Fermi surfaces large and small: unifying theories of the Kondo lattice and Hubbard models

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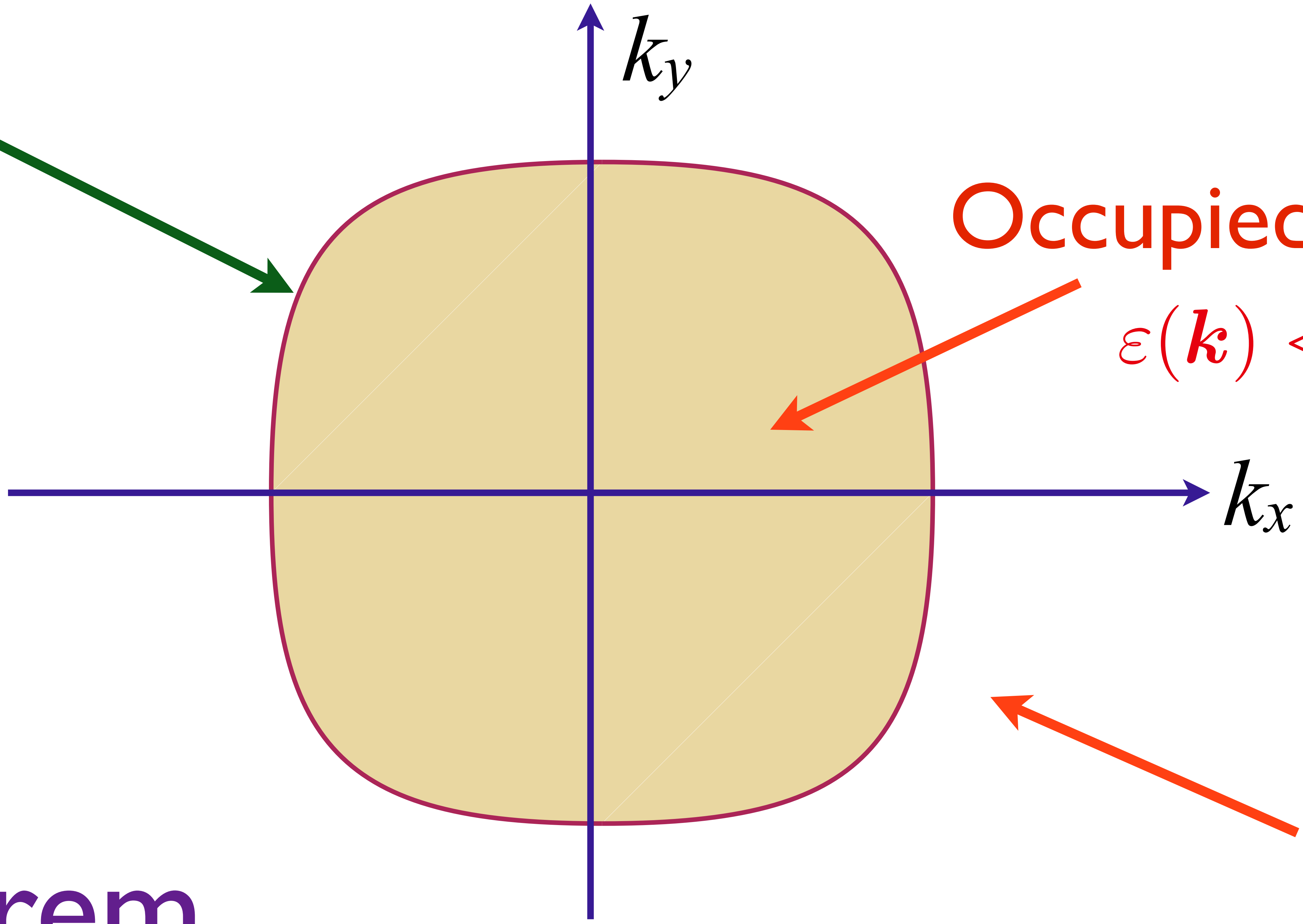
Ordinary metals

Electrons move with momentum **k** through the lattice with dispersion $\varepsilon(\boldsymbol{k})$

Fermi surface



Occupied states

$\varepsilon(\boldsymbol{k}) < E_F$

Empty states

$\varepsilon(\boldsymbol{k}) > E_F$

Luttinger theorem

$$2 \times \frac{\text{Volume inside Fermi surface}}{(2\pi)^d} = \text{density of electrons (mod 2)}$$

1. Kondo lattice model: the heavy Fermi liquid (HFL) as the Higgs phase of a $U(1)$ gauge theory
2. Kondo lattice model: the FL* phase — fractionalization, emergent gauge fields, and Luttinger violation
3. Hubbard model: the vanilla FL phase
4. Hubbard model: the FL* phase at small doping p, using ancilla qubits

