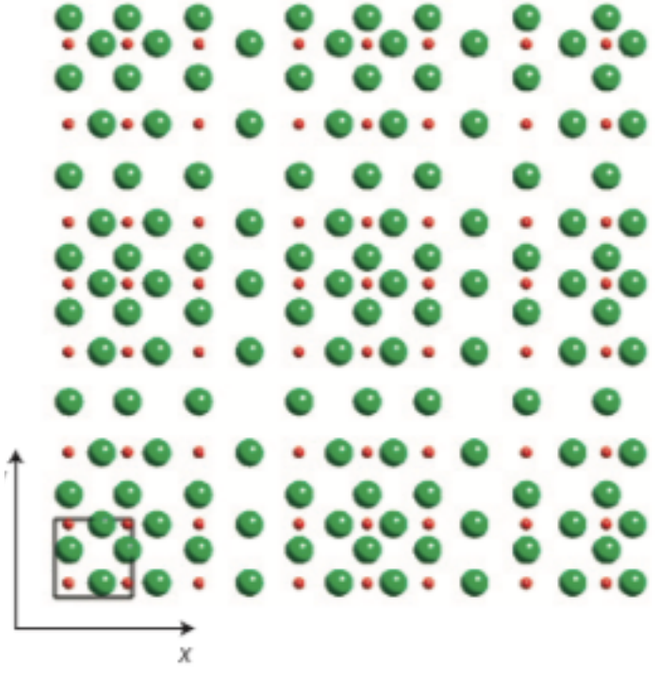
We pin the length of CDW modulation vector

$Q \approx 0.31$ in YBCO

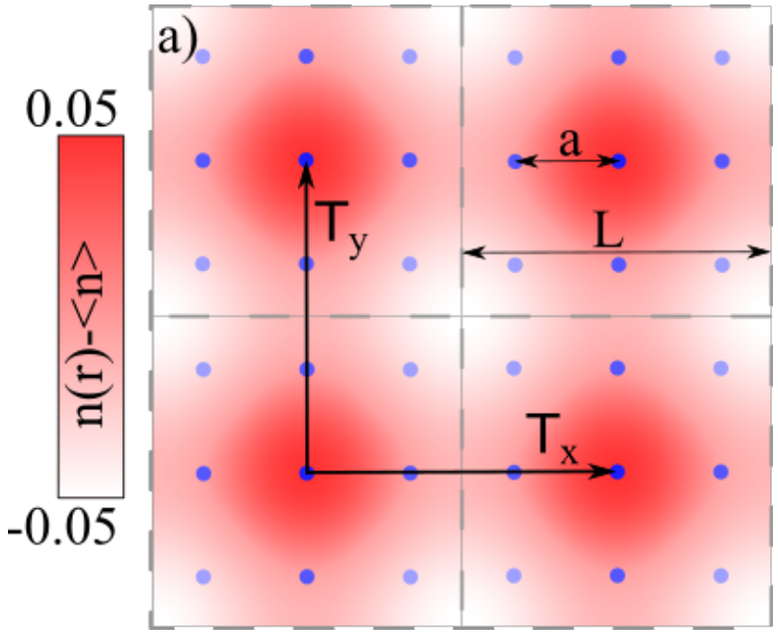
Checkerboard pattern:



