Exceptional van Hove Singularities in Pseudogapped Metals

Marcello Civelli

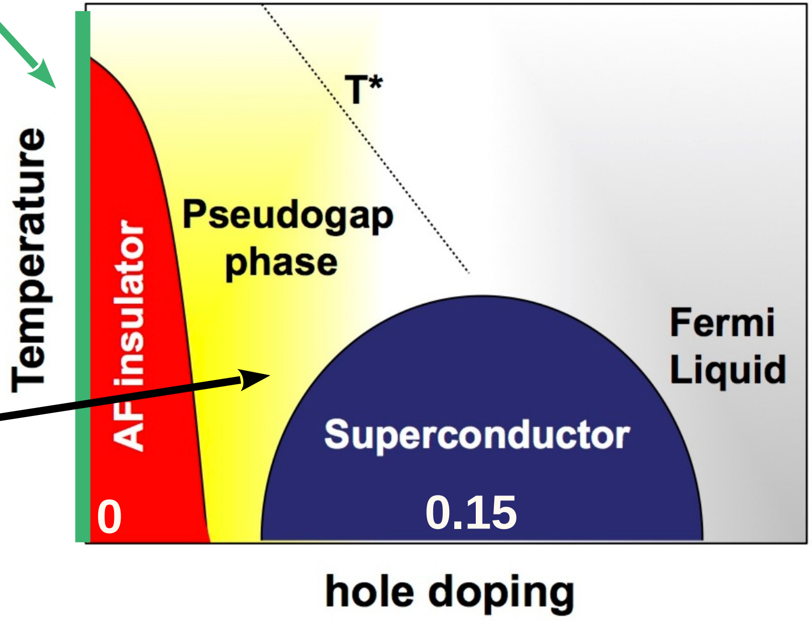
arXiv:2210.01830
to appear in PRB Letters

In collaboration with
I. Paul (MPQ Paris Cité)

High-Tc Supra : the mysterious PseudoGap

Superconductivity appears upon doping an uncon-ventional **insulator (Mott)**

The normal state, the **PseudoGap, is** also **an unconventional metal**



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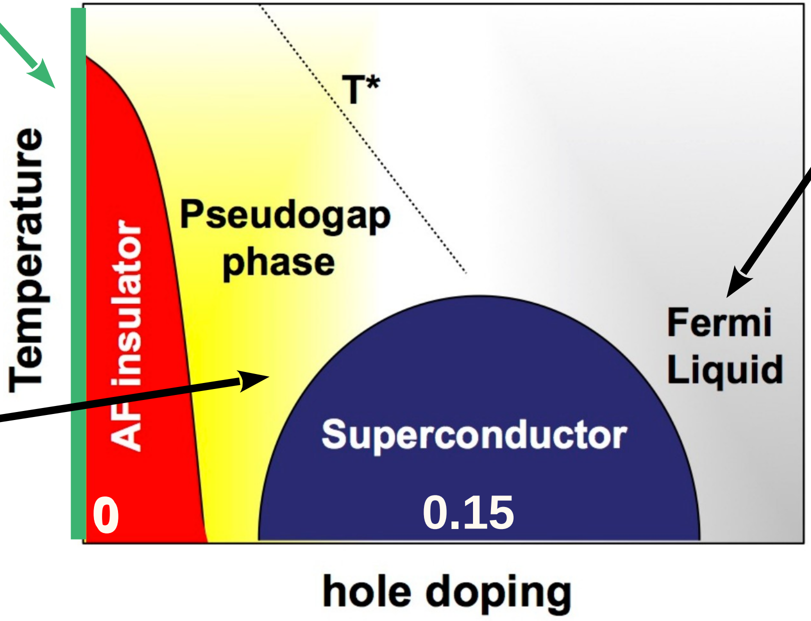

At high doping we find a **conventional metal : Fermi Liquid**

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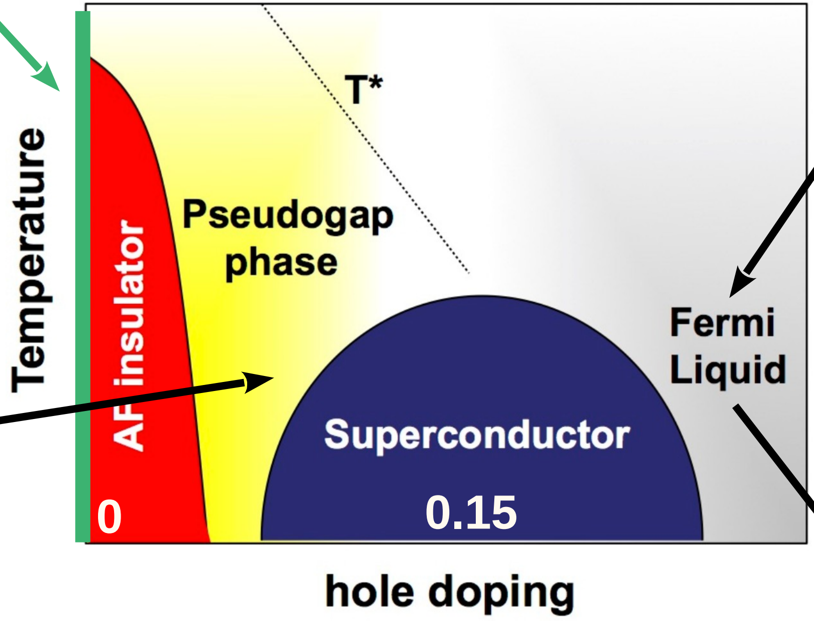

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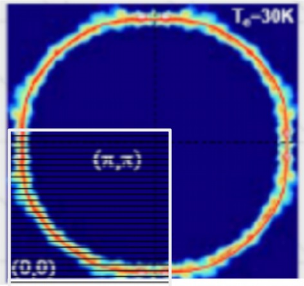
We can measure by photo-emission (ARPES) **the Fermi Surface in the momentum *k* space**

métal standard



Platé et al, PRL 05

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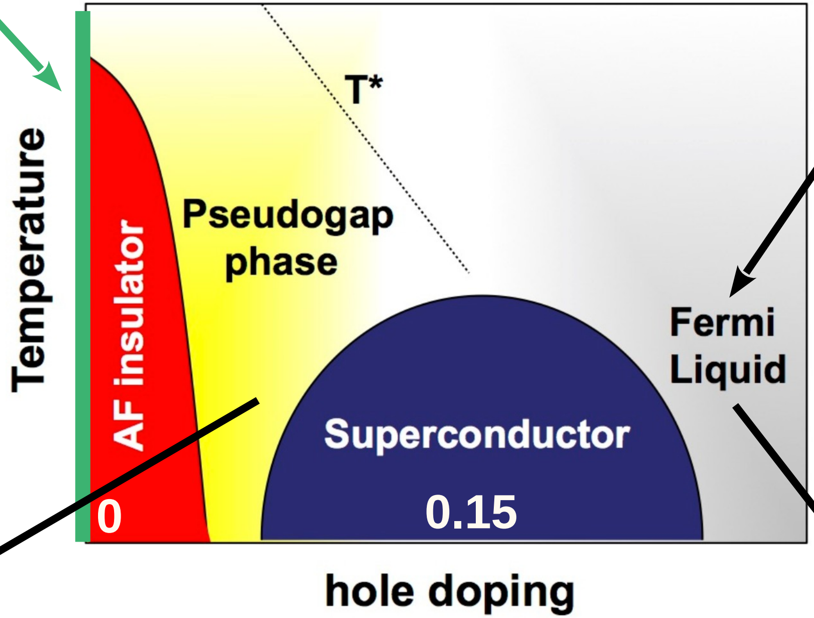

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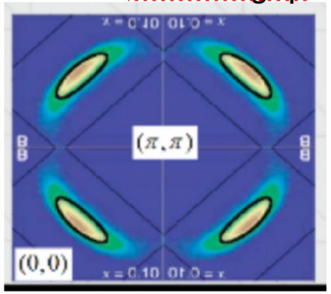

K.M. Shen et al. Science 05

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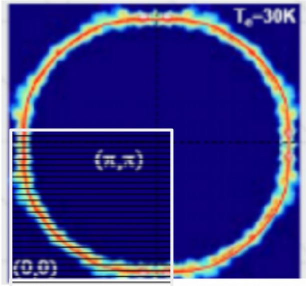

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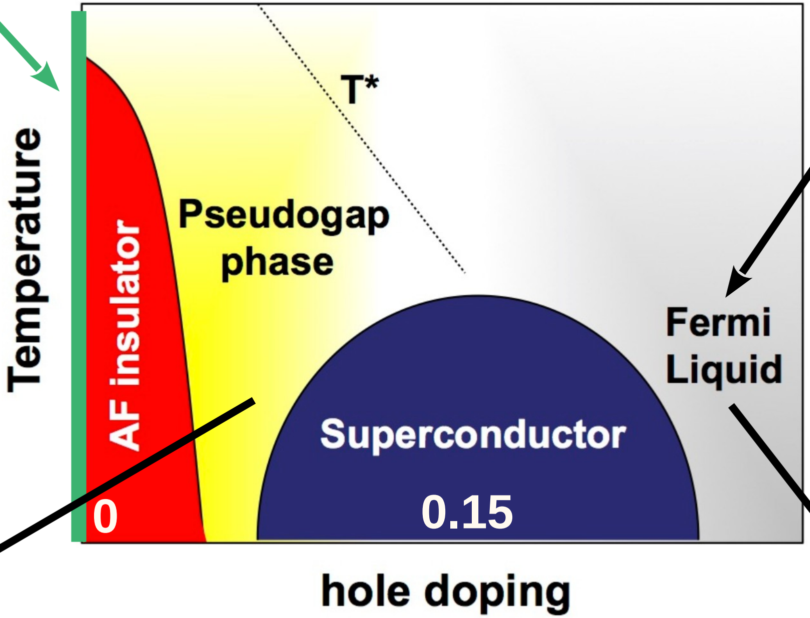

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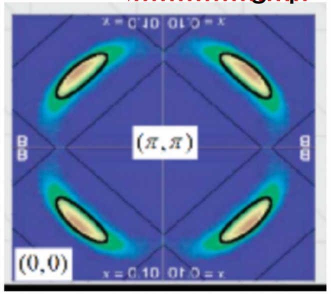
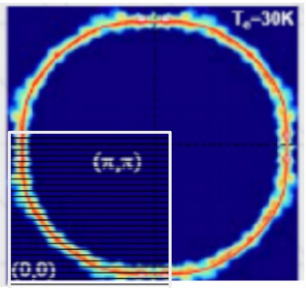


K.M. Shen et al. Science 05

Fermi Surface breaks into pieces : **Mystery !**

métal standard



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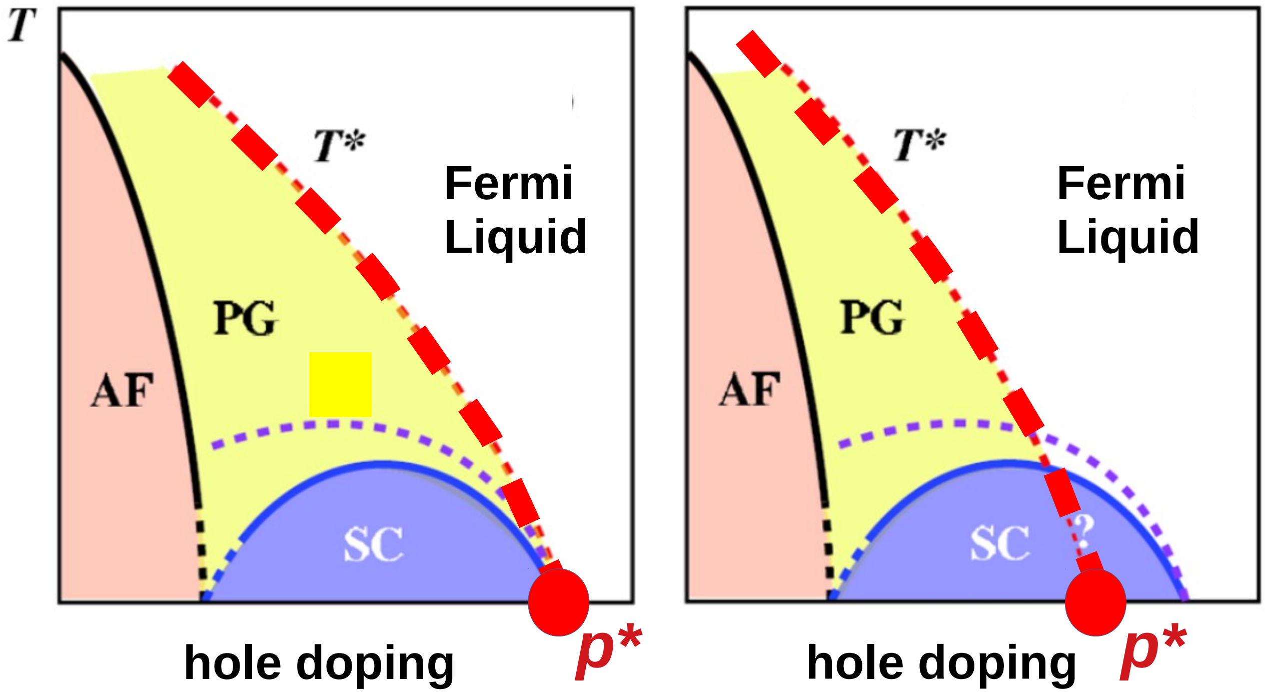
Focus : the rising point of the Pseudogap *p**

F. Rullier-Albenque,a and H. Alloul, EPJ Web of Conferences 23, 00016, 2012



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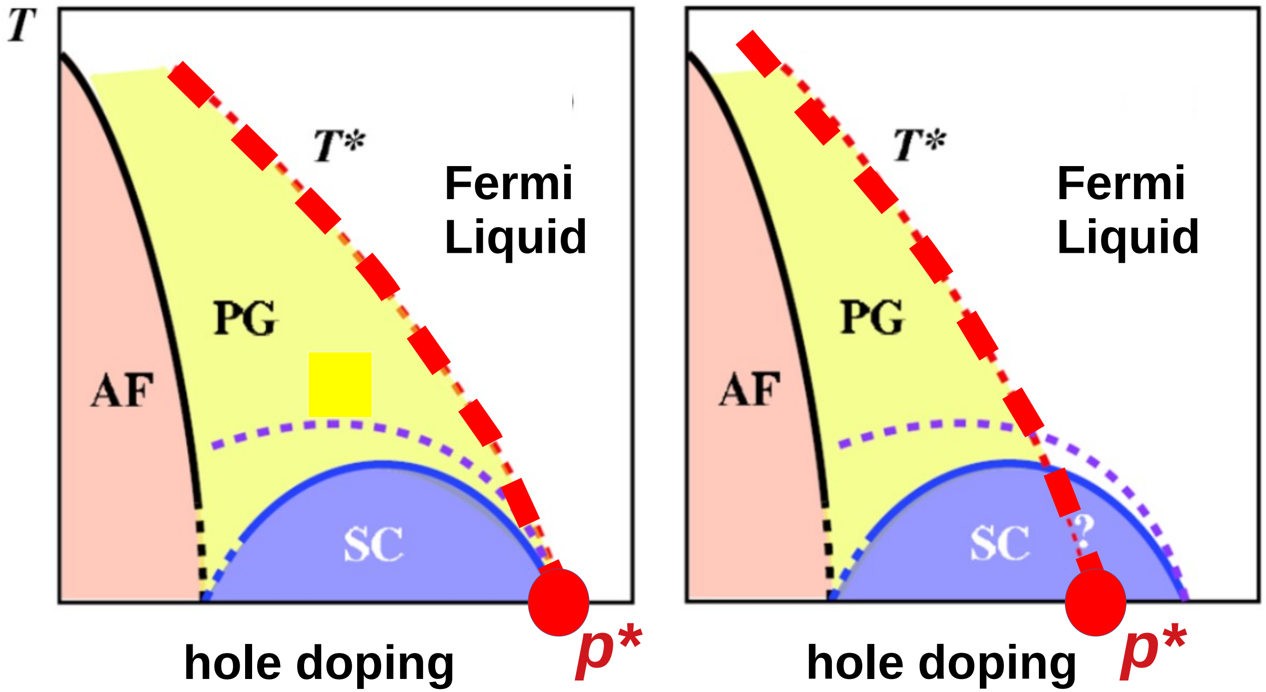