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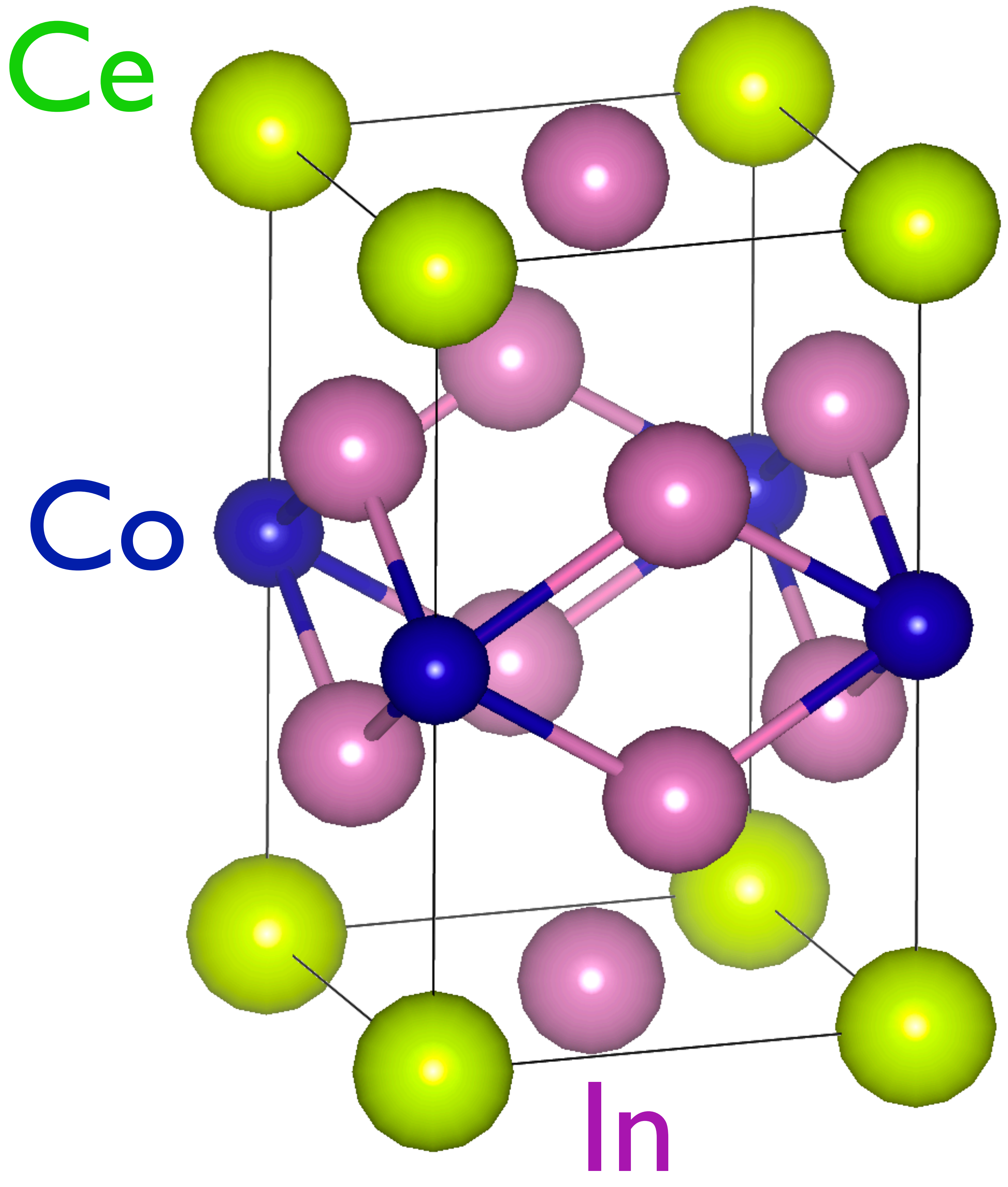
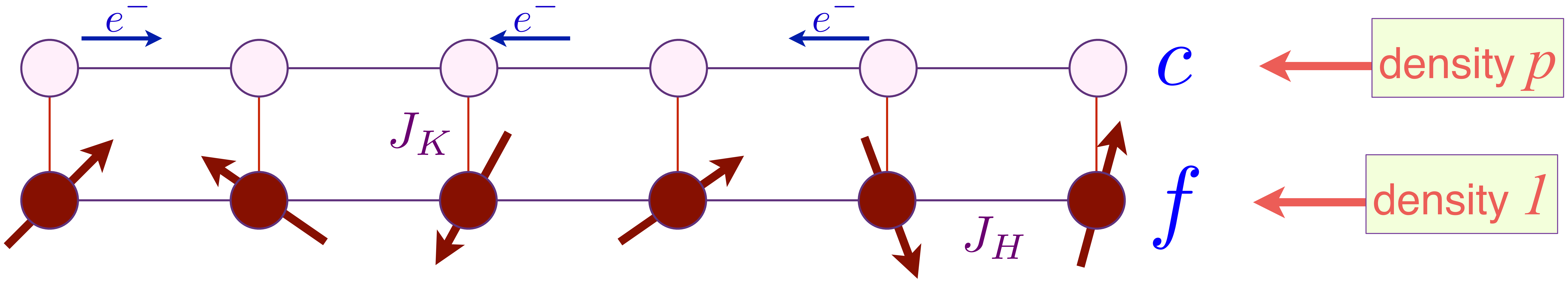


Strong on-site repulsion U only on Ce sites

$CeCoIn_5$

$$\mathcal{H}_{KL} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c^{\dagger}_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma} + \sum_{i} J_K \, c^{\dagger}_{i\sigma} \frac{\boldsymbol{\tau}_{\sigma\sigma'}}{2} c_{i\sigma'} \cdot \boldsymbol{S}_i + \sum_{\langle ij \rangle} J_H \, \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