R. Comin et al., NMat 14, 796 (2015)

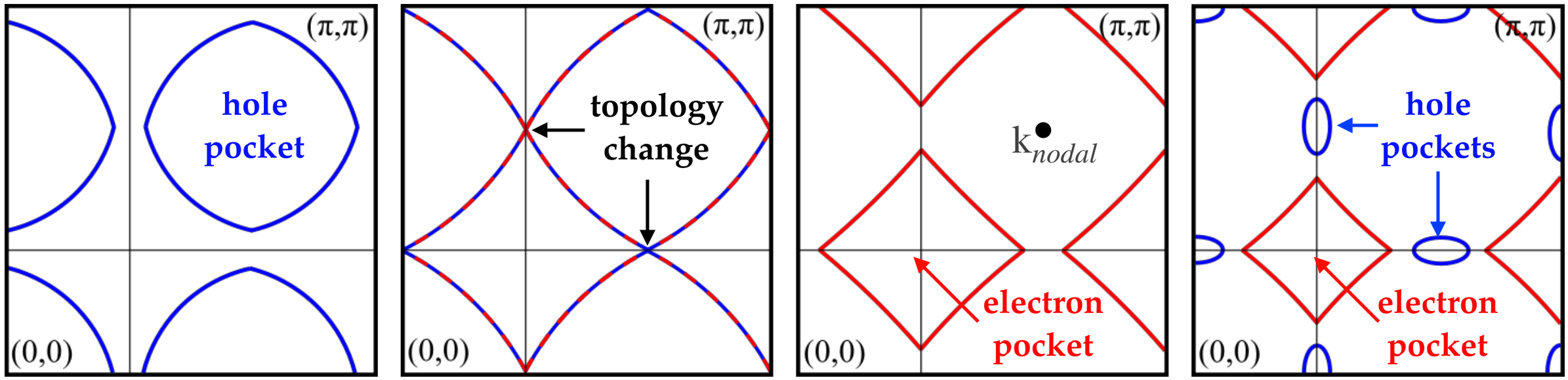


J. Chang et al., NPhys 8, 871 (2012)



Fermi surface reconstruction

$\delta = 0.08$ $\delta \approx 0.09$ $\delta = 0.11$ $\delta = 0.13$

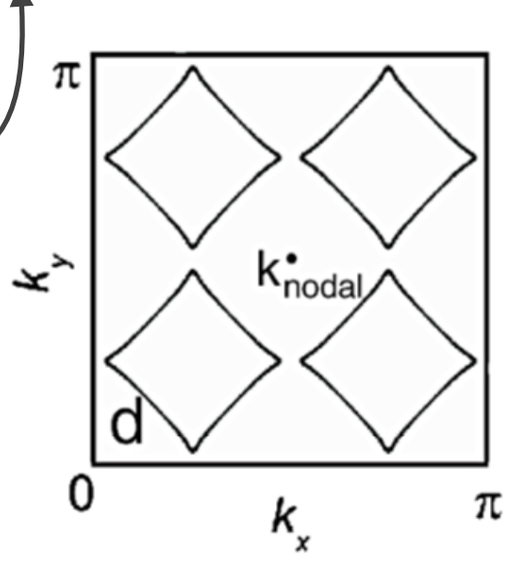


$$H_t = \sum_{ij\sigma} t_{ij} \tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma}$$

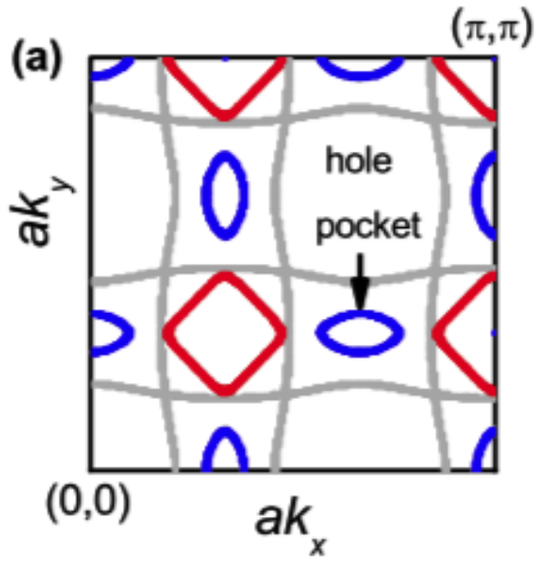
constrained electron
+ Coulomb repulsion