Understanding how the **pseudogap** rises in the phase diagram could reveal the **theory of the high Tc superconductivity**

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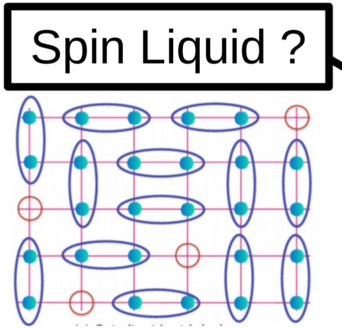
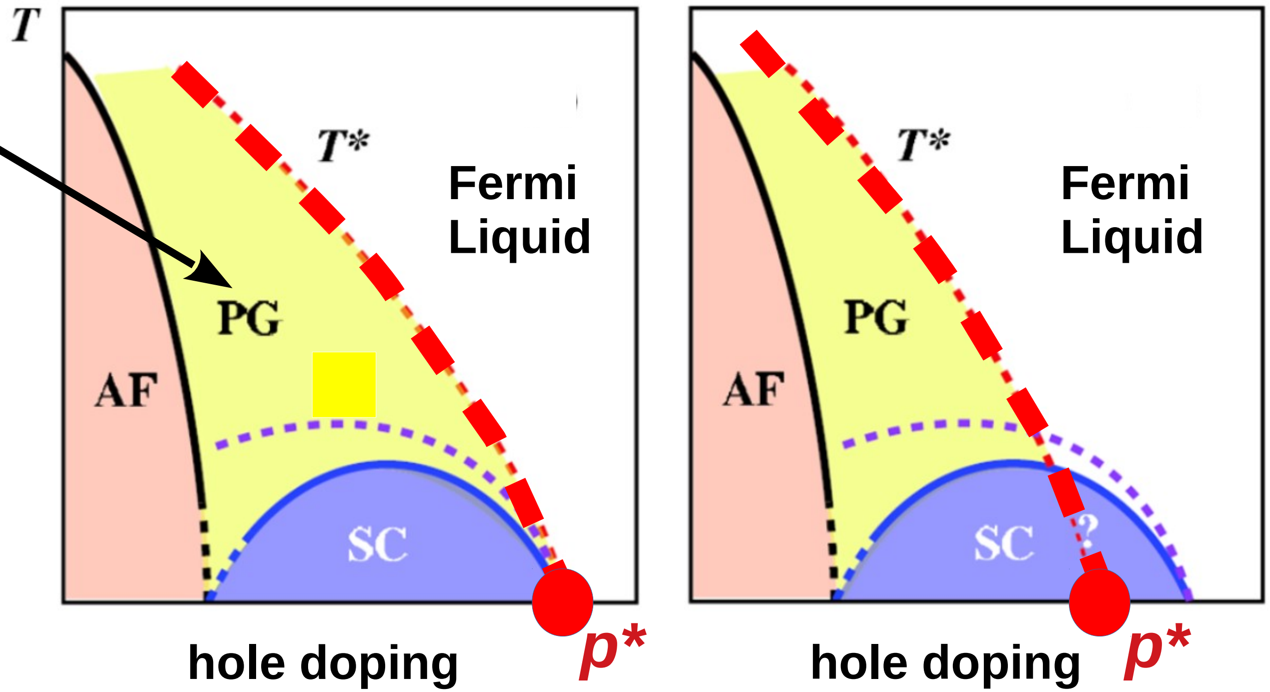


PW Anderson
E. Fradkin
S. Kivelson
S.Sachdev…..



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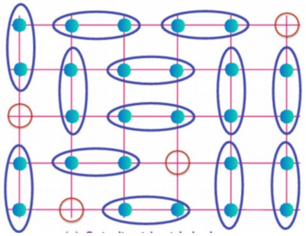
Spin Liquid ?



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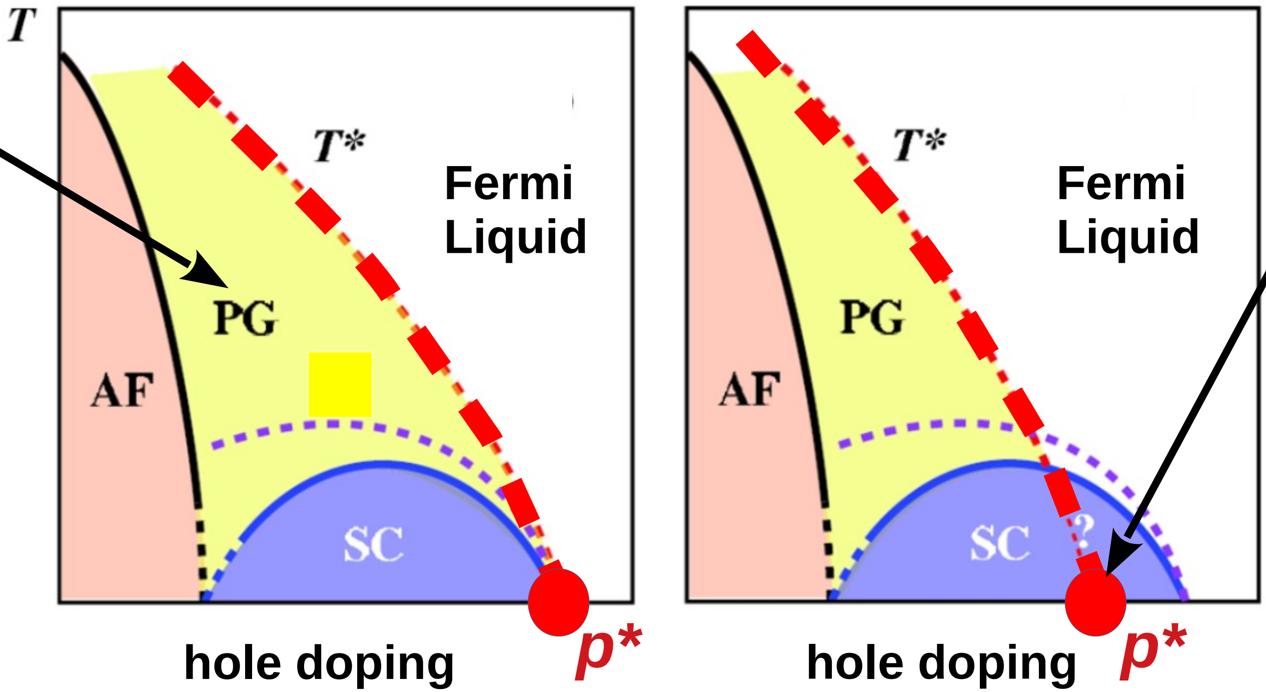


Quantum Critical Point

But what's the broken order ?

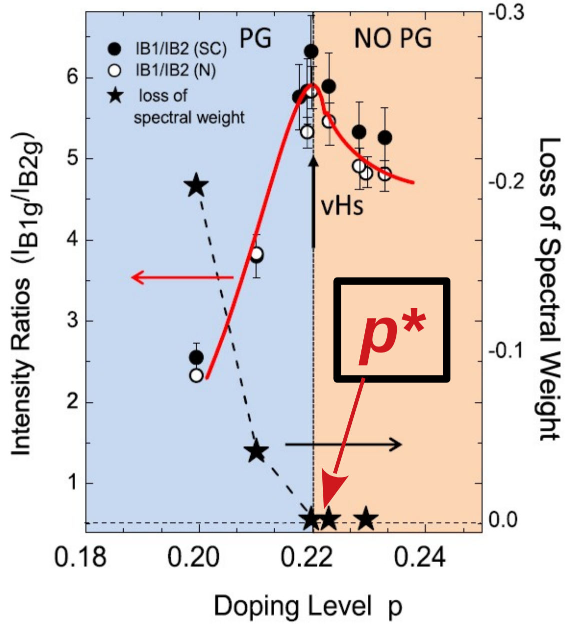
exotic magnetism
charge density waves
loop currents …..

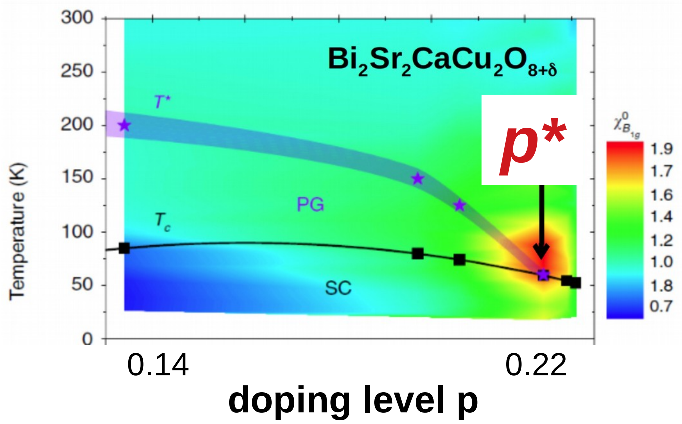
Understanding how the **pseudogap** rises in the phase diagram could reveal the **theory of the high Tc superconductivity**

Key experiments about p*
and open questions

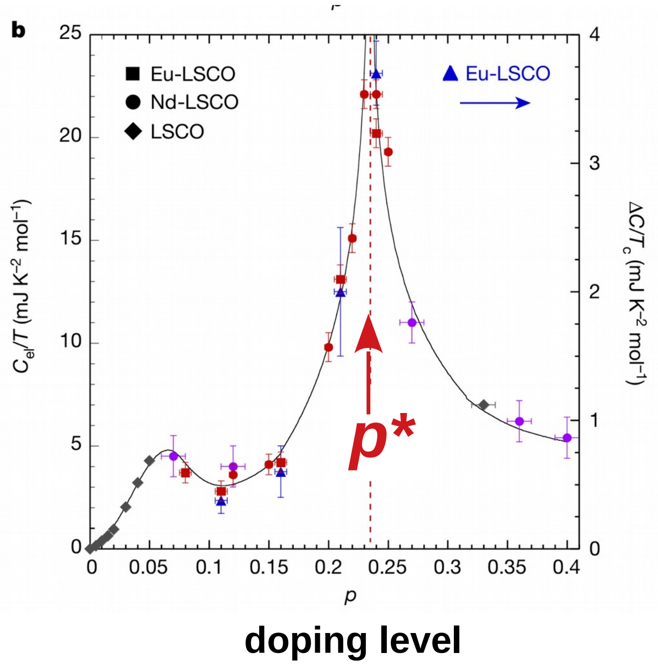
3 key experiments to determine *p**

Raman spectroscopy, A. Sacuto & Y. Gallais group MPQ



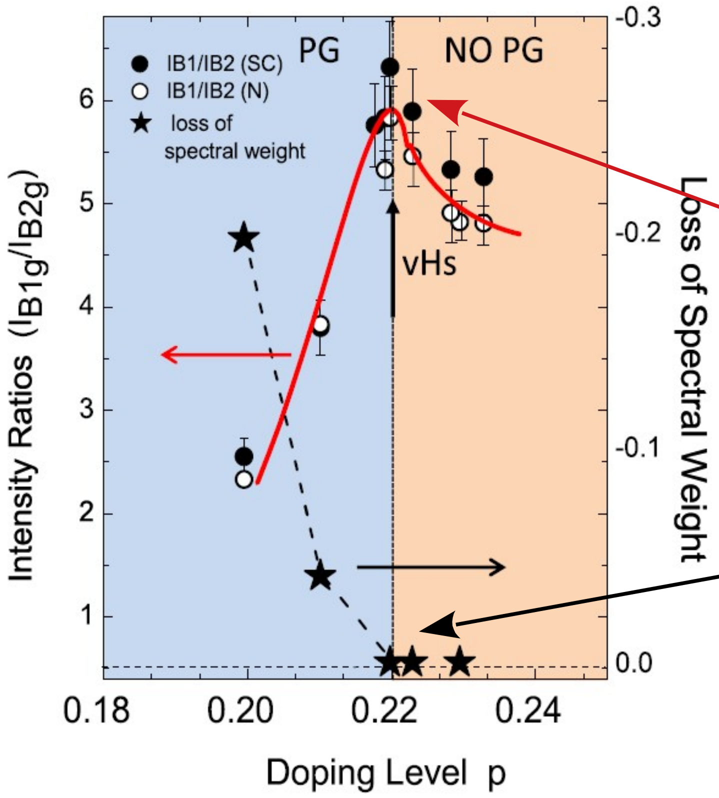


Specific Heat
L. Taillefer Group Sherbrooke



Raman spectroscopy through *p**

S. Benhabib, A. Sacuto, MC, I Paul, et al,
PRL **114**, 147001 (15) **on Bi2212**



Alain Sacuto
U. Paris Cité

Siham Benhabib
IPS Orsay

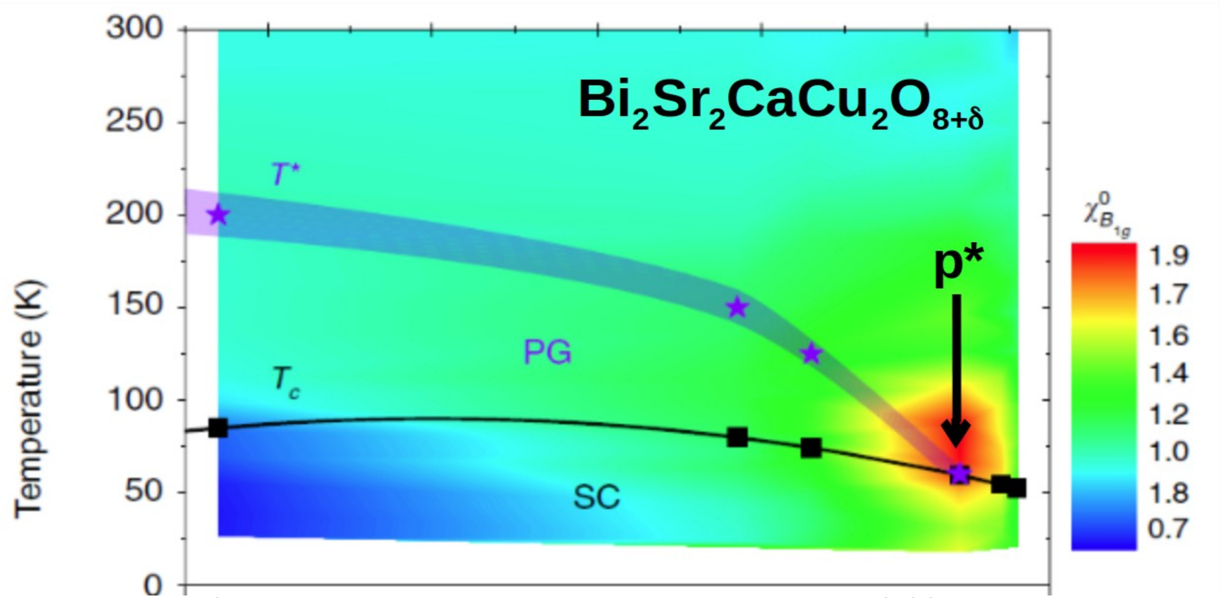
Dorothée Colson
CEA Saclay

- At ***p* ~ 0.22*** Raman Intensity has a sharp intensity **enhancement**

★ At the same doping **PseudoGap collapses**

Raman spectroscopy through *p**

N. Auvray, Y. Gallais, I Paul, et al., Nat. Comm **10:5209** (19)



0.14 0.22

doping level p

Y. Gallais

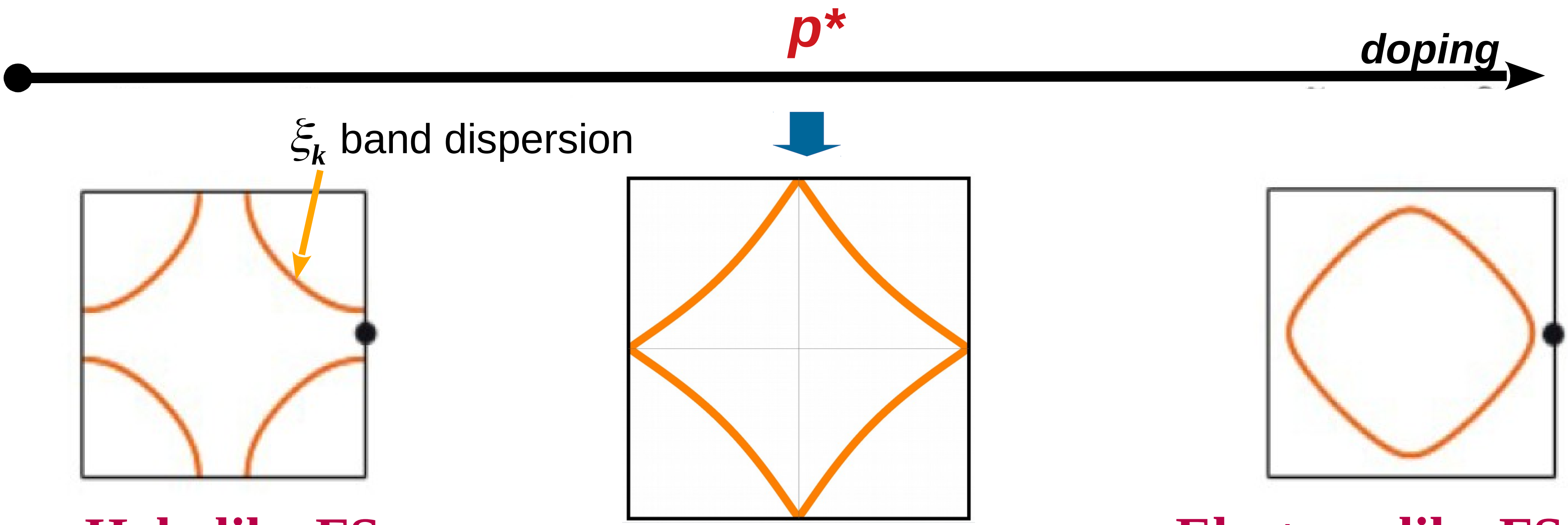
I. Paul

static nematic susceptibility χ_{B1g}

$$\Re\chi_{B1g}=\frac{2}{\pi}\int_0^\infty d\omega\ \frac{\Im\chi_{B1g}(\omega)}{\omega}$$

Enhanced Raman χ_{B1g} **fluctuations appear at** ***p* ~ 0.22***

Could the Raman enhancement at *p** be a Lifshitz transition effect?