Kondo lattice



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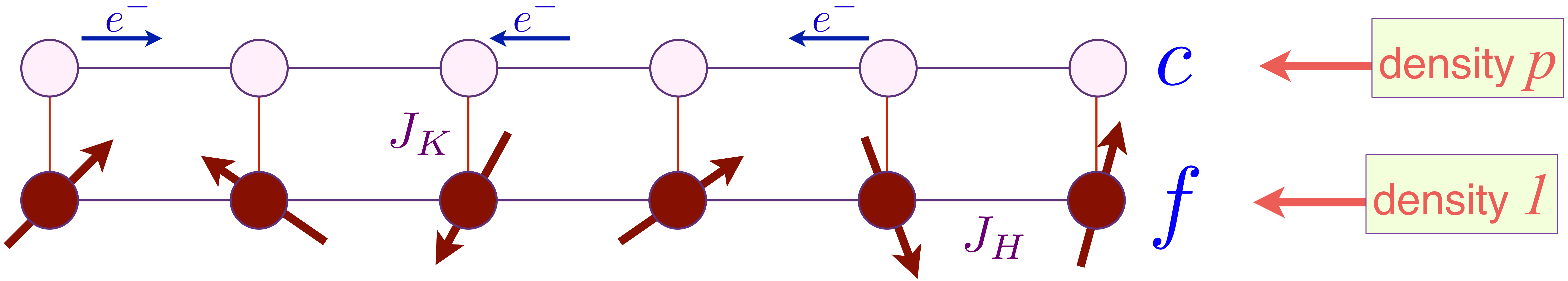
- Spinon fractionalization: $\boldsymbol{S}_i = \frac{1}{2} f^\dagger_{i\sigma} \boldsymbol{\tau}_{\sigma\sigma'} f_{i\sigma}, \; \sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} = 1.$

Kondo lattice



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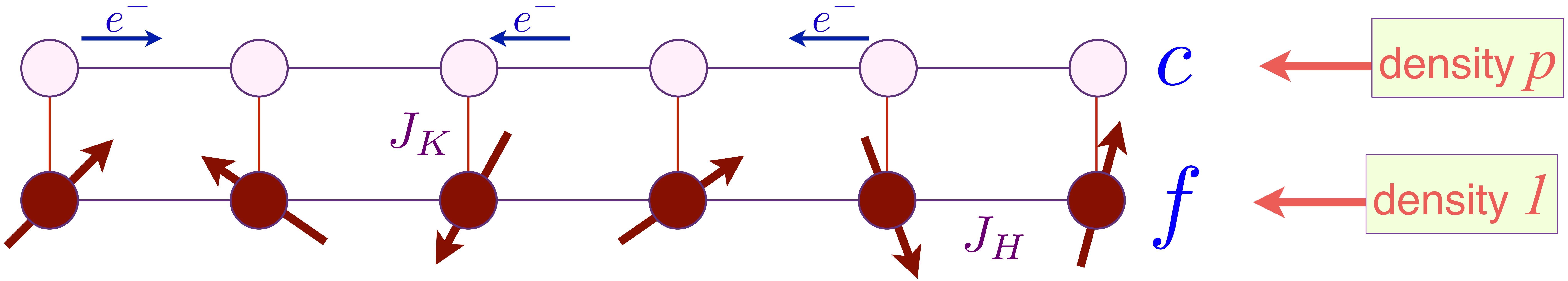
- The spinon number constraint introduces a $\mathrm{U}(1)_{\text{gauge}}$ gauge symmetry $f_{i\sigma} \to f_{i\sigma} e^{-i\vartheta_i}$. So the total symmetry is $\mathrm{U}(1)_{\text{gauge}} \times \mathrm{U}(1)$.

Coleman, Read, Newns, Millis, P.A. Lee, Auerbach, Levin

Kondo lattice



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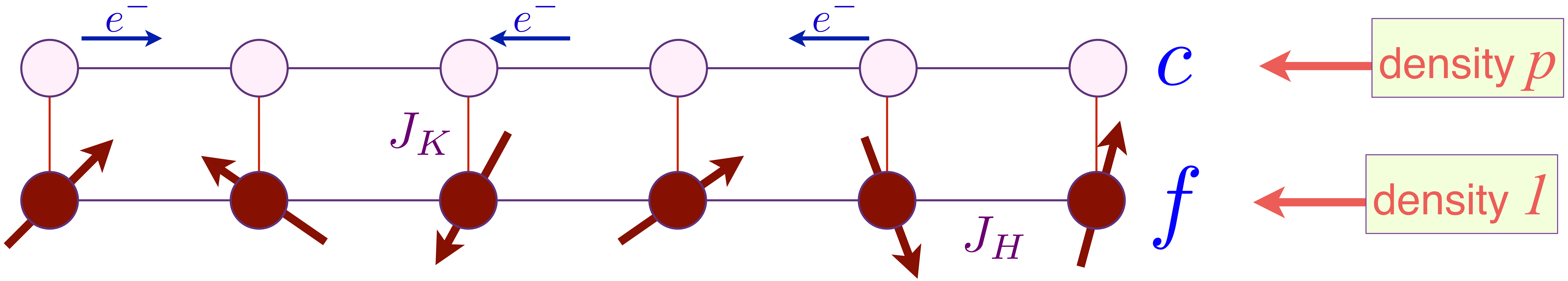

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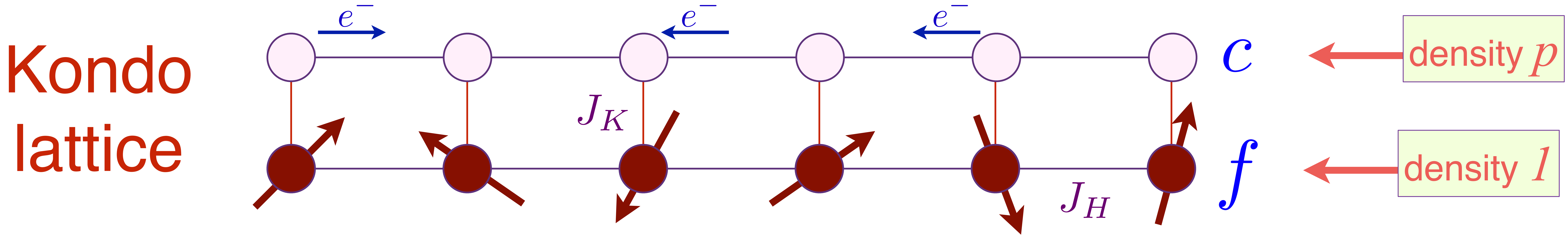

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- The Fermi surface is *large*, of size $1 + p$, and we obtain the HFL state.