$$H_t = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma}$$

unconstrained electron
+ long-range ordering

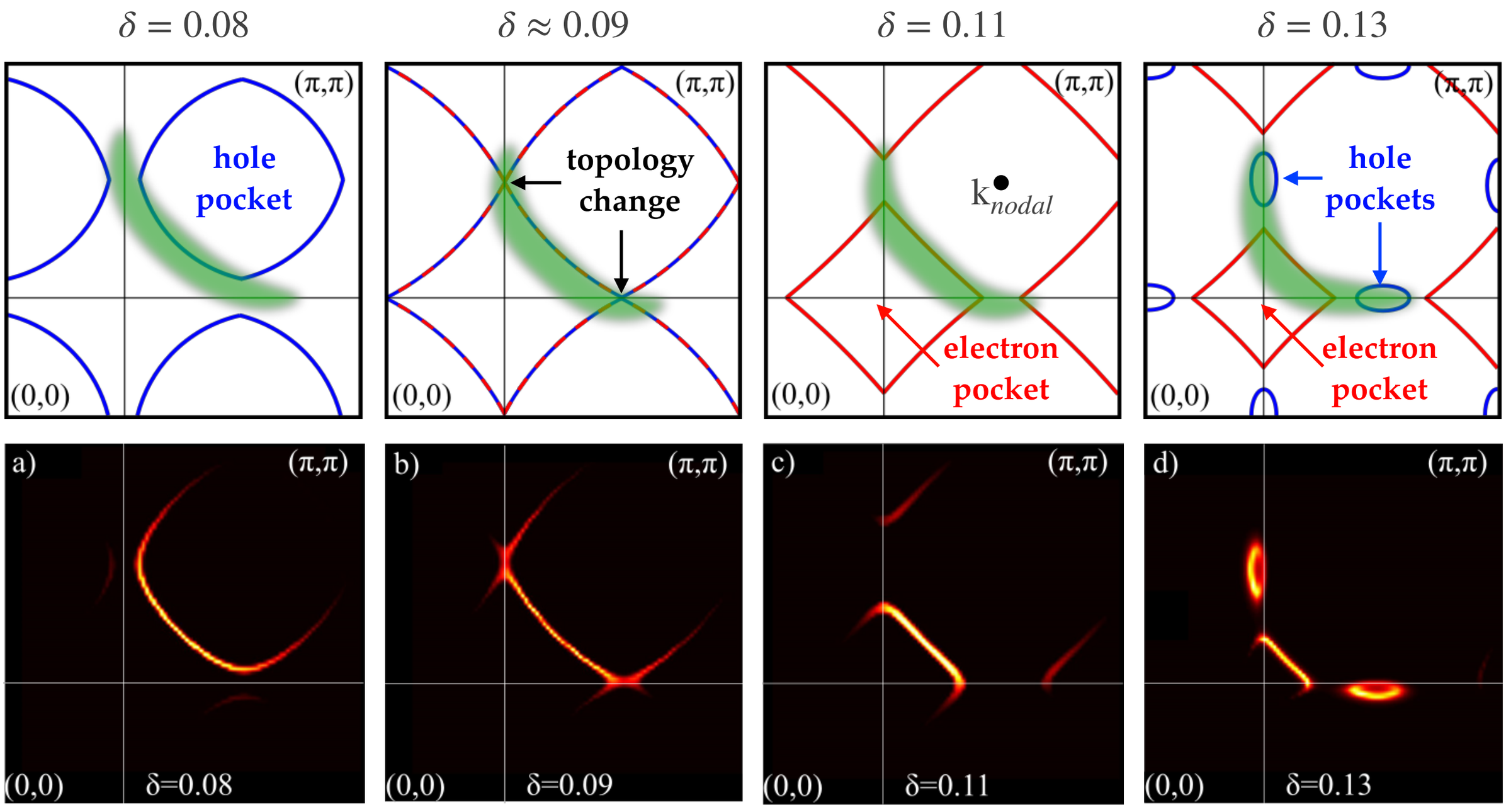


N. Harrison, S.E. Sebastian,
PRL 106, 226402 (2011).

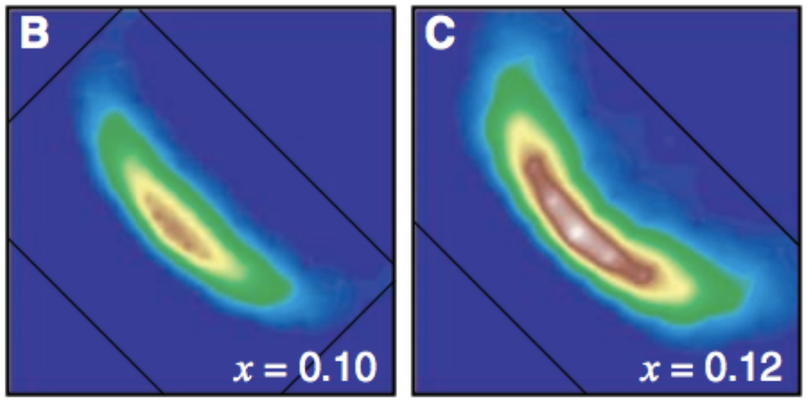


N. Harrison, S.E. Sebastian,
PRB **92**, 224505 (2015)

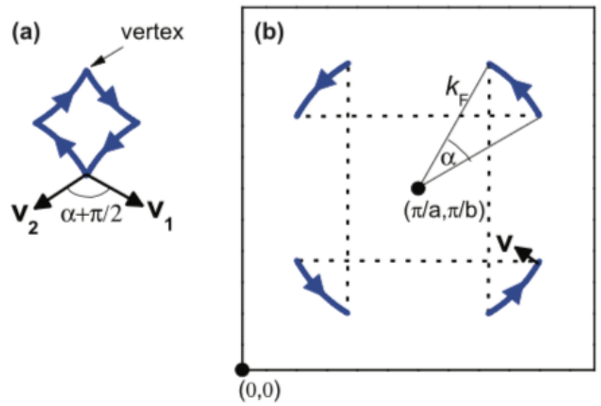
Fermi surface reconstruction



Fermi surface reconstruction



K.M. Shen et al., Science **307,** 901 (2005)



N. Harrison and S.E. Sebastian,
PRB 92, 224505 (2015)

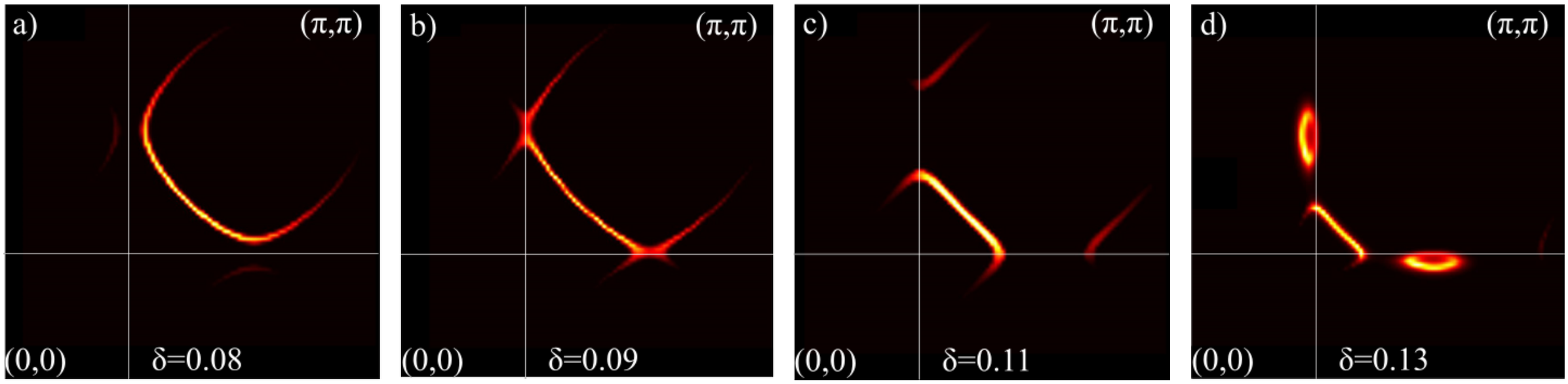
Hole pockets?