Hole-like FS **Electron-like FS**

density of states

$$N(\xi) = \int_{\xi=\xi_k} dk \frac{1}{|\nabla_k \xi_k|}$$

if $\nabla_k \xi_k = 0$ one has a huge response

This happens at high symmetry points $(0, \pm\pi)$ $(\pm\pi, 0)$

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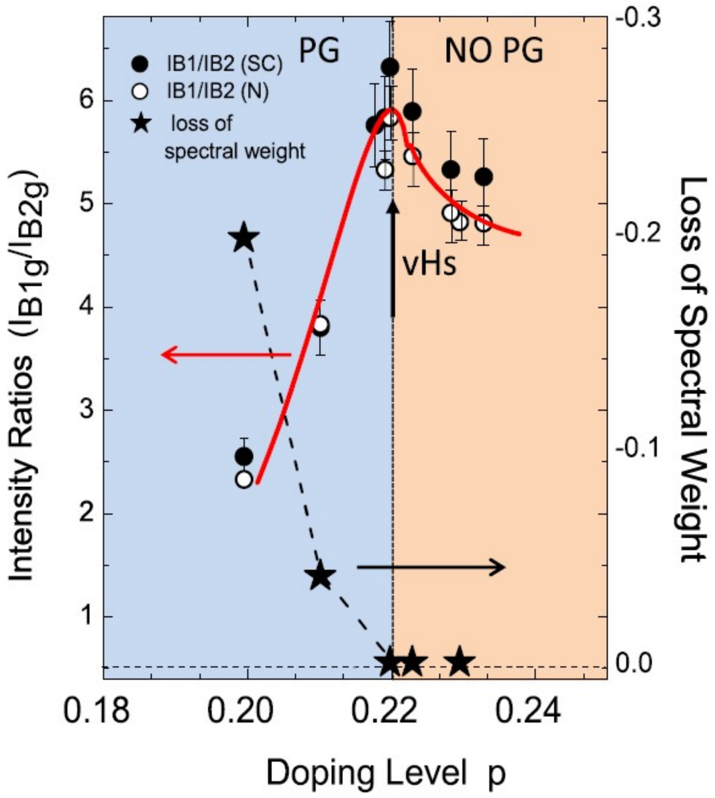
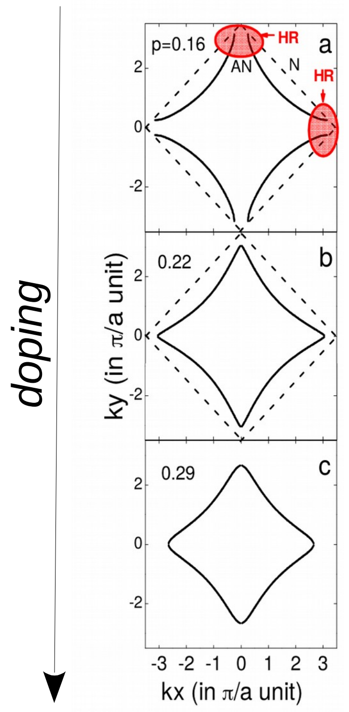


Fermi Surface



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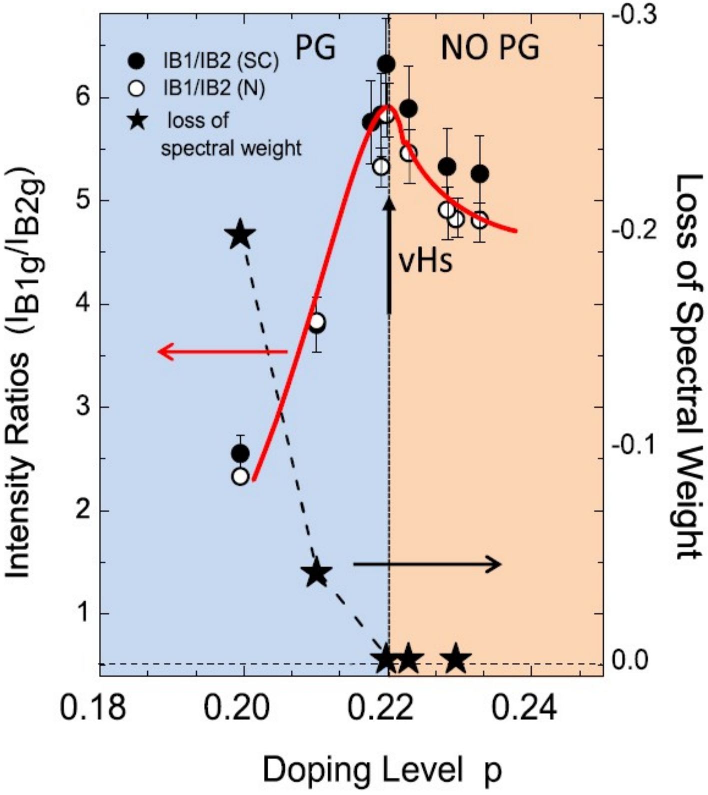

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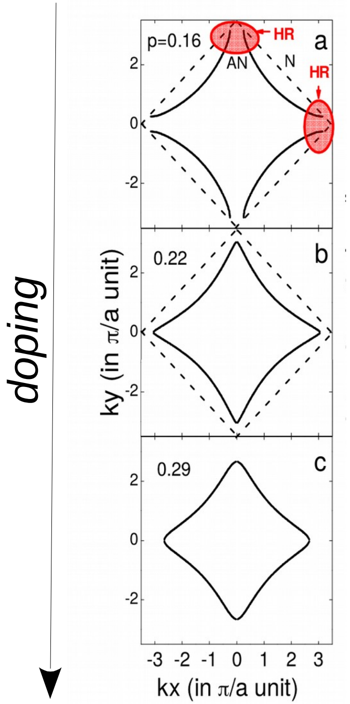
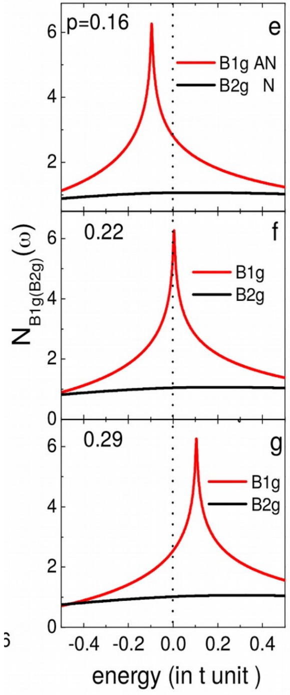
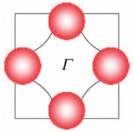


Weighted *B1g* density of states





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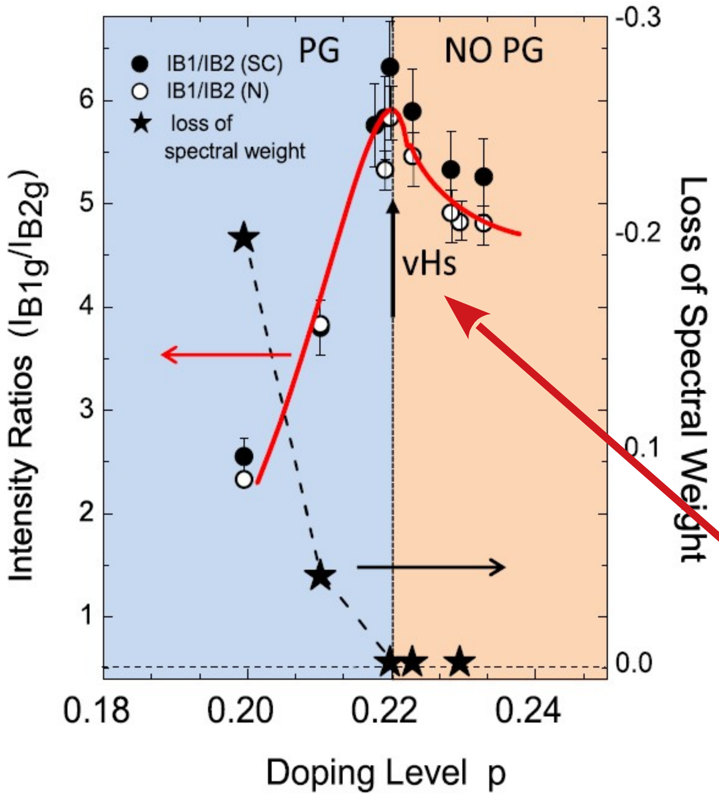

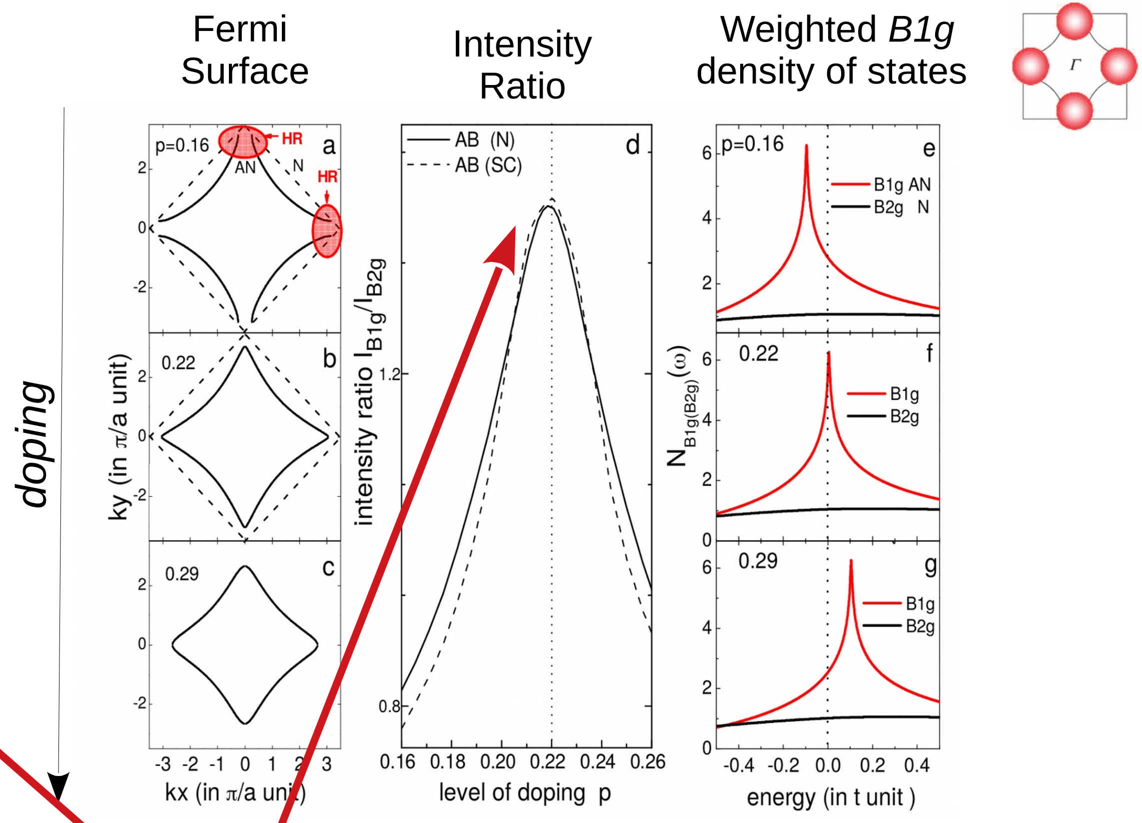

*p**

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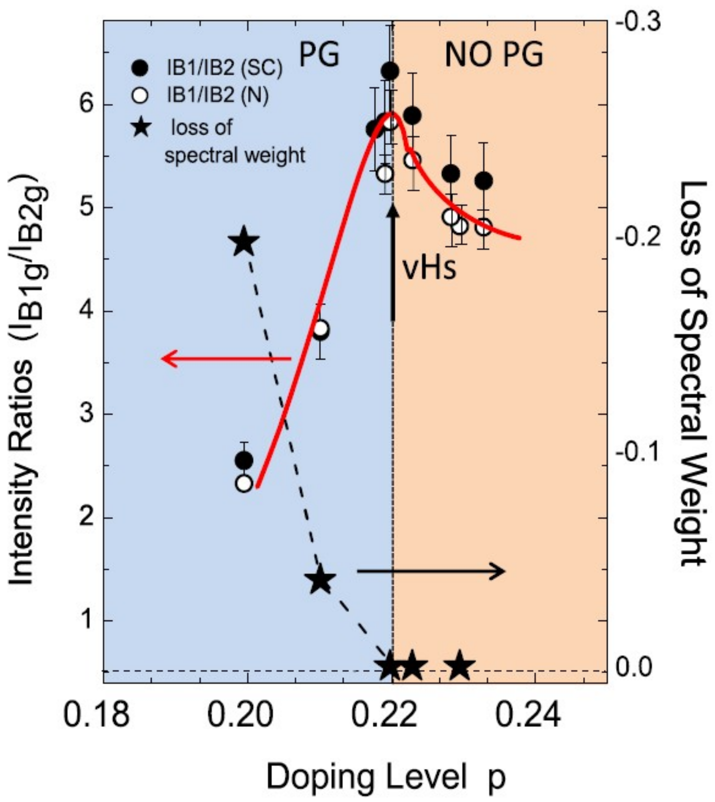
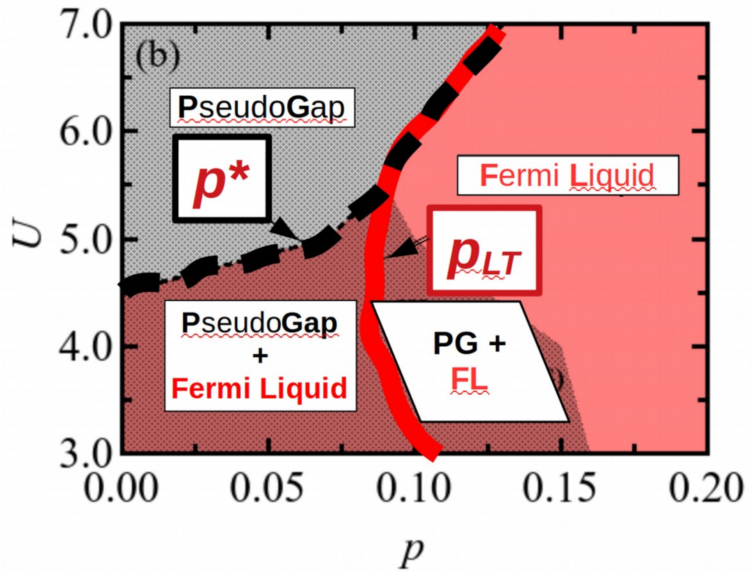