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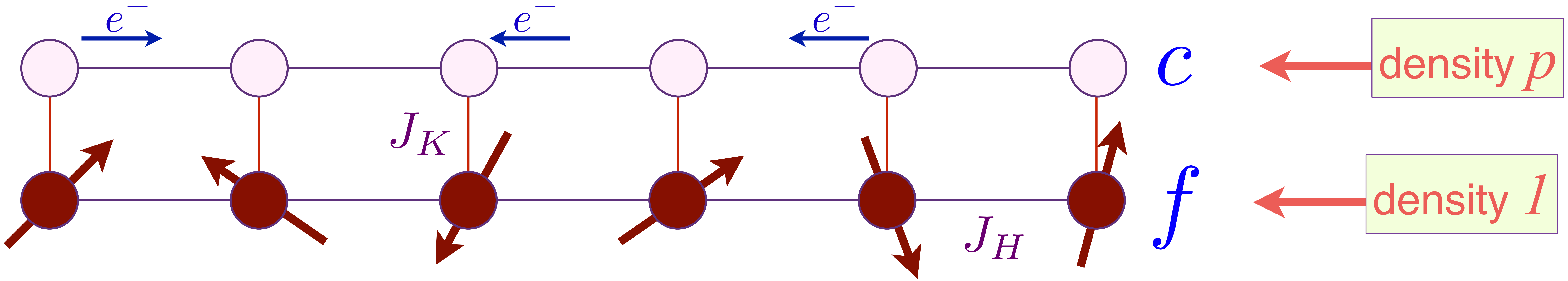
Kondo lattice



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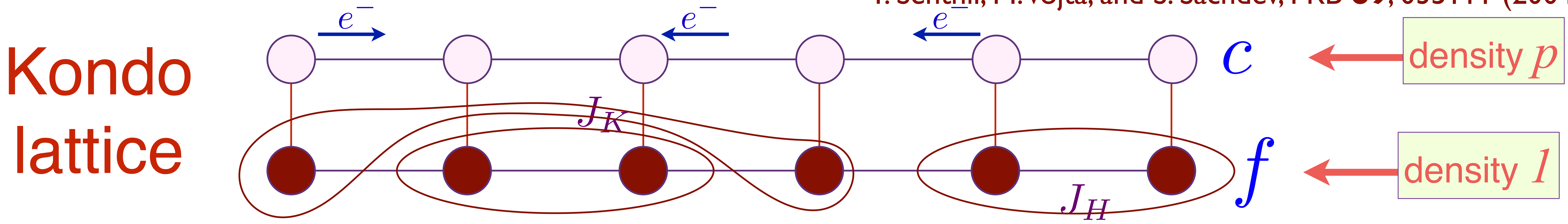
T. Senthil, M. Vojta, and S. Sachdev, PRB **69**, 035111 (2004)



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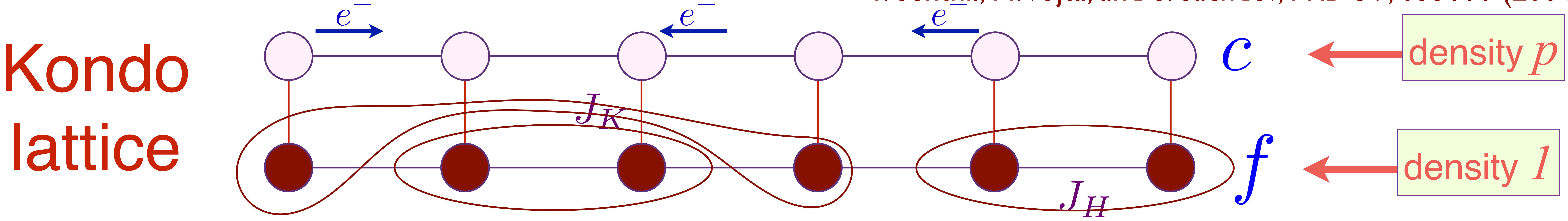

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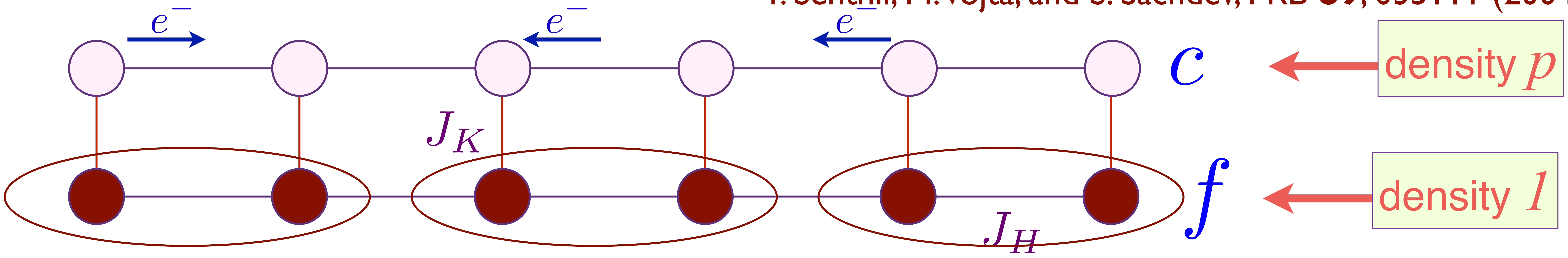