Pseudogap

Topological transition

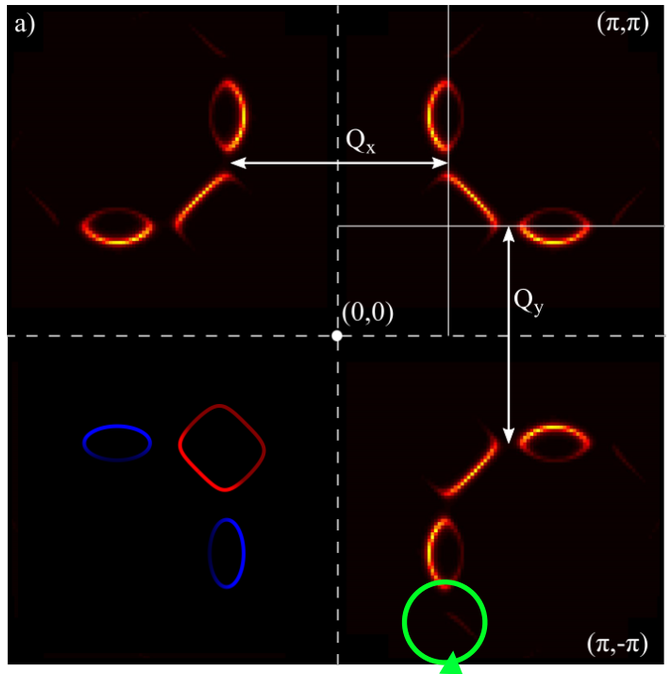
Electron pocket

Electron pocket + 2 hole pockets



PG vs FL behavior

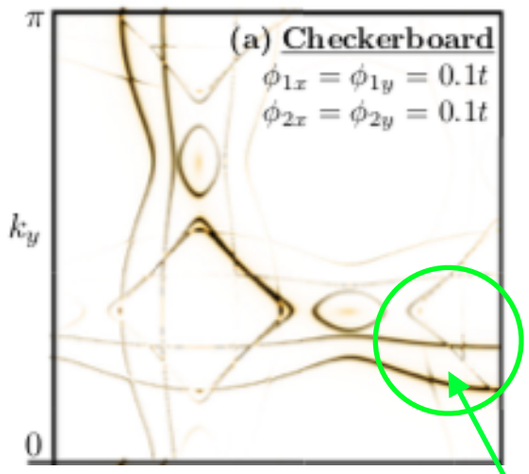
This work



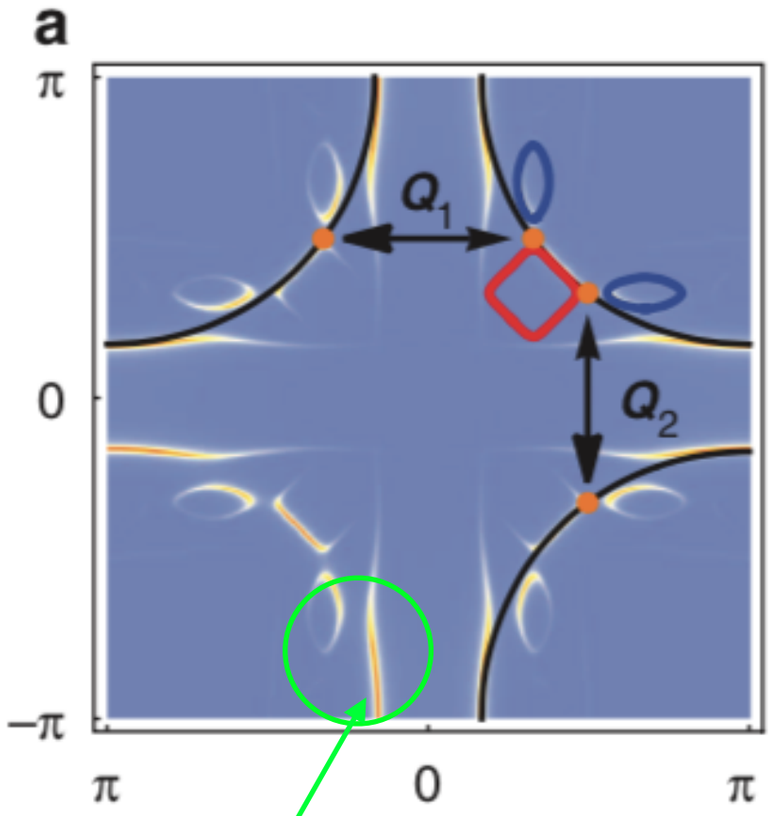
Zero spectral weight
in the antinodal region

A.V. Maharaj, P. Hosur, S. Raghu,

PRB 90, 125108 (2014)