H. Braganca et al. PRL *120, 067002 (2018)*



CDMFT calculations have shown a tight **relation between** the PseudoGap endpoint ***p**** **and the Lifshitz transition doping** ***p_{LT}*** **without invoking a broken order phase**

see also Wu, Georges, Ferrero, et al, PRX **8**, 021048 (18)

Raman spectroscopy through *p**

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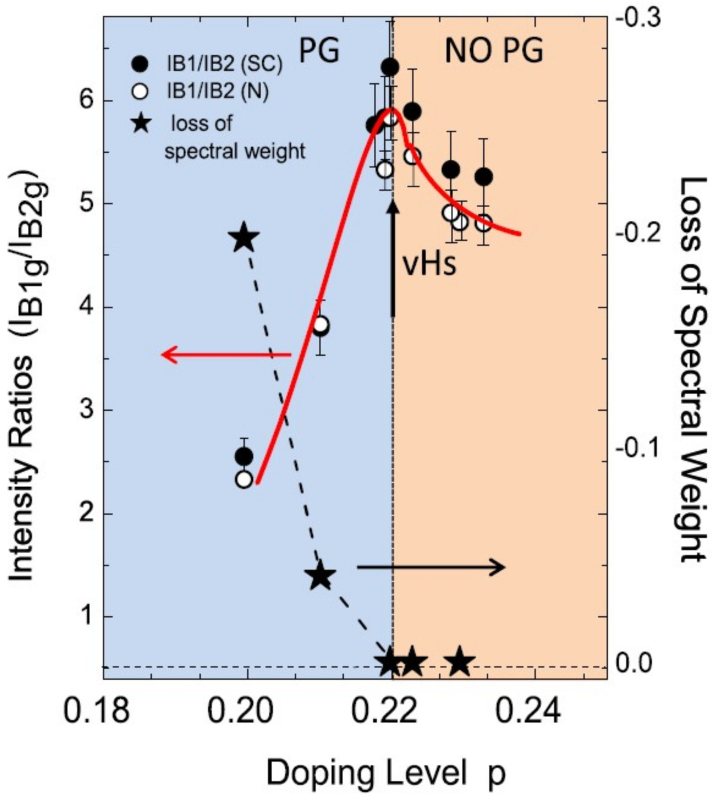
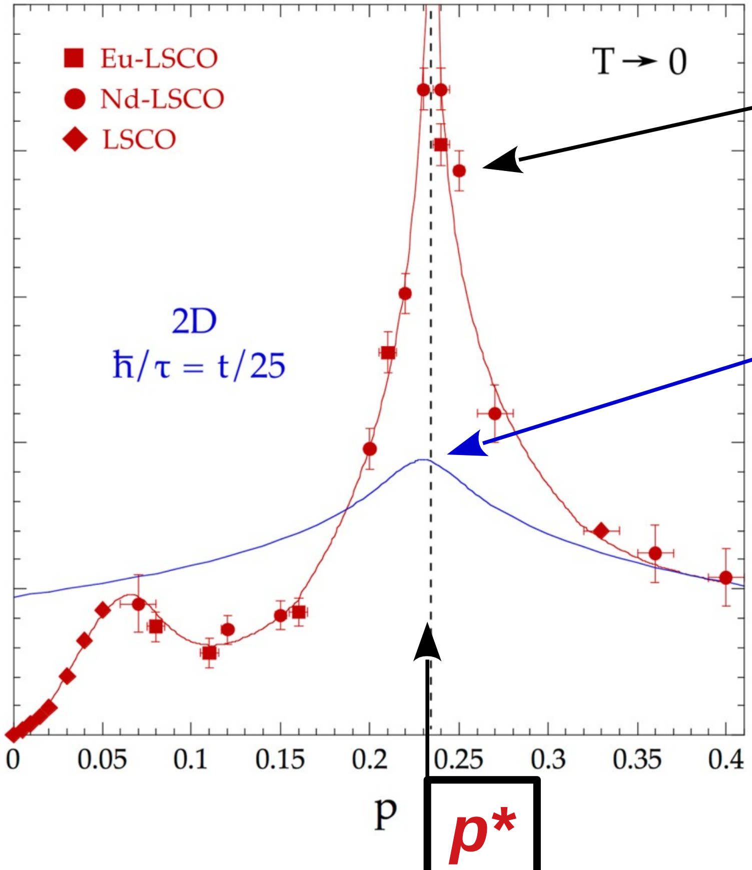


Transport and thermal transport measures from the group of L. Taillefer **confirmed this scenario of a PG tight to a Lifshitz transition** :
see e.g Doiron-Leyraud, N., Cyr-Choinière, O., Badoux, S. et al.
Pseudogap phase of cuprate superconductors confined by Fermi surface topology.
Nat Commun 8, 2044 (2017).

Recent specific heat measures at p*
have questioned the Lifshitz transition scenario

Michon, Taillefer, T. Klein, et al,
Nature **567**, 218 (19)



The specific heat coefficient **$\gamma = C_v/T$** at very low T→ 0 **is diverging at p***

The **divergence of γ is incompatible with a Lifshitz transition** as soon as one consider a finite scattering time τ, due to disorder, or the third dimensionality of a real systems: Density of states ***N(ω) ~ log (ω) weak!***

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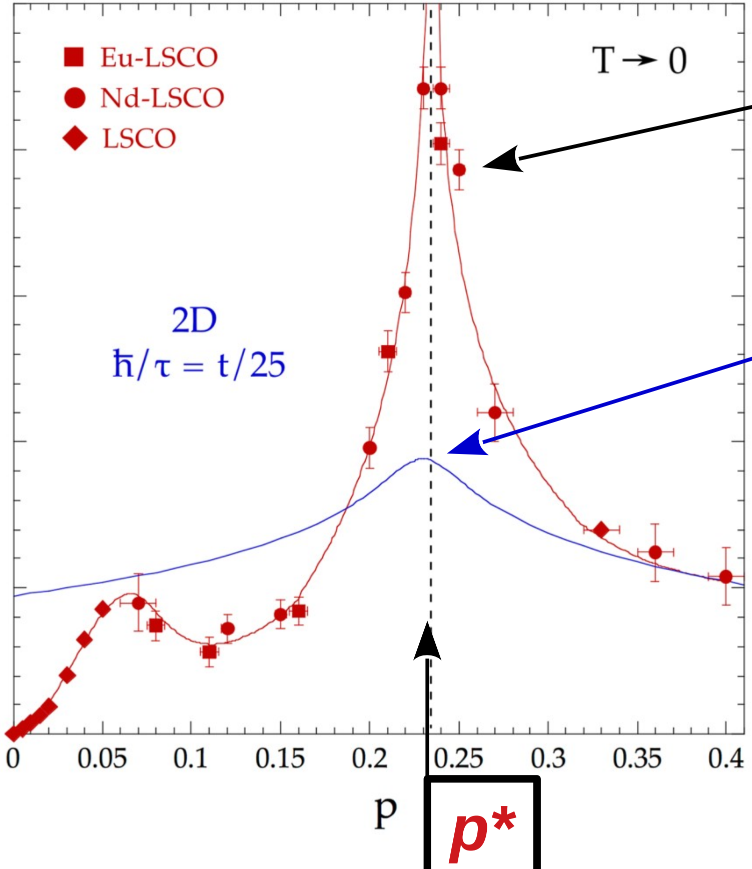

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Is the Lifshitz transition in the Pseudogap phase the same as a regular one ?

Lifshitz transition in the PseudoGap phase: the role of correlations

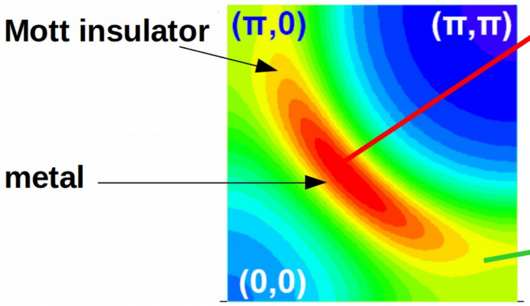
Our understanding of the PseudoGap from strong correlations

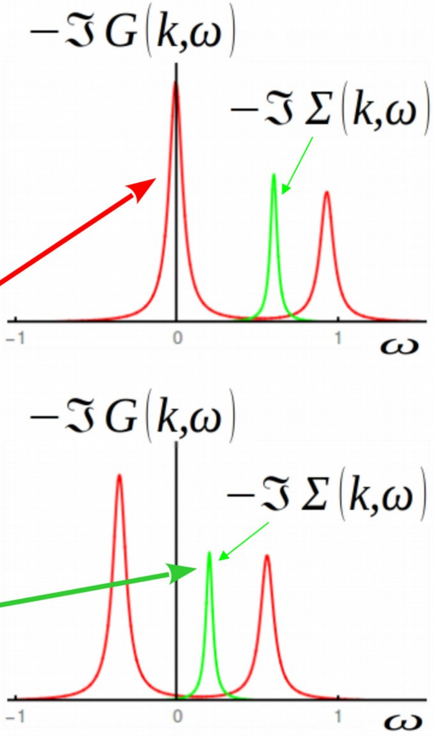
Cluster Dynamical Mean Field Results
on the Hubbard Model

A **pole-like singularity develops in the self-energy**: breaking of the FL in some regions of momentum space

$$G(k,\omega)=\frac{1}{\omega-\xi_k-\Sigma(\omega,k)}$$

$$\Sigma(k,\omega\to 0)\approx\frac{P_k^2}{\omega-\varepsilon_k}$$





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[22] T. D. Stanescu and G. Kotliar, Phys. Rev. B **74**, 125110 (2006).
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[25] S. Sakai, Y. Motome, and M. Imada, Phys. Rev. Lett. **102**, 056404 (2009).
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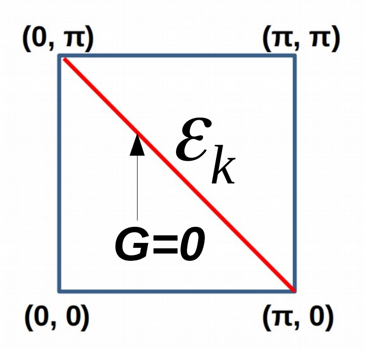
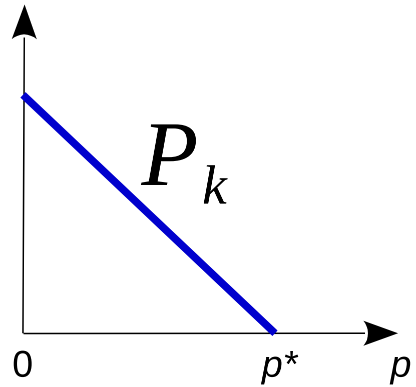
[27] W. Wu, M. S. Scheurer, S. Chatterjee, S. Sachdev, A. Georges, and M. Ferrero, Phys. Rev. X **8**, 021048 (2018).
[28] H. Bragança, S. Sakai, M. C. O. Aguiar, and M. Civelli, Phys. Rev. Lett. **120**, 067002 (2018).
[29] G. Sordi, K. Haule, A.-M.S. Tremblay, Phys. Rev. Lett. **104**, 226402 (2010).
[30] G. Sordi, K. Haule, A.-M. S. Tremblay, Phys. Rev. B **84**, 075161 (2011).

Low energy ω → 0 approach: the Yang-Zhang-Rice model

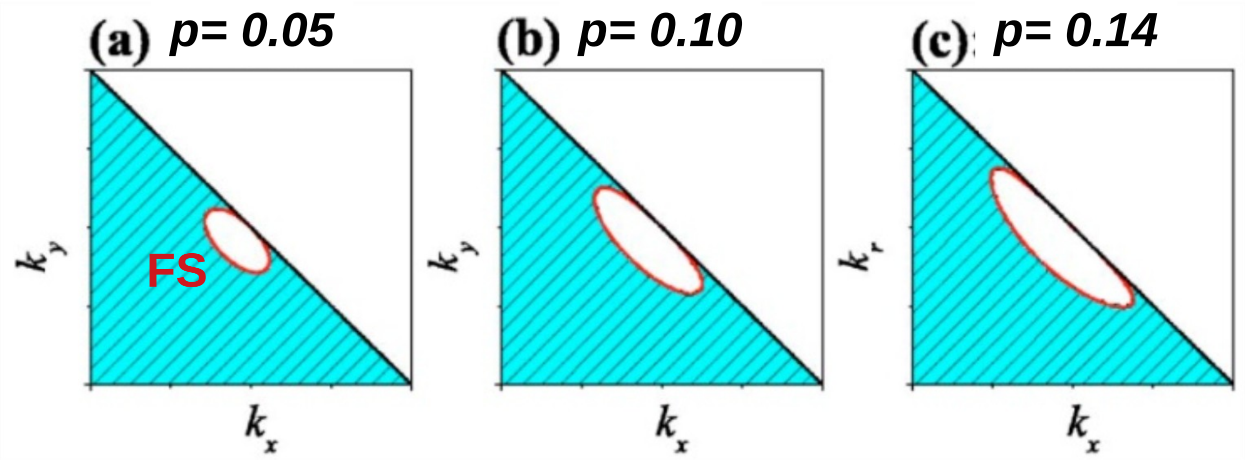
Yang, Rice, Zhang, PRB **73**, 174501 (06)

$$G(k,\omega)^{-1} = \omega - \xi_k - \frac{P_k^2}{\omega - \varepsilon_k}$$





Appearance of FS pockets



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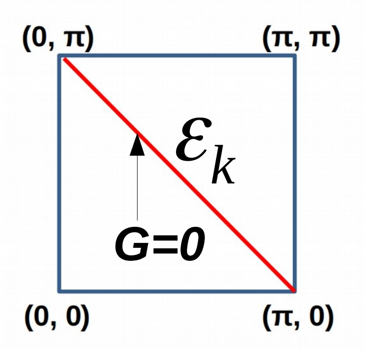
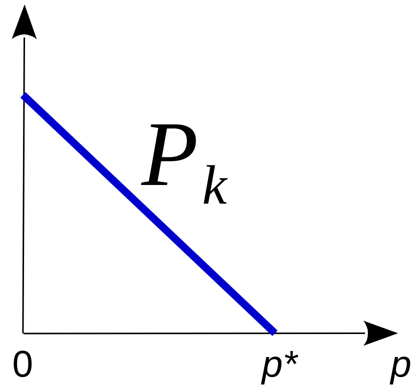
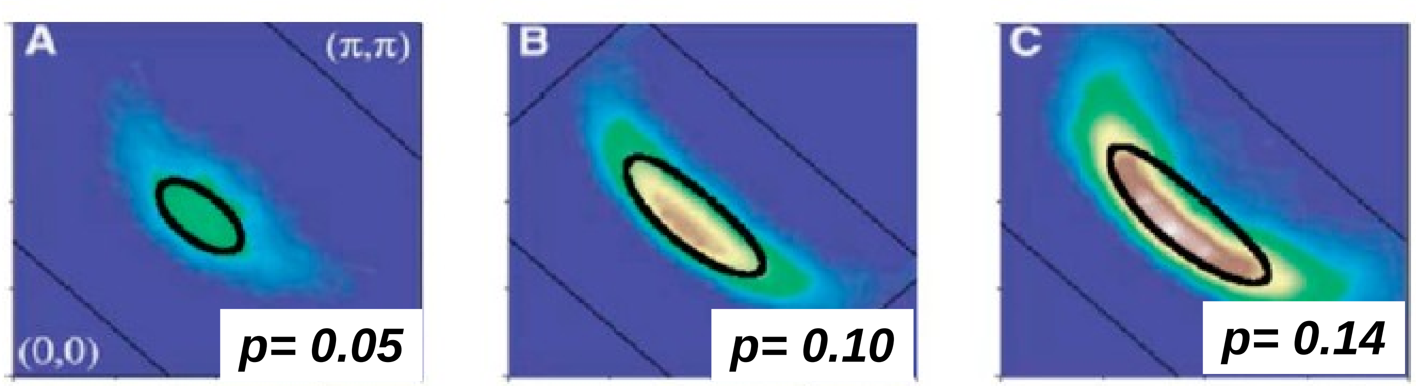