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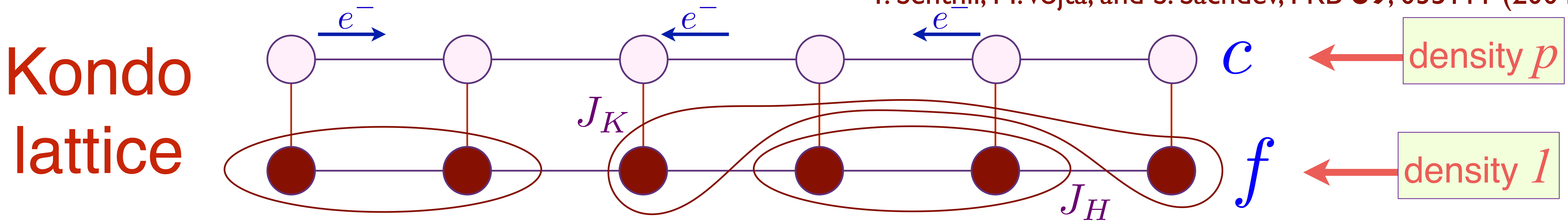

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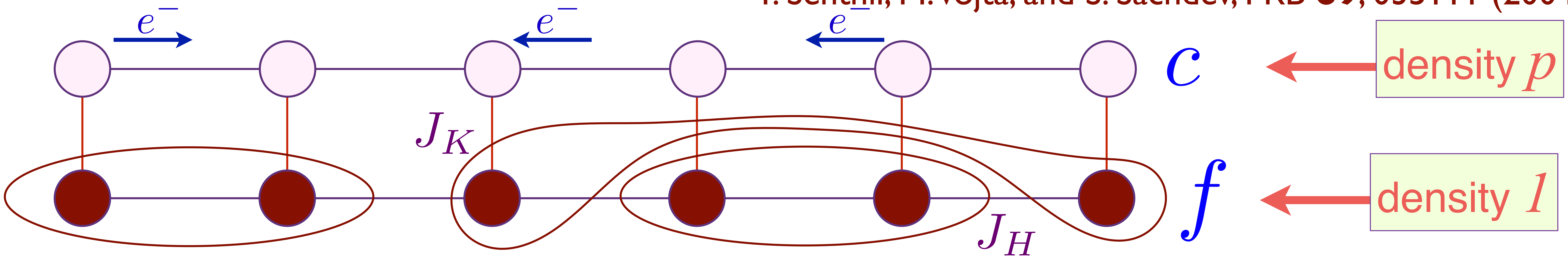

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- The Luttinger arguments applied to $\mathrm{U}(1)$ lead to a *small* Fermi surface of electrons of size p.
- The Luttinger arguments applied to $\mathrm{U}(1)_{\mathrm{gauge}}$ lead to 'symmetry enriched topological (SET)' or 'symmetry fractionalization' constraints on the spin liquid sector.

P. Bonderson, M. Cheng, K. Patel, E. Plamadeala, arXiv:1601.07902

T. Senthil, M. Vojta, and S. Sachdev, PRB **69**, 035111 (2004)

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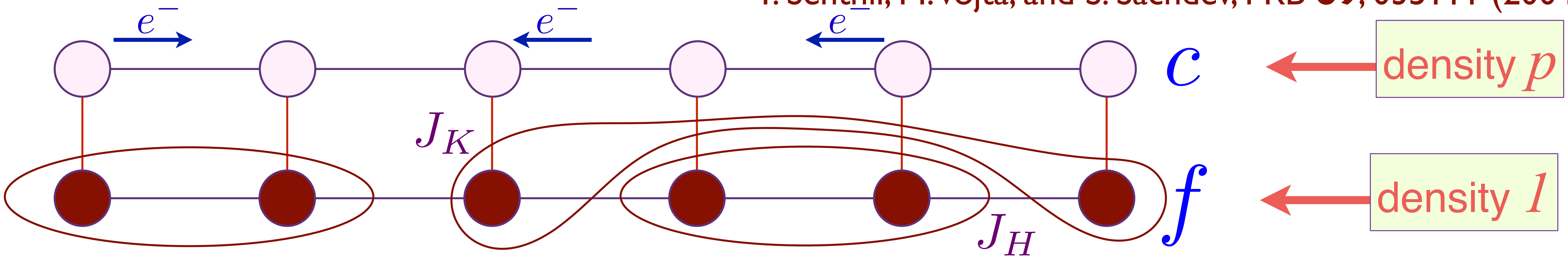
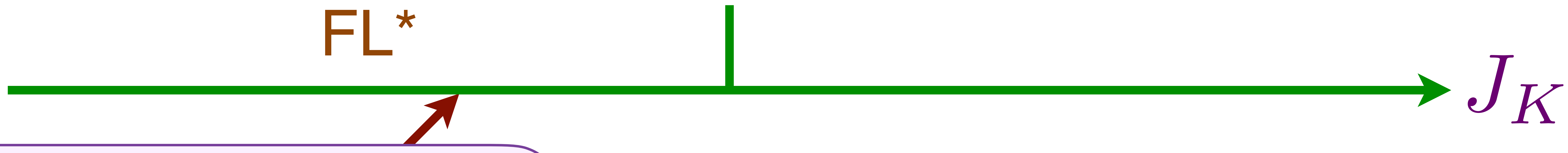


FL* phase in ***Kondo lattice*** models

Kondo lattice of f electron spins coupled
to a conduction band of c electrons of density p.