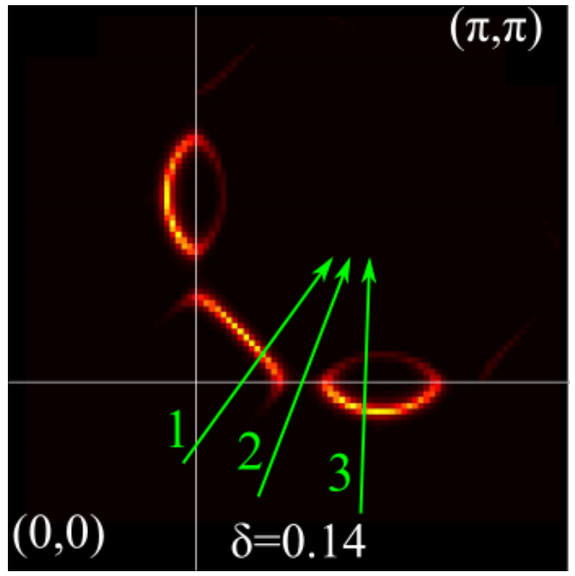
A. Allais, D. Chowdhury, S. Sachdev,
Nat. Commun. 5, 5771 (2014)



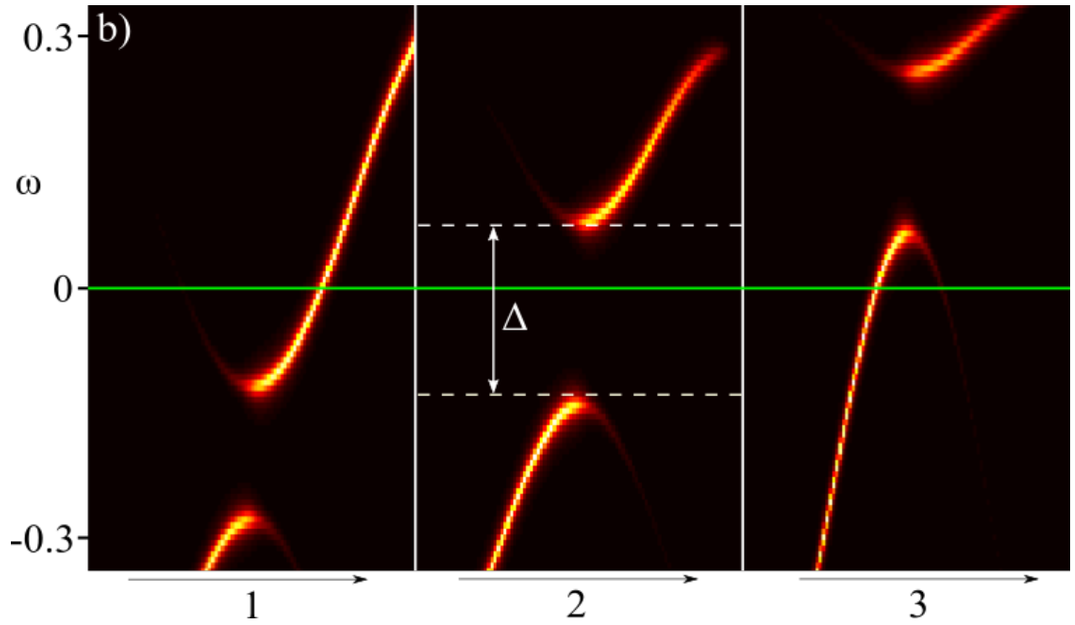
Additional branches
in the antinodal region