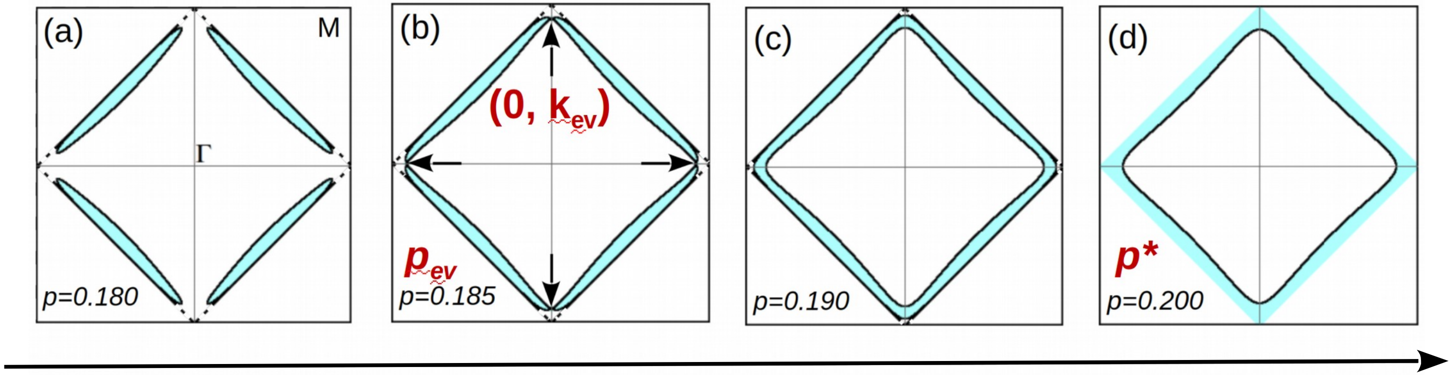


Describes Fermi Arcs seen in ARPES



The *correlated* Lifshitz Transition: an « exceptional » van Hove singularity

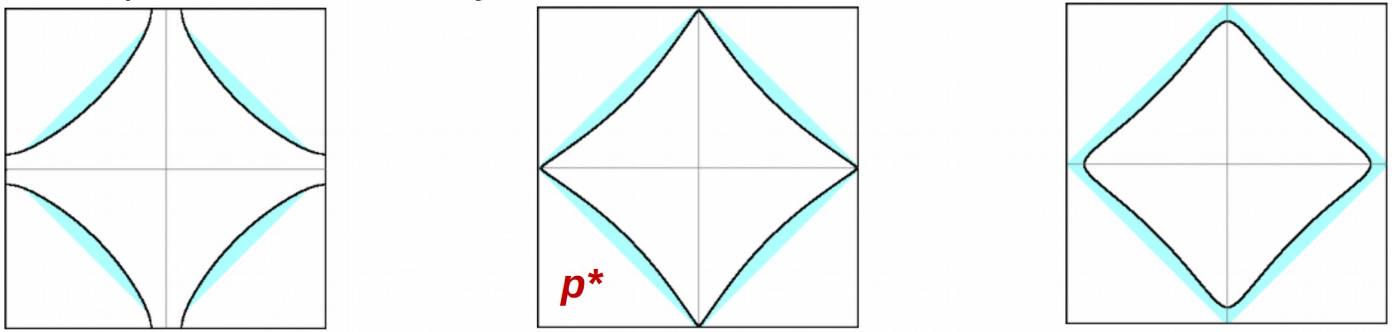
I Paul, MC, arxiv 2210.01830



The Lifshitz transition takes place :

- At $p_{ev} < p^*$ (where PG → 0)
- Saddle points are on $(0,\pm k_{ev})$ and $(\pm k_{ev},0)$, *which are not high symmetry points*
- ***How Density of states diverges ?***

to compare with the weakly correlated one



The Lifshitz transition takes place :

- At p^* (where PG → 0)
- Saddle points are on *high symmetry points* $(0,\pm\pi)$ and $(\pm\pi,0)$
- ***Density of states weakly diverges $N(\omega) \sim \log(\omega)$***

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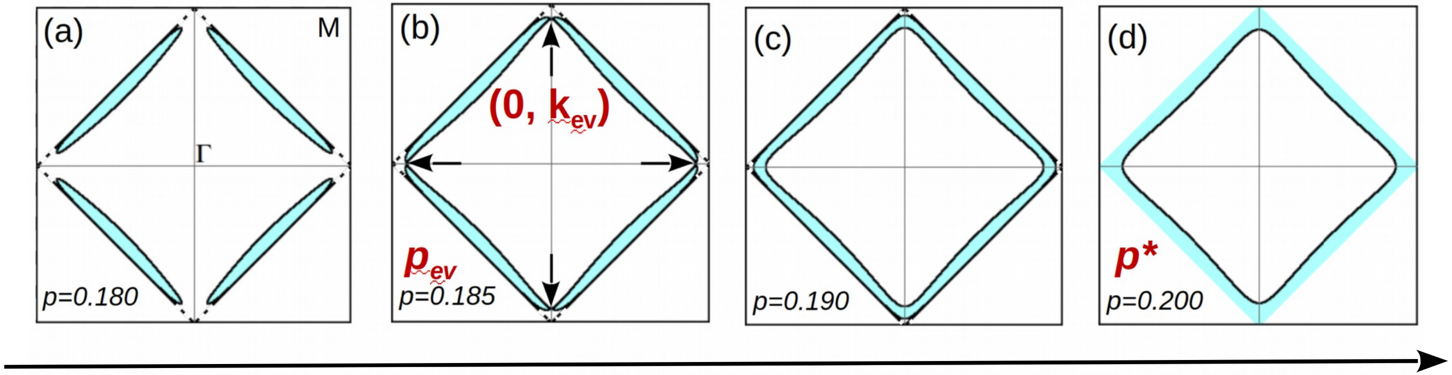

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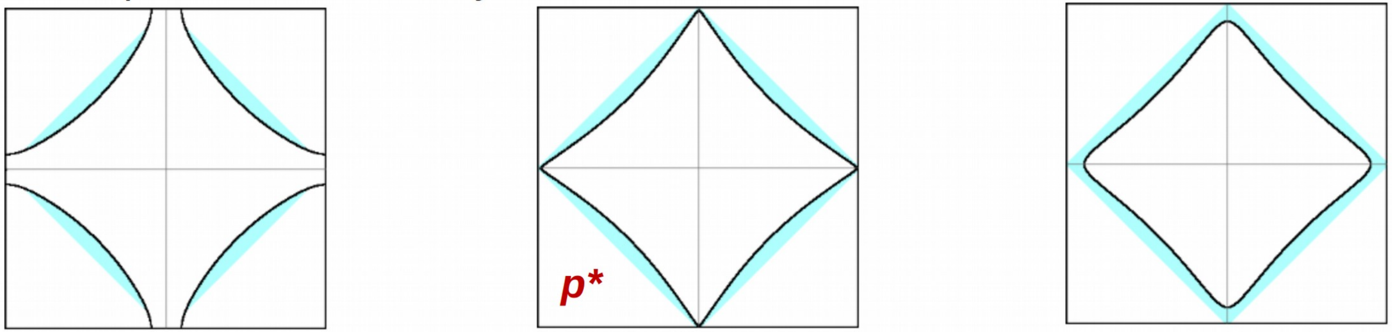

The Lifshitz transition takes place :

- At $\boldsymbol{p_{ev} < p^*}$ (where PG → 0)
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- ***How Density of states diverges ?***

The Lifshitz transition takes place :

- At ***p**** (where PG → 0)
- Saddle points are on *high symmetry points* ***(0,±π) and (±π,0)***
- ***Density of states weakly diverges N(ω) ~ log (ω)***

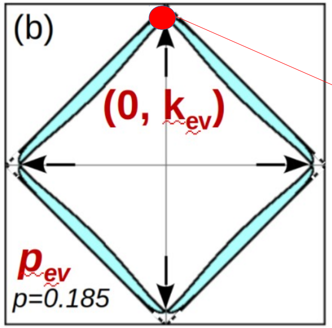
ARTICLE

https://doi.org/10.1038/s41467-019-13670-9 OPEN

Magic of high-order van Hove singularity

Noah F.Q. Yuan[1], Hiroki Isobe[1] & Liang Fu[1*]

Could it be that ***(0,±k$_{ev}$)* and *(±k$_{ev}$,0)*** *are a* ***second order van Hove singularity ?***



$$G(k,\omega)^{-1} = \omega - \xi_k - \frac{P_k^2}{\omega - \varepsilon_k} \qquad E(\mathbf{k}) = (\xi_\mathbf{k} + \varepsilon_\mathbf{k}) - \sqrt{(\xi_\mathbf{k} - \varepsilon_\mathbf{k})^2 + 4P_\mathbf{k}^2}/2$$

Expand around $\mathbf{k}_{ev} = (0, k_{ev})$ $\quad \mathbf{q} = \mathbf{k} - \mathbf{k}_{ev}$

$$E(\mathbf{k} - \mathbf{k}_{ev}) = \nabla E_\mathbf{q} \cdot \mathbf{q} + \mathbf{q} \cdot \hat{\mathbf{D}} \cdot \mathbf{q} + \ \ldots$$

$$\nabla E_\mathbf{q} = 0 \quad as \quad it\, is\, a\, VHS$$

$$E(\mathbf{k} - \mathbf{k}_{ev}) = \alpha q_x^2 - \beta q_y^2 + \ \ldots$$

1) $\alpha \neq 0,\ |\hat{\mathbf{D}}| \neq 0$ ***regular VHS***

$N(\omega) \sim \log(\omega)$

2) $\alpha = 0,\ |\hat{\mathbf{D}}| = 0$ ***2nd Order VHS***

$N(\omega) \sim \omega^{-1/4}$

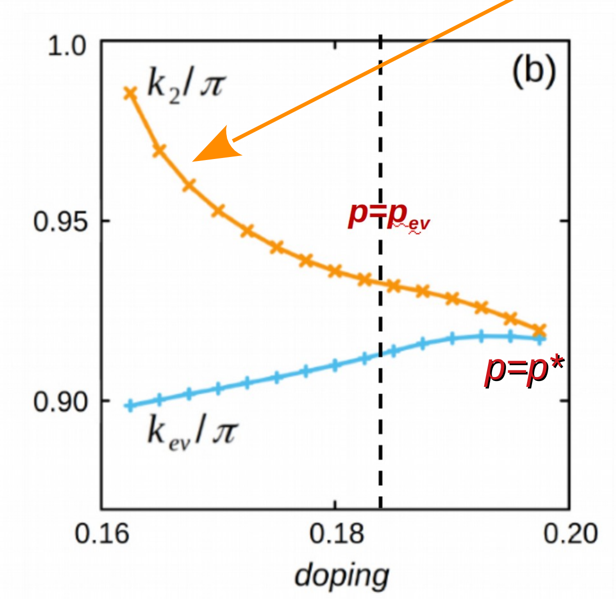
divergence is strong !

Could it be that ***(0,±k_{ev})* and *(±k_{ev},0)*** *are a* ***second order van Hove singularity ?***

Actually not !

I Paul, MC, arxiv 2210.01830

$\alpha = \partial^2 E_{\mathbf{k}} / \partial^2 k_x = 0$ in $(0, k_2)$



$k_2 \neq k_{ev}$ hence VHS is never 2nd order

It is however very close
closer and closer *p* → *p we approach the 2nd VHS limit**

If $\alpha \to 0$ the density of states can be strongly enhanced
(though never algebraically $\omega^{-1/4}$ strictly speaking)

$$N(\omega) = \frac{1}{2\pi^2\sqrt{\alpha\beta}}\left[\mathrm{Re}\left[\frac{1}{(1+u)^{1/4}}K(r_1)\right]\right.$$
$$\left.-\mathrm{Im}\left[\frac{1}{(1+u)^{1/4}}K(r_2)\right]\right].$$

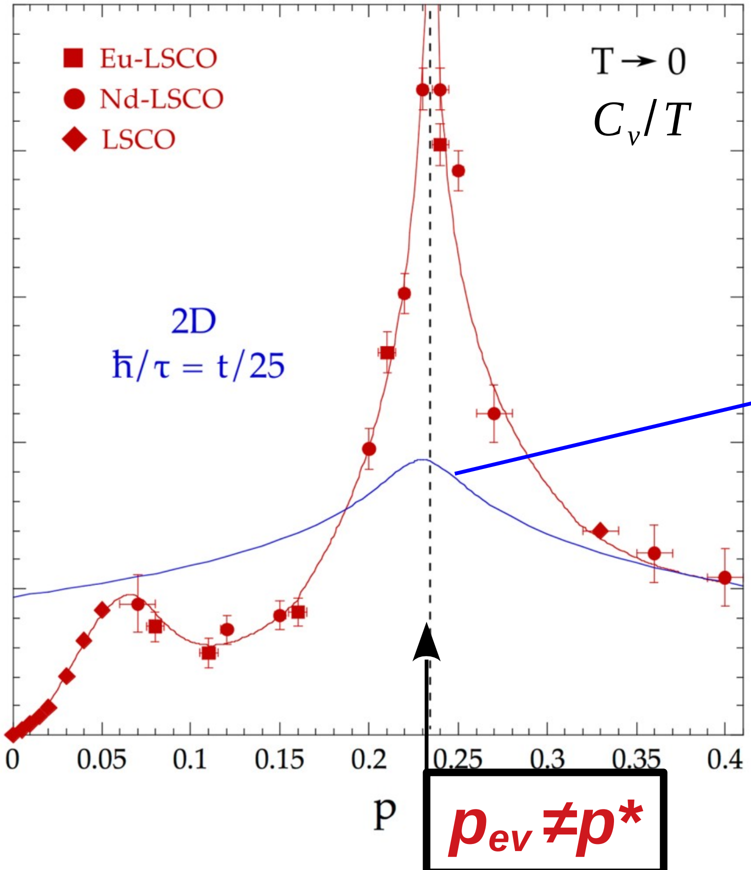
Here, $u = (\omega + i\Gamma)/E_0$, $E_0 = \alpha^2\beta/\gamma^2$, $r_{1,2}^2 = [1 \pm 1/(1+u)^{1/2}]/2$, and $K(r) \equiv \int_0^{\pi/2} d\theta/\sqrt{1 - r^2 \sin^2\theta}$ is the complete elliptic integral of the second kind, and $\Gamma = 0.01t$ is a frequency independent inverse lifetime.