Small Fermi surface of size p

$$
\begin{aligned}
|\mathrm{FL}*\rangle = &[\text{Projection onto one } f \text{ per site}] \\
&\bowtie |\text{Slater determinant of } f\rangle \\
&\otimes |\text{Slater determinant of } c\rangle
\end{aligned}
$$

S. Burdin, D. R. Grempel, and A. Georges, PRB **66**, 045111 (2002)
T. Senthil, M. Vojta, and S. Sachdev, PRB **69**, 035111 (2004)
A. Paramekanti and A. Vishwanath, PRB **70**, 245118 (2004)

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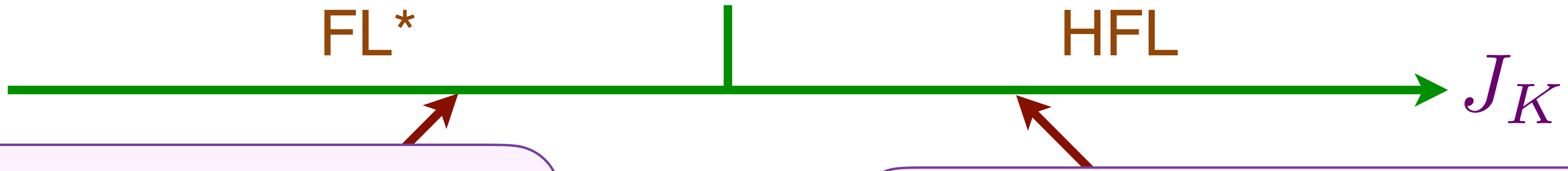

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Large Fermi surface of size $1 + p$

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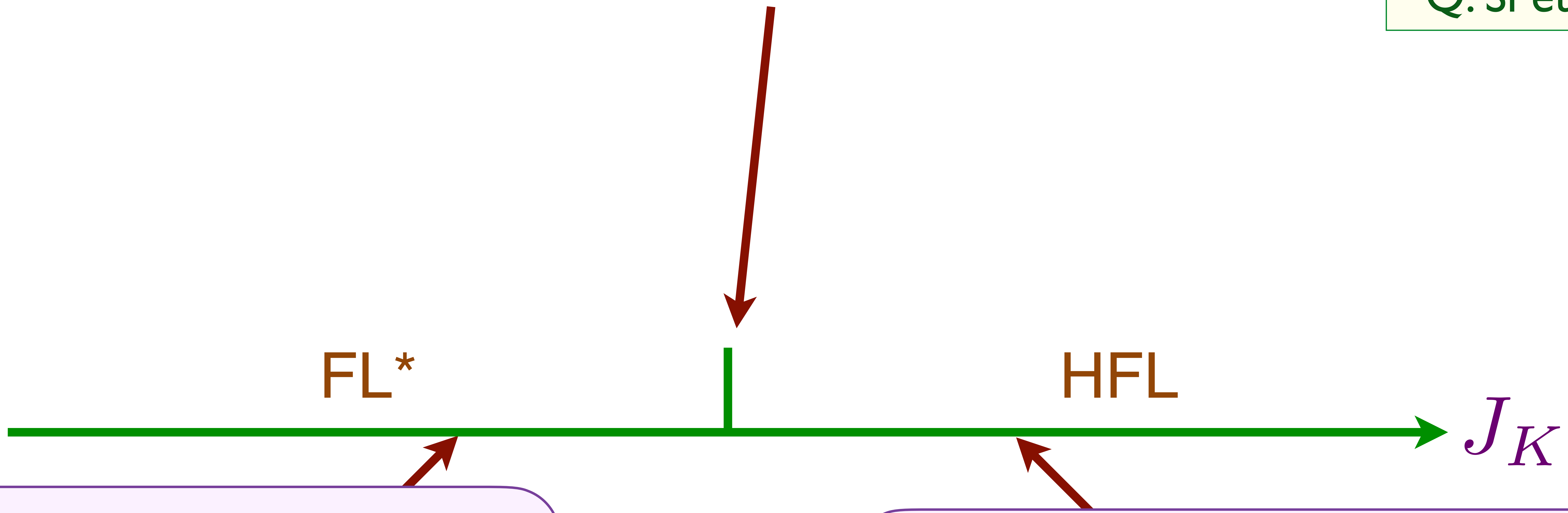
A. Sengupta (2000)
Q. Si et al. (2001)

Kondo-breakdown transition



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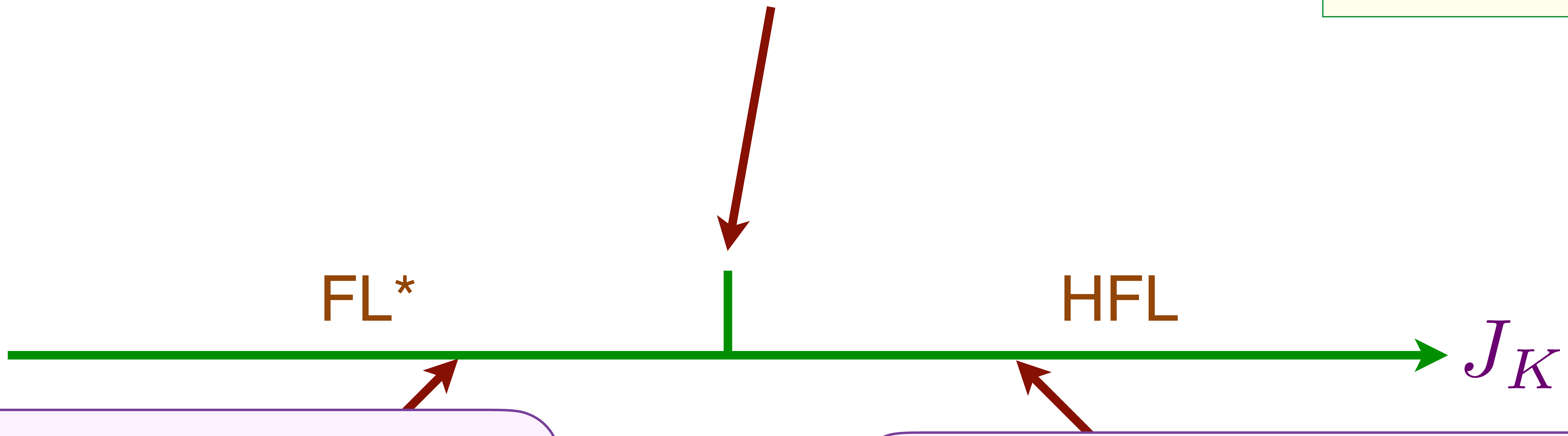
Kondo-breakdown transition
'Selective Mott' transition