CDW gap

Strong Coulomb repulsion leads to the gap opening



Band splitting

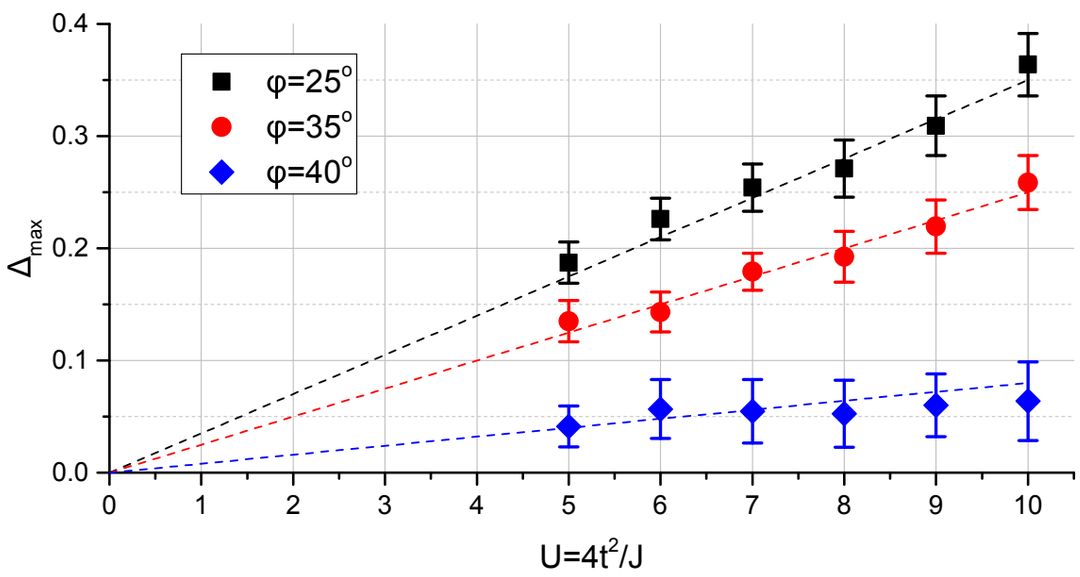


Electron-like pocket

Gap

Hole-like pocket

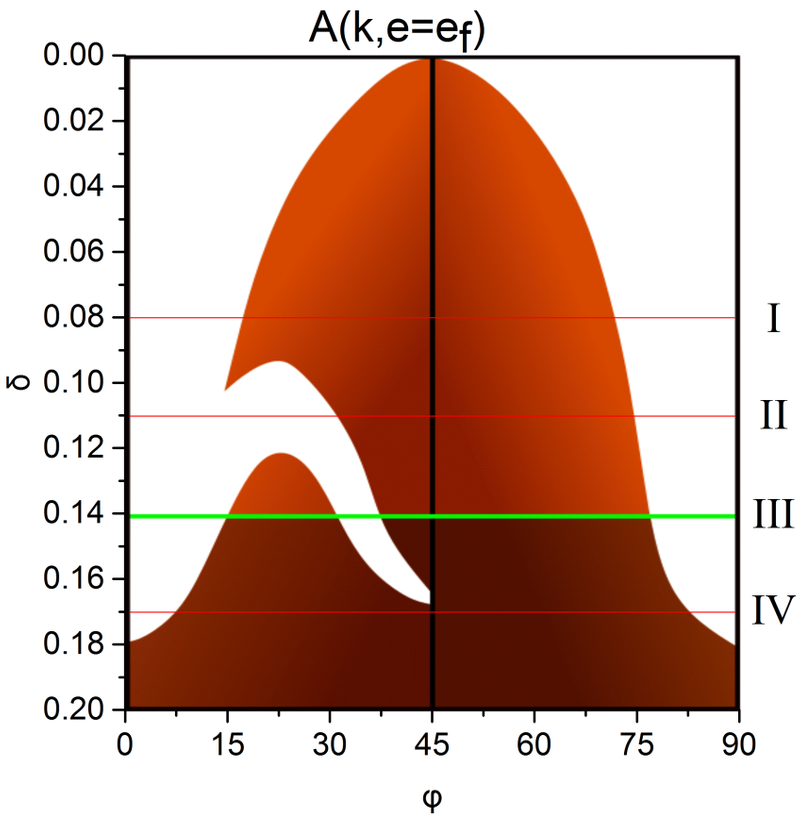
Value of the gap is linearly depends on U

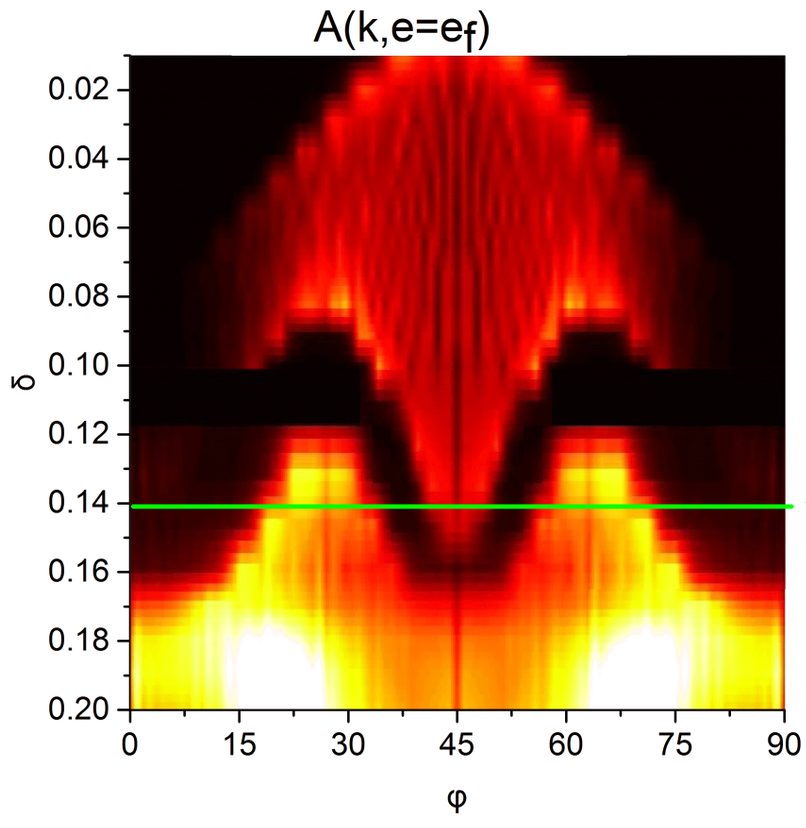


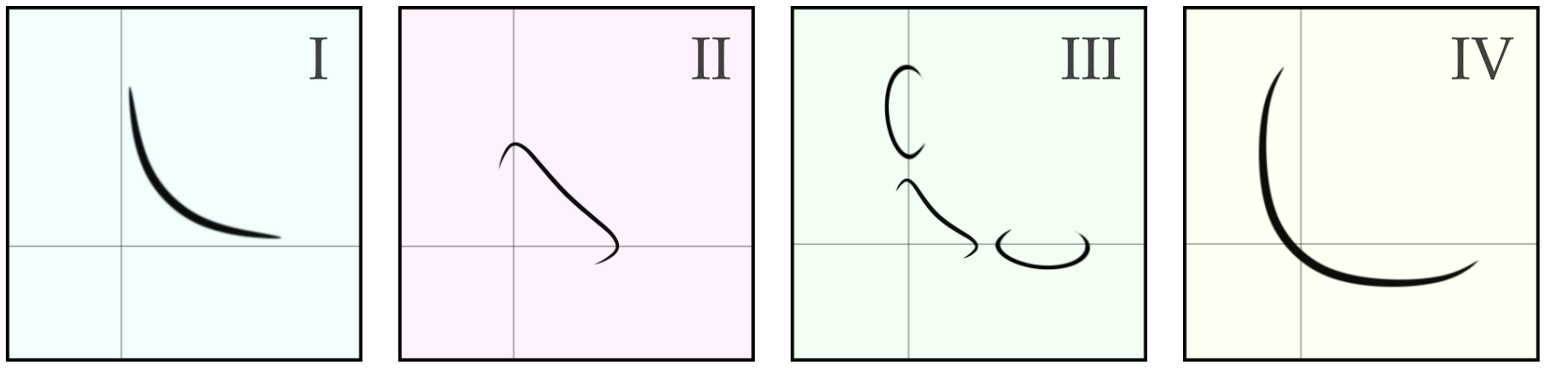
In the limit U=0 surface becomes the large FL-like cylinder