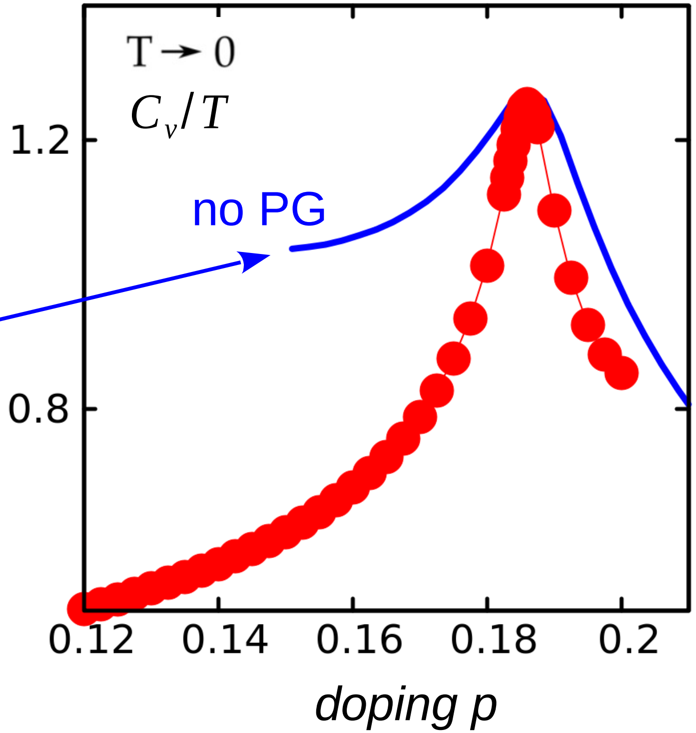
Comparison with specific heat and nematic susceptibility

Result 1: specific heat

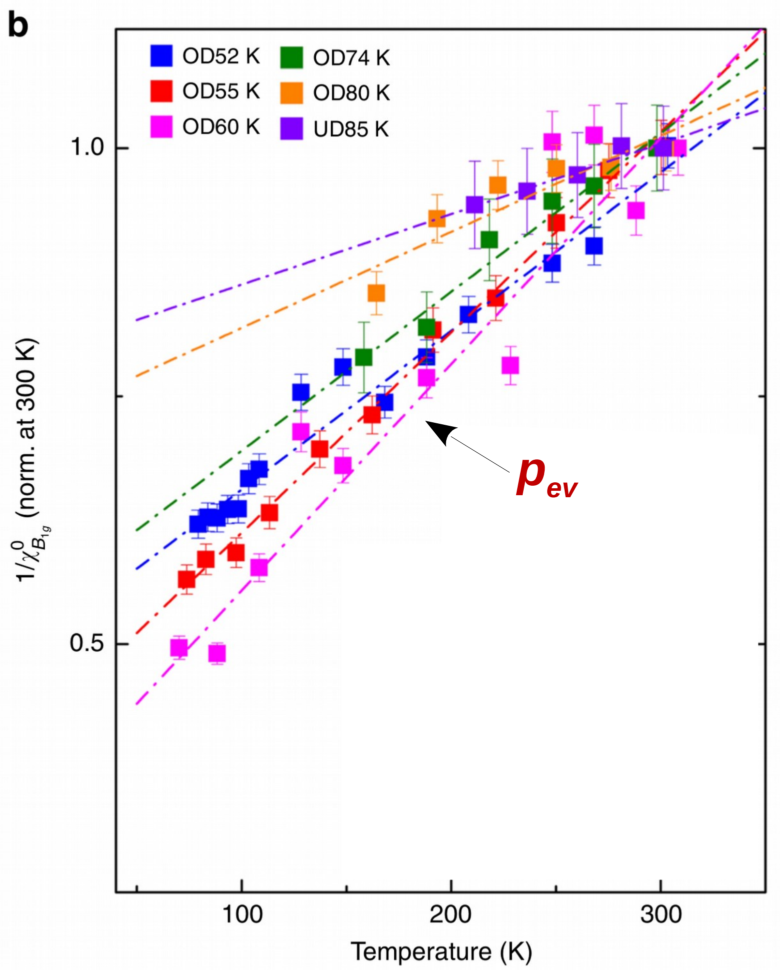
Michon, Taillefer, T. Klein, et al,
Nature **567**, 218 (19)

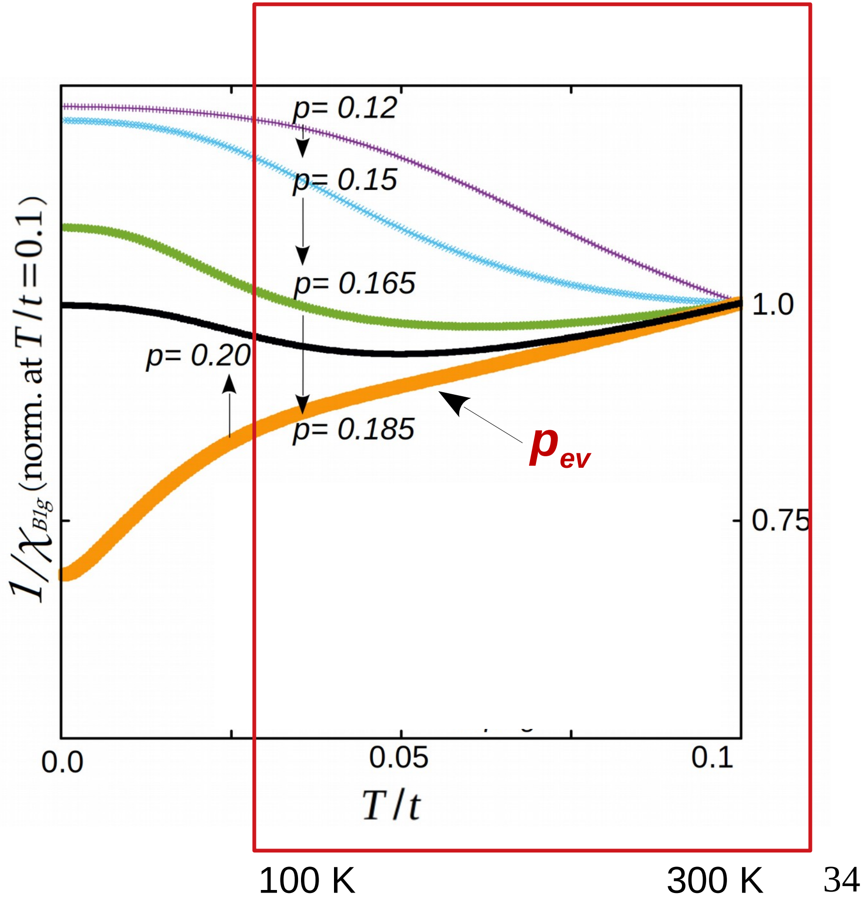
I, Paul, MC, arxiv 2210.01830





Result 2: Nematic Susceptibility χ_{B1g}





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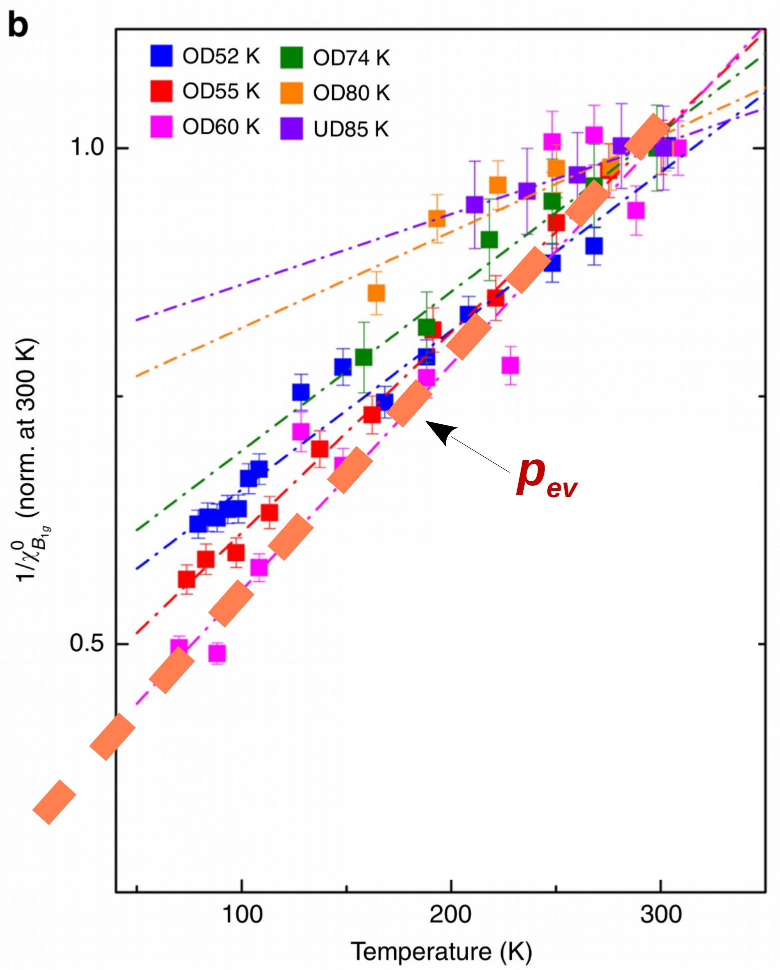

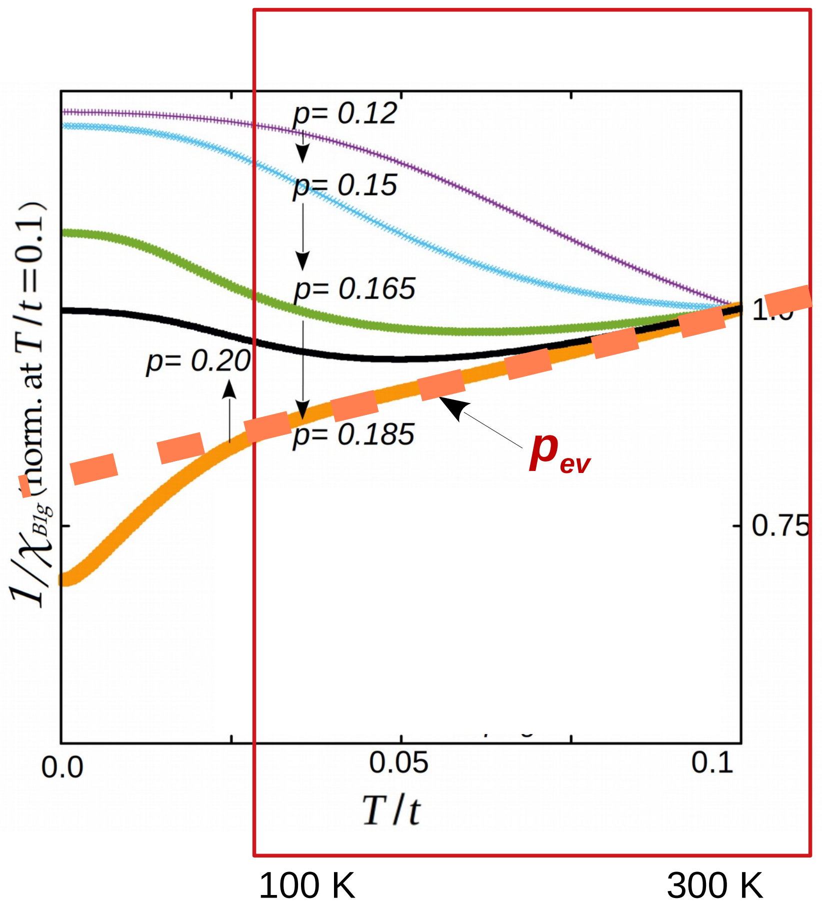

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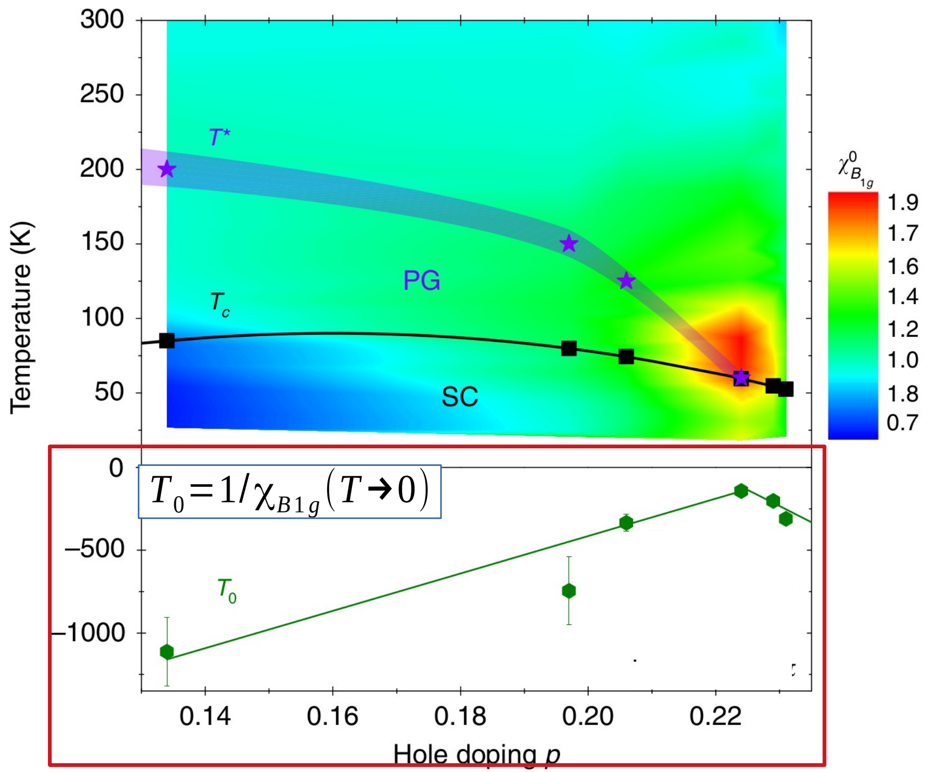
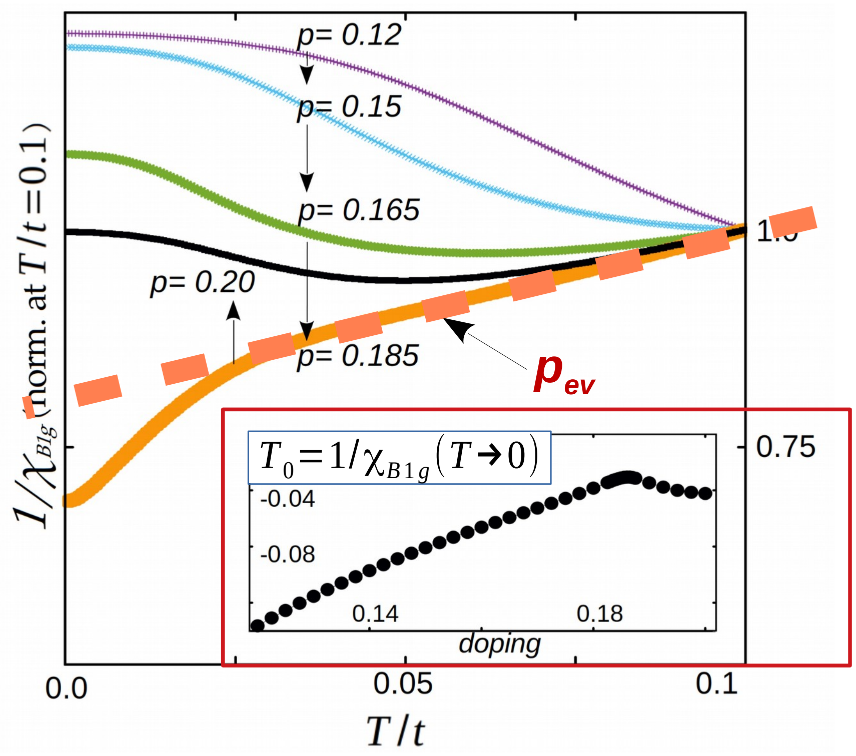
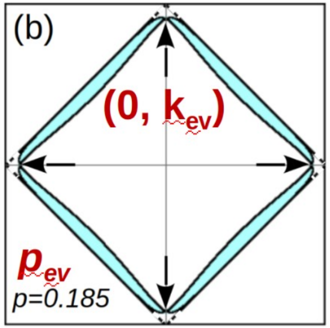


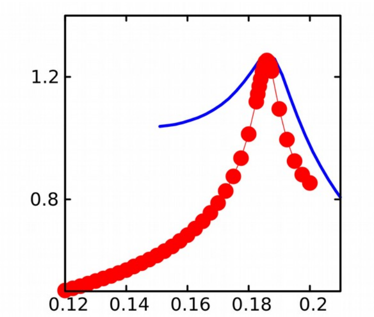


Conclusions

- We propose the existence of a new type of **correlated doping-driven Lifshitz transition**, characterized by **an « exceptional » VHS** point, which is relevant for the **rising point of the PseudoGap** phase of cuprates.



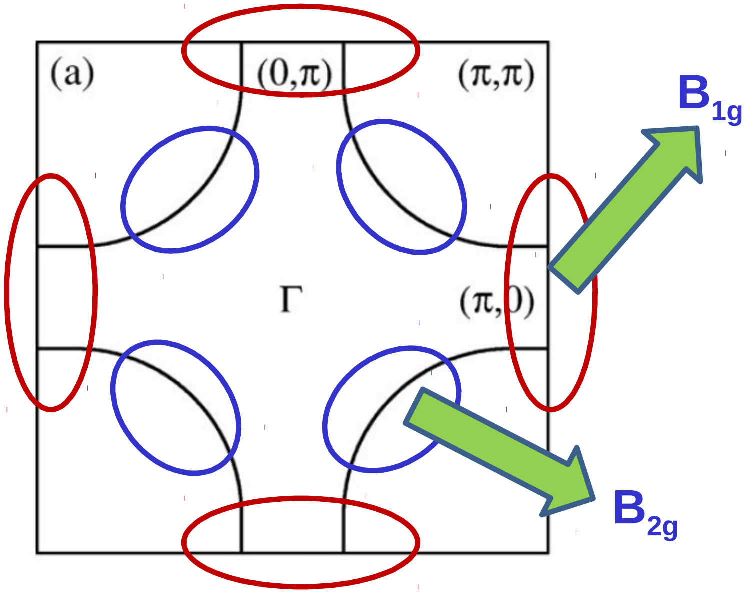
- « Exceptional » VHS is close to a second order VHS, and **can produce enhanced divergence in key responses, like the nematic susceptibility and the specific heat**, without invoking mysterious broken orders.