V. Anisimov *et al.* (2002)
L. de' Medici *et al.* (2005)



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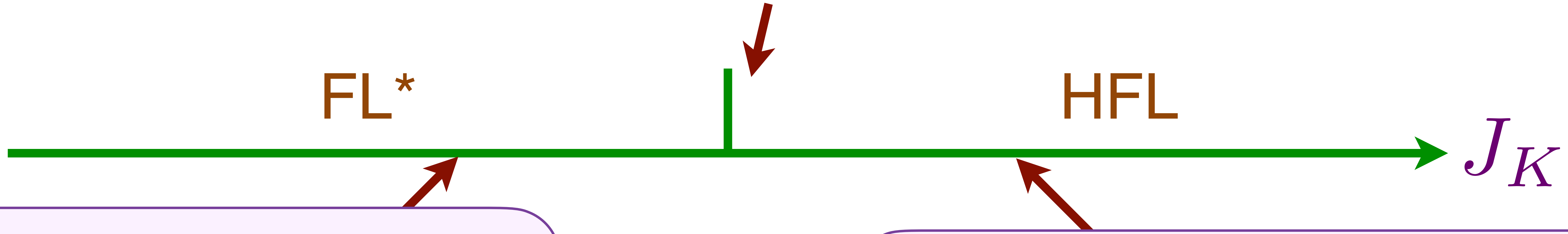
Kondo-breakdown transition
'Selective Mott' transition
Deconfined criticality of a U(1) gauge theory with a
Higgs field, spinons, and a small Fermi surface of electrons.
(FL* can be replaced by a confining phase with AFM or VBS order).