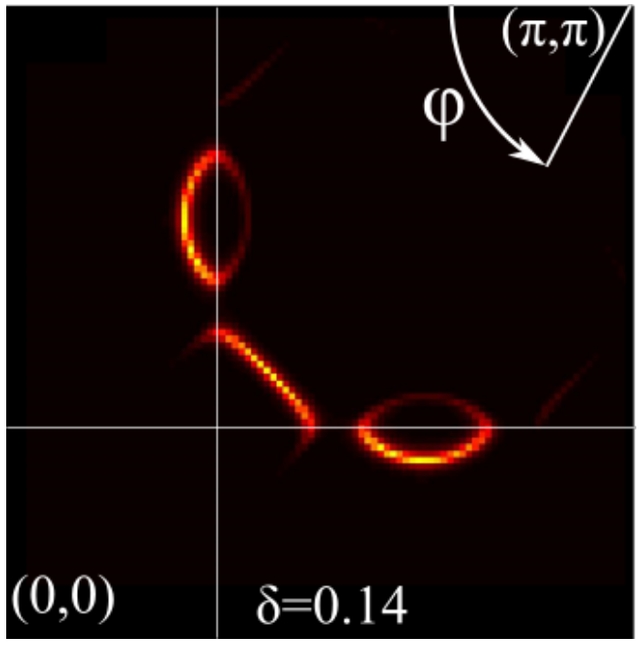
Fermi surface structure

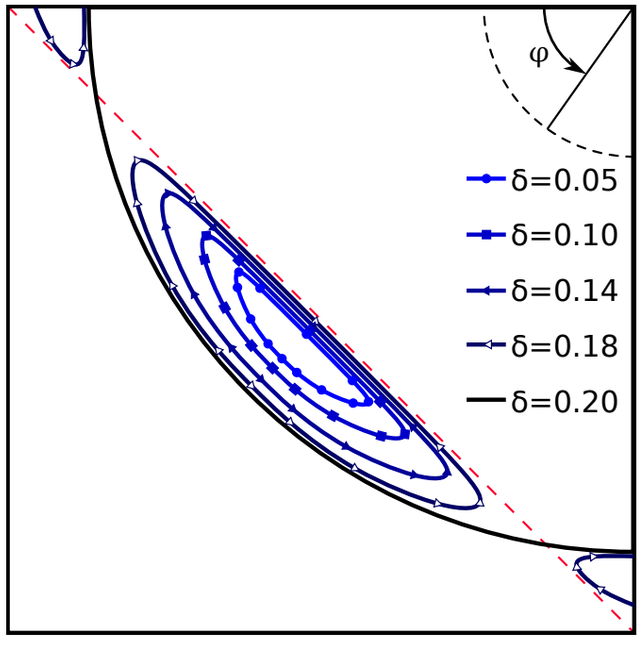
$$\delta_1^{CDW} < \text{anisotropic gap} < \delta_2^{CDW}$$