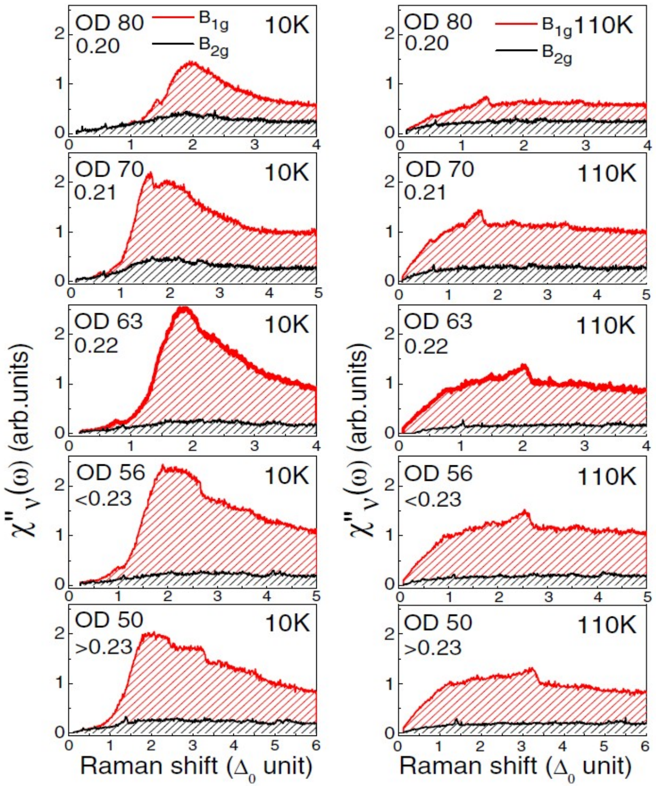


- This may solve an apparent contradiction with previous results that claim that the endpoint of the **PG is strongly tight to a VHS in many cuprates.** (Prediction : $p_{ev} < p^*$)

Acknowledgments : S. Sakai, M. C. Aguair, H. Bracanca

Extras

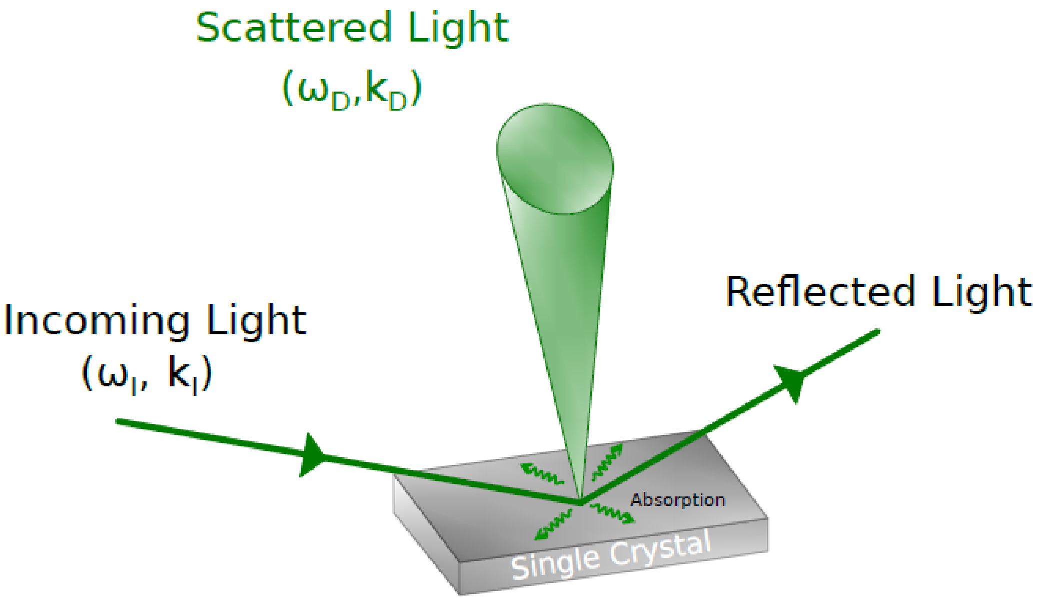




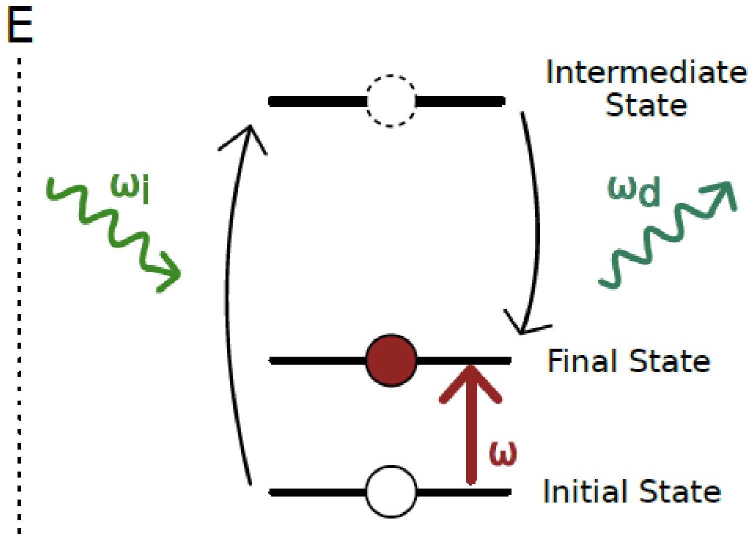
Peak in the antinodal B_{1g} response. Coincides with pseudogap end point doping p*

S. Benhabib, A. Sacuto, MC, IP, et al, PRL **114**, 147001 (15)

Electronic Raman Scattering



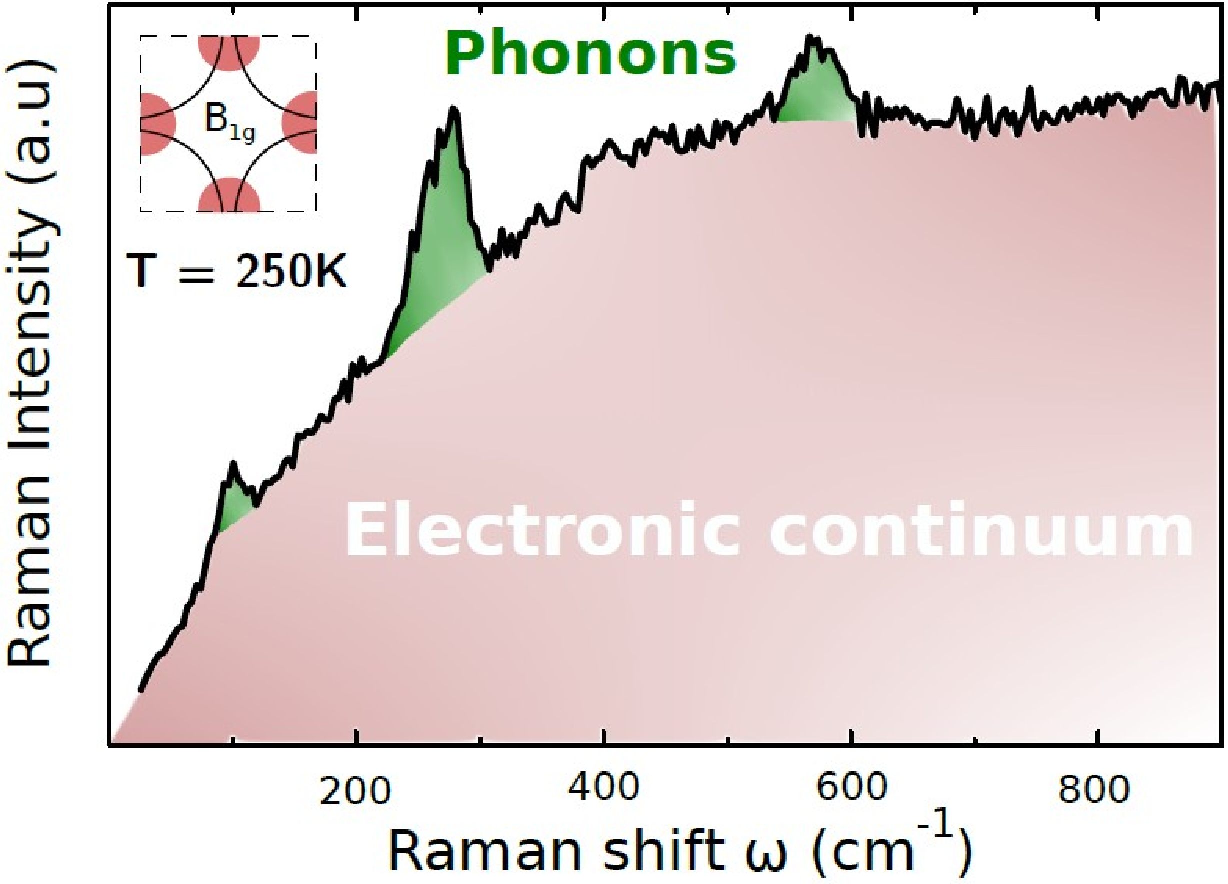
Inelastic scattering of light



Electronic process

What do we measure with Raman diffusion ?

Underdoped Bi-2212 ($T_c = 75$ K) at the antinodes



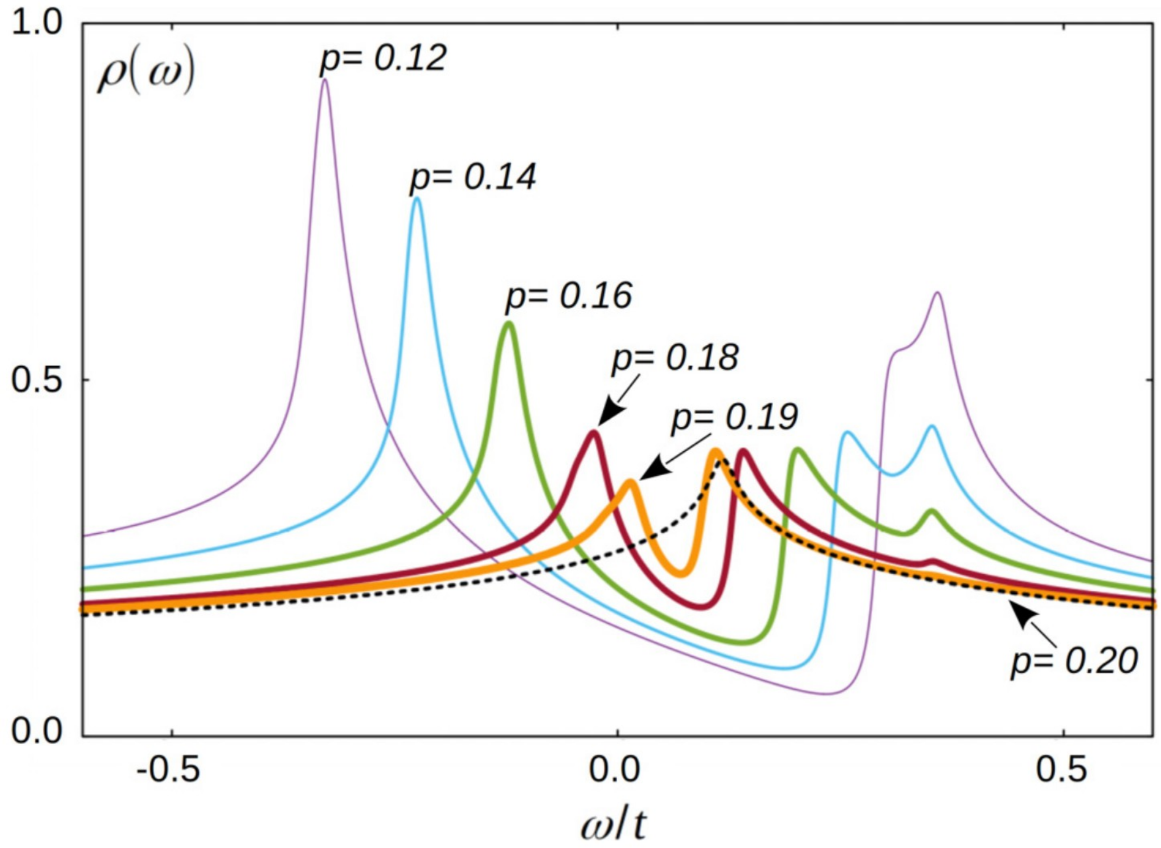
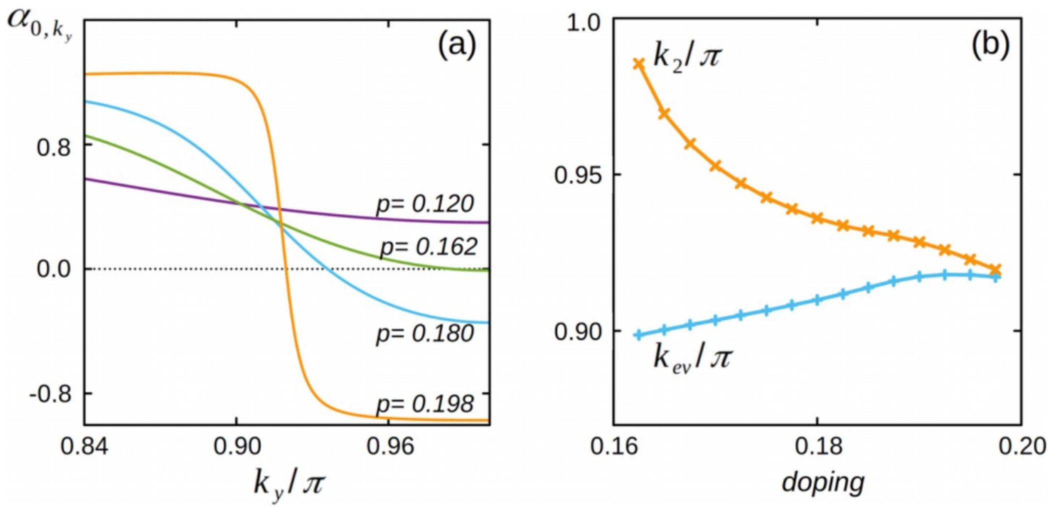
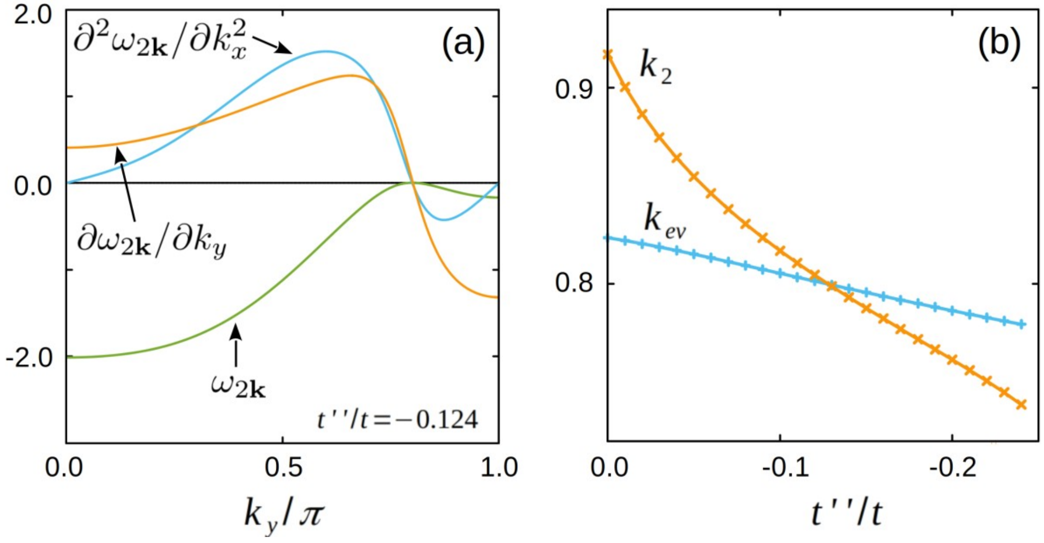


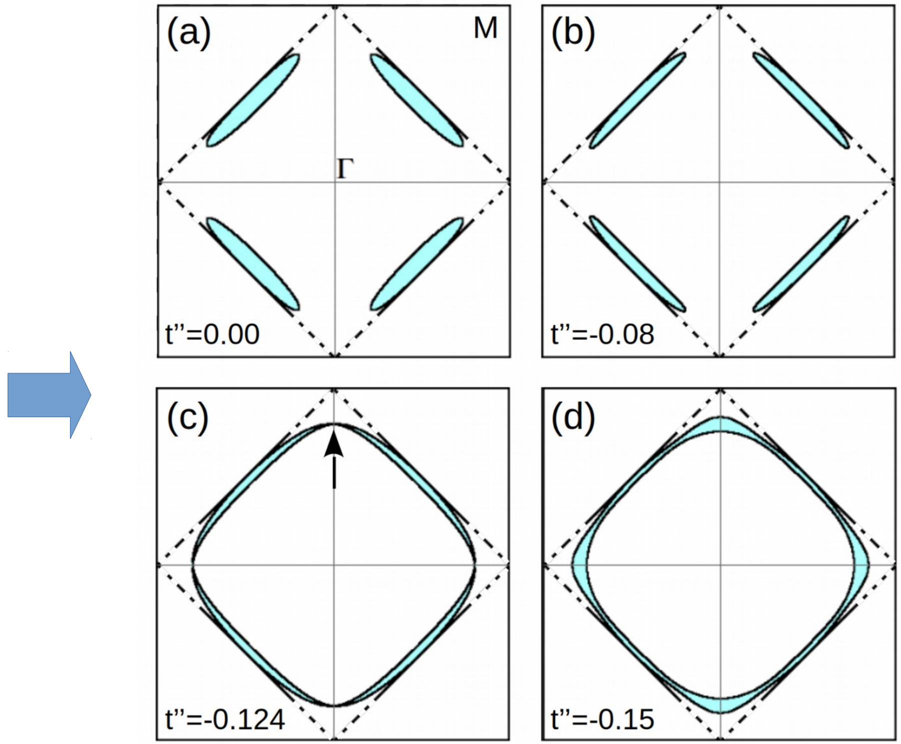
FIG. 2. Density of states $\rho(\omega)$ for various dopings. The exceptional van Hove singularity manifests as a peak which is at negative energies ω for low doping. The peak height diminishes as the pseudogap potential decreases with doping. The peak crosses $\omega = 0$ at $p_{ev} \approx 0.185$.



α_{0,k_y}
(a)
0.8
0.0
-0.8
p= 0.120
p= 0.162
p= 0.180
p= 0.198
0.84
0.90
0.96
k_y/π
(b)
1.0
0.95
0.90
k_2/π
k_{ev}/π
0.16
0.18
0.20
doping



2.0
0.0
-2.0
(a)
$\partial^2\omega_{2\mathbf{k}}/\partial k_x^2$
$\partial\omega_{2\mathbf{k}}/\partial k_y$
$\omega_{2\mathbf{k}}$
$t''/t=-0.124$
0.0
0.5
1.0
k_y/π
(b)
0.9
0.8
k_2
k_{ev}
0.0
-0.1
-0.2
t''/t



(a)
M
Γ
t''=0.00
(b)
t''=-0.08
(c)
t''=-0.124
(d)
t''=-0.15

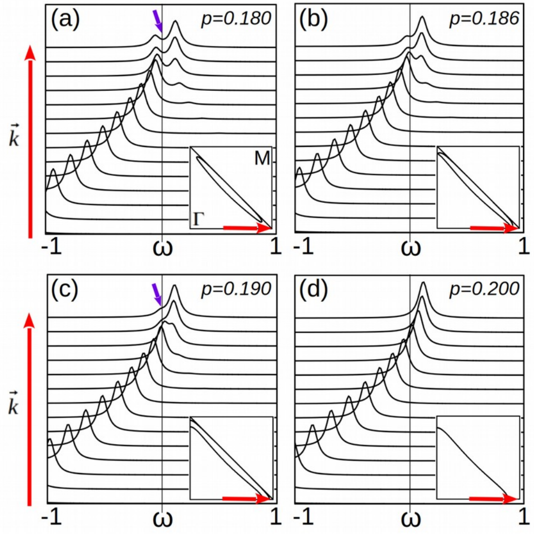


FIG. S3. (Color Online). Spectral peak dispersion of $A(\mathbf{k},\omega)$ vs ω, accessible by ARPES, plotted along the high symmetry line $(0,0)\rightarrow(\pi,0)$, for various doping p across the exceptional van Hove singularity.

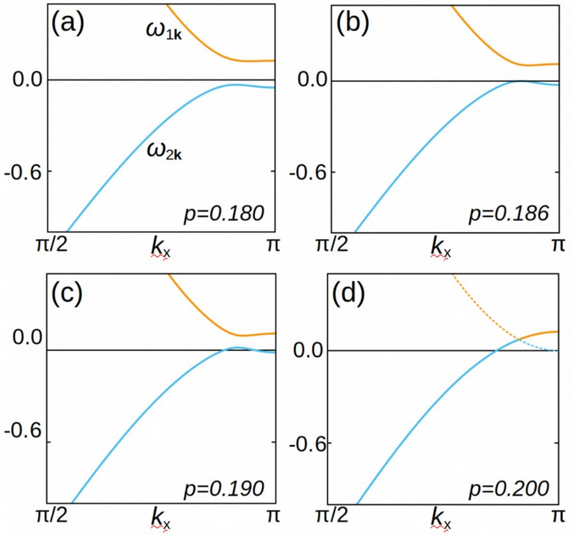
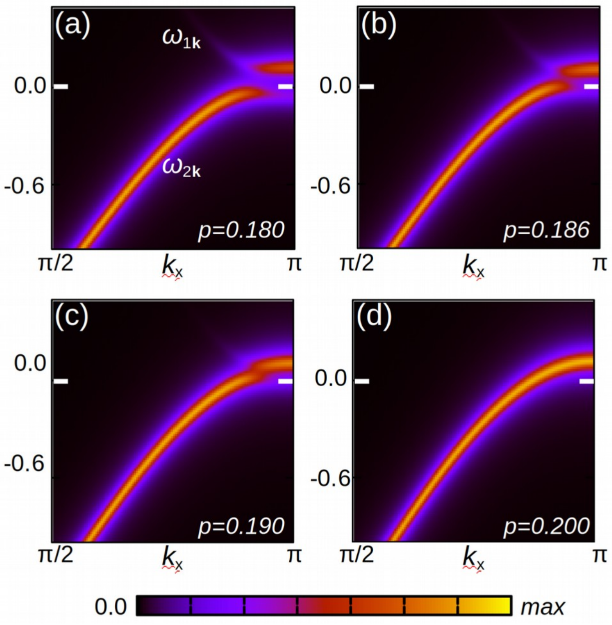


FIG. S4. (Color Online). Band dispersions $\omega_{1\mathbf{k},2\mathbf{k}}$ along the high symmetry line $(0,0)\rightarrow(\pi,0)$ for various doping p across the exceptional van Hove singularity.



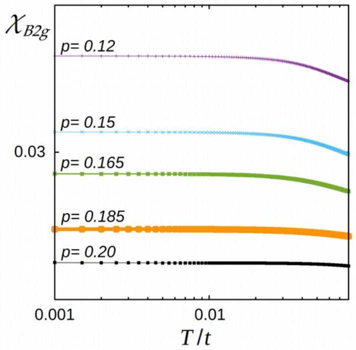
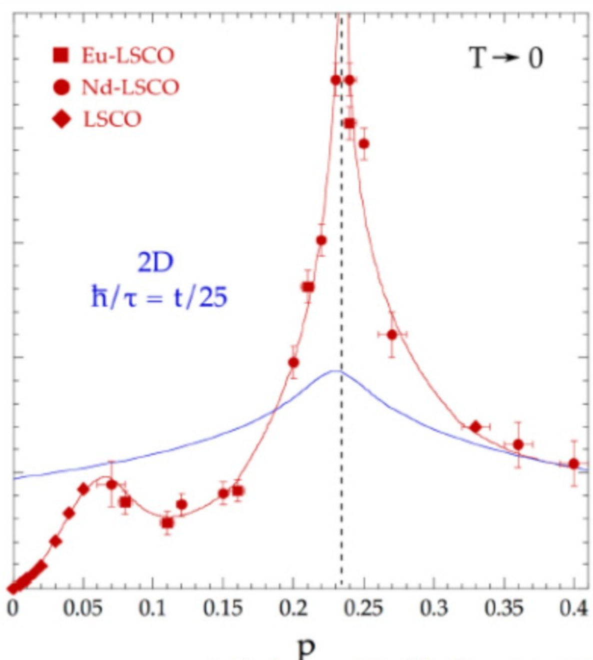
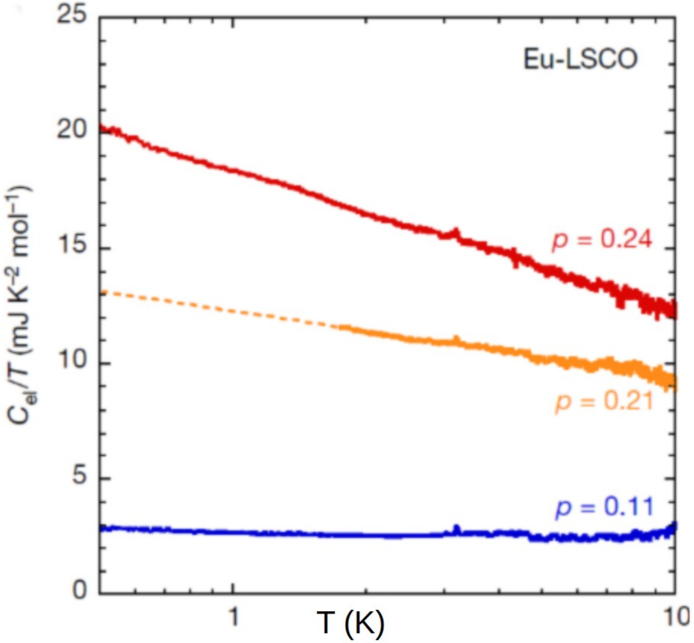


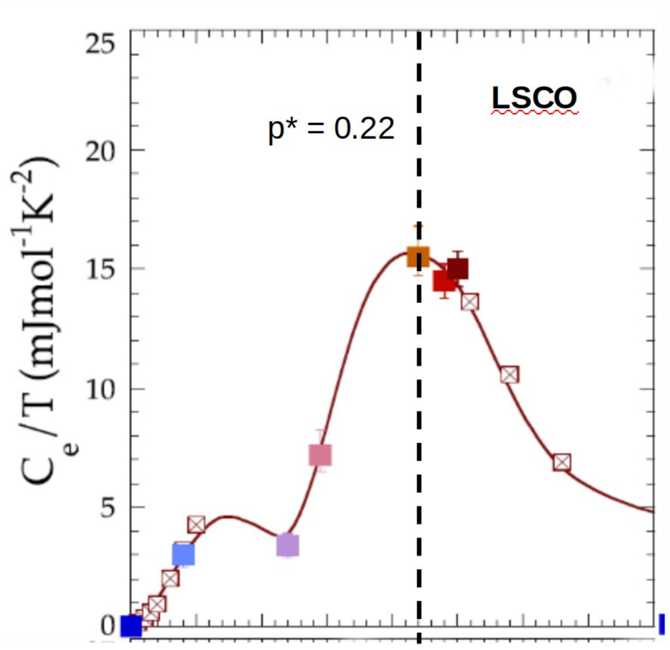
FIG. S7. (Color Online). Temperature dependence of the $\chi_{B_{2g}}(T)$ for various doping p across the exceptional van Hove singularity.

Specific heat





Michon, Taillefer, T. Klein, et al, Nature **567**, 218 (19)



Girod et al, PRB **103** 214506 (21)

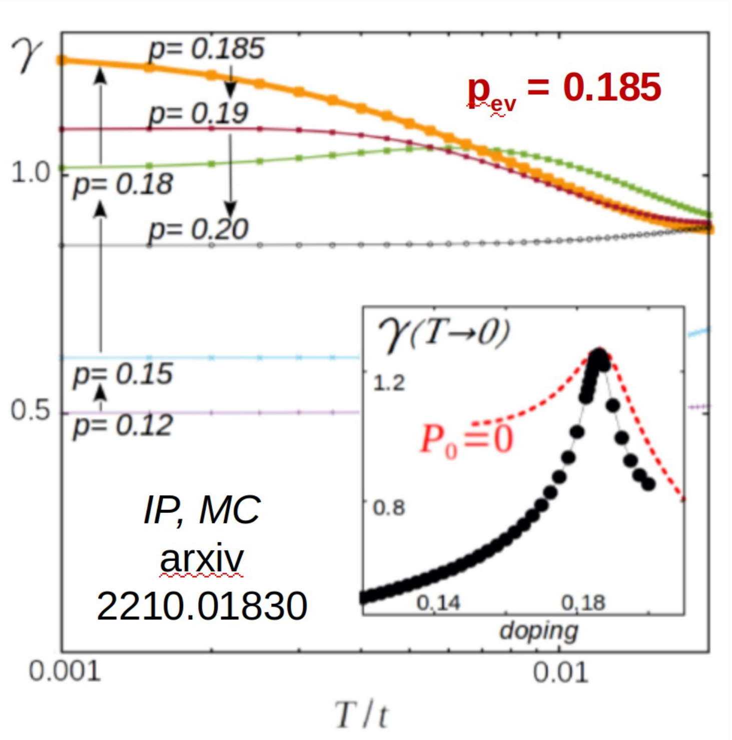
Specific heat coefficient γ = C/T large around p*

γ (T) ~ log (1/T), reminiscent of quantum critical behavior

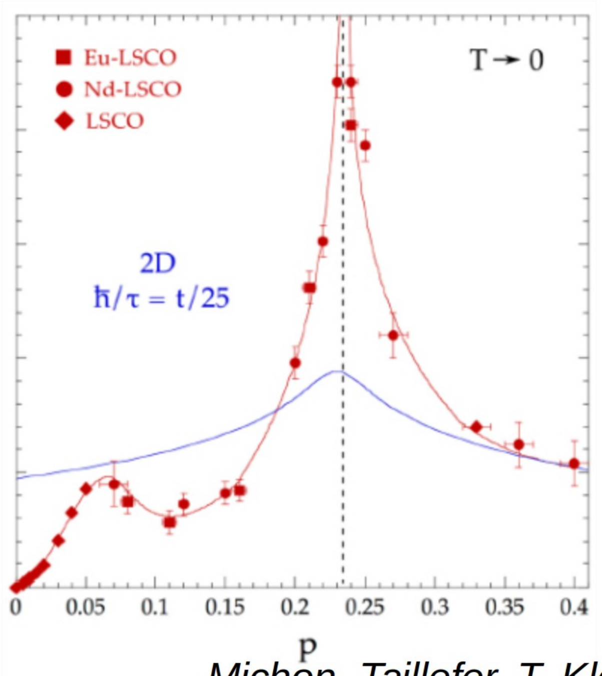
Effect is too sharp for an ordinary van Hove singularity

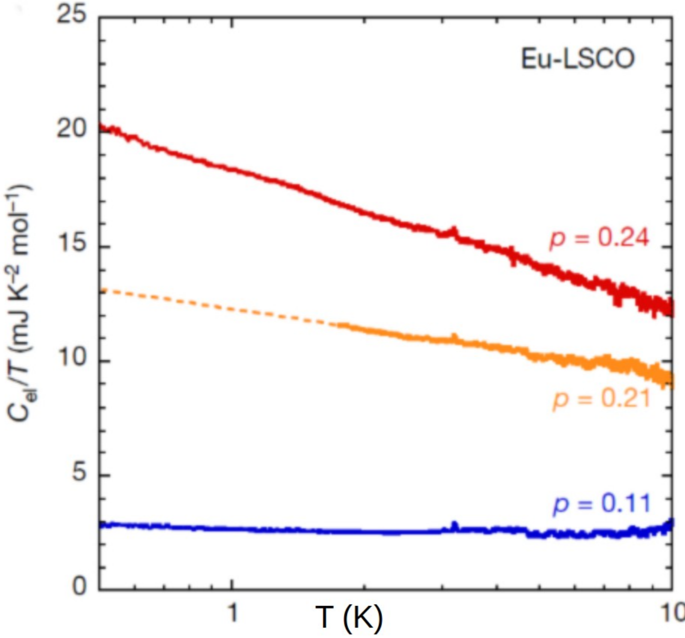
seen also in LSCO, Ca doped YbCO, $Bi_{2+y}Sr_{2-x-y}La_xCuO_{6+\delta}$

Exceptional van Hove: Specific



IP, MC arxiv 2210.01830





Michon, Taillefer, T. Klein, et al, Nature **567**, 218 (19)

C/T is T-independent away from exceptional van Hove point

C/T increases, has substantial T dependence near exceptional van Hove singularity at p = p_{ev}

C/T has sharp peak at a given doping