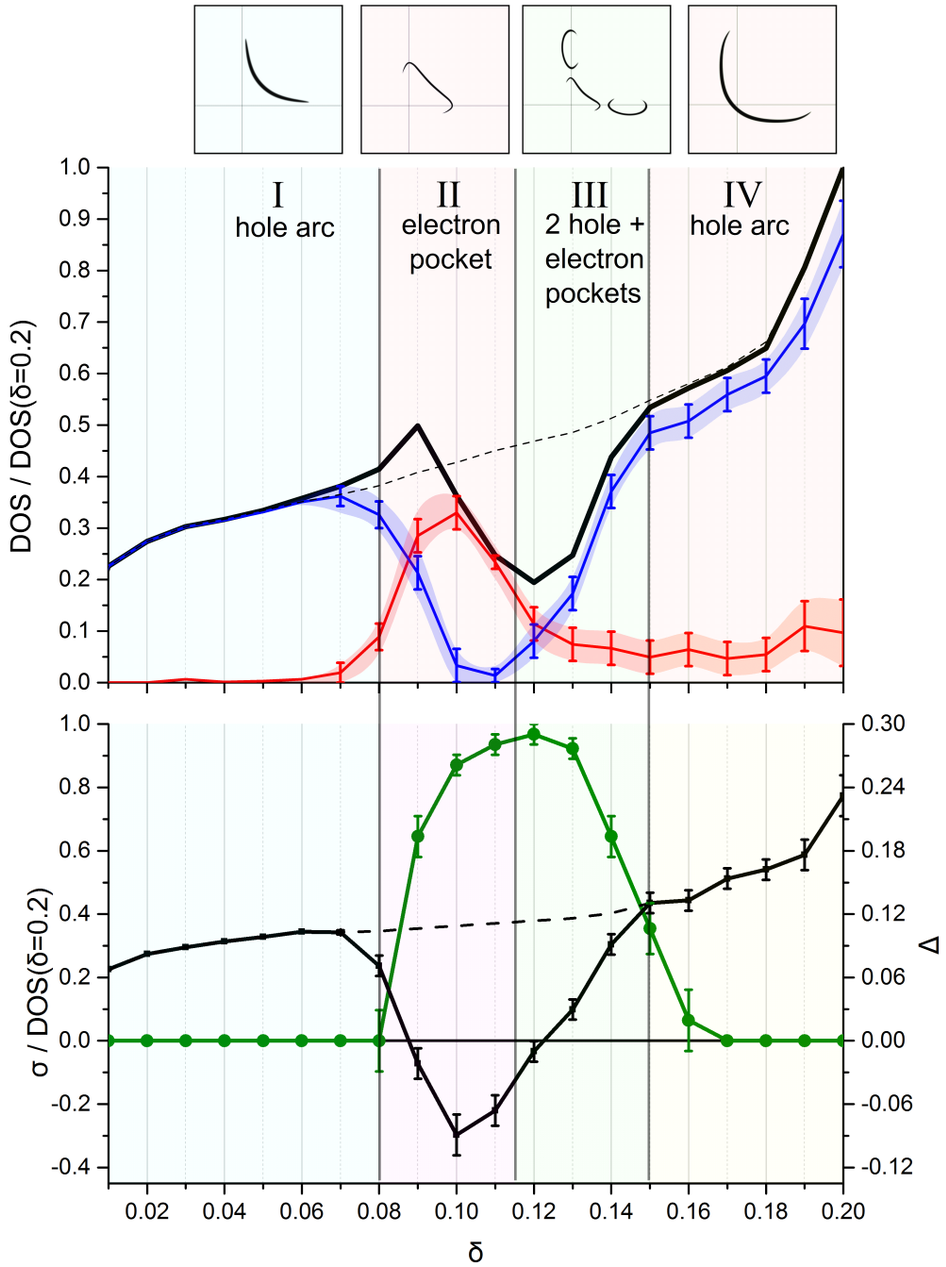






T.Y. Yang, T.M. Rice and F.C.Zhang, PRB 73, 174501 (2006).

DOS and sign of carriers



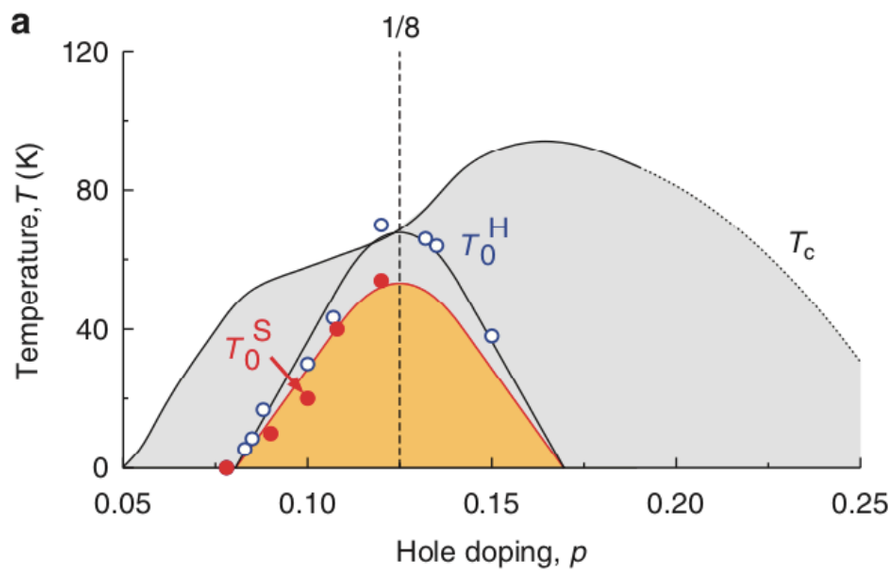
$$\sigma = \int_{BZ} \mathrm{sign}(m_{eff}) A(\mathbf{k}, \varepsilon_f) d\mathbf{k}$$

this work: $\delta_1^{CDW} \approx 8.5\,\%$

$\delta_2^{CDW} \approx 15\,\%$

for YBCO: $\delta_1^{CDW} \approx 8\,\%$

$\delta_2^{CDW} \approx 16\,\%$



F. Laliberte et al, Nat. Commun. 2, 432 (2011).

e pocket / *e*+2*h* pockets: $\delta_{1-2}^{CDW} \approx 11.5\,\%$

Conclusion

- The CDW Fermi surface reconstruction is reproduced:
  - with taking into account the strong Coulomb repulsion.
  - without including any long-range ordering term.

- Both the he electron pocket alone or in the company with the two hole-like pockets are present in different doping regime.

- A whole evolution of the Fermi surface in underdoped cuprates was reproduced.

Thanks for your attention!