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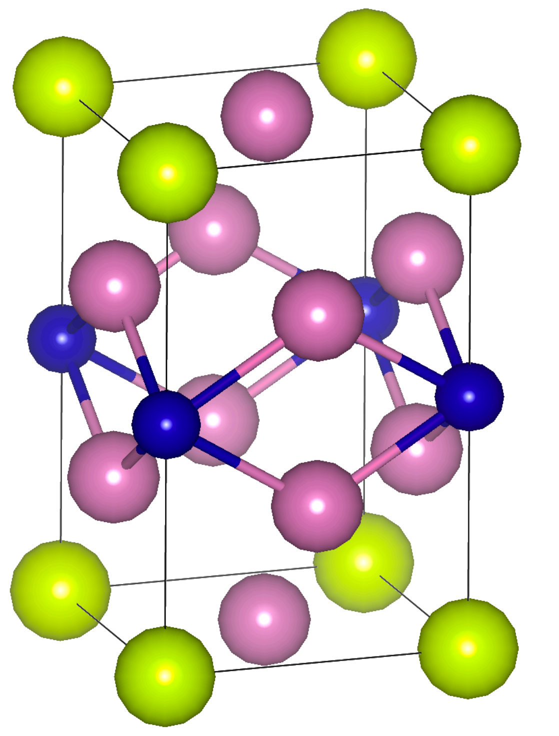
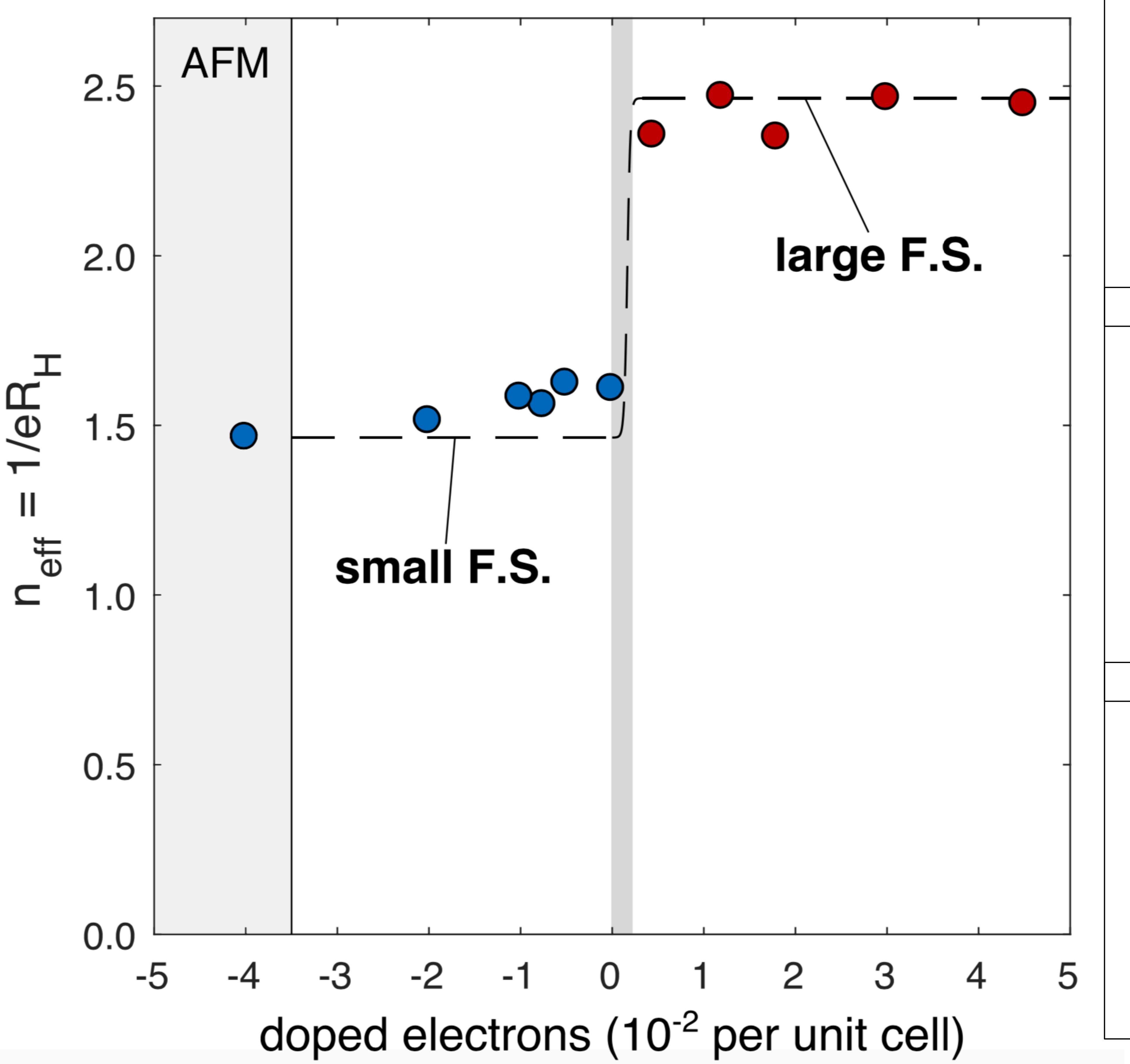
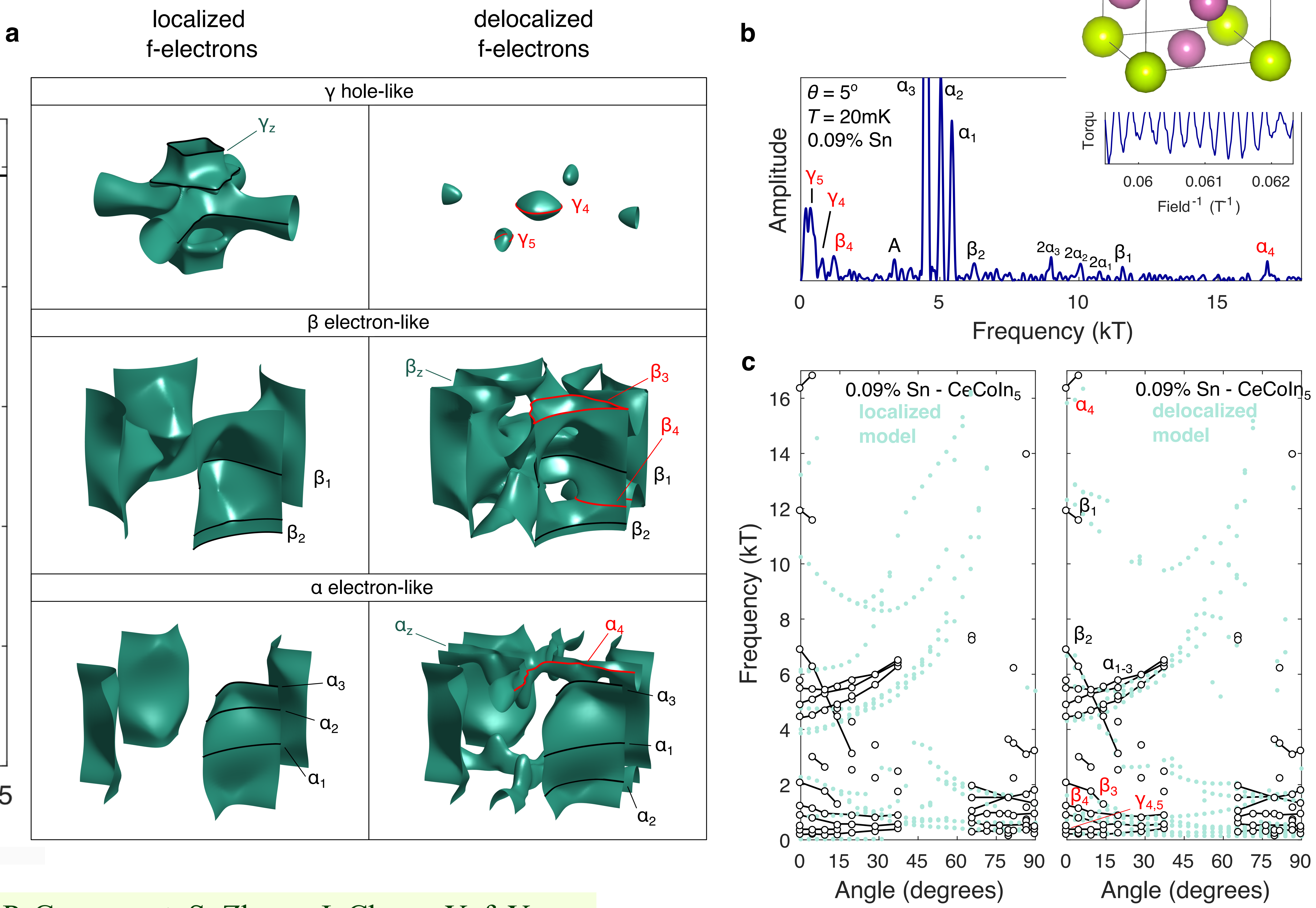


arXiv:2011.12951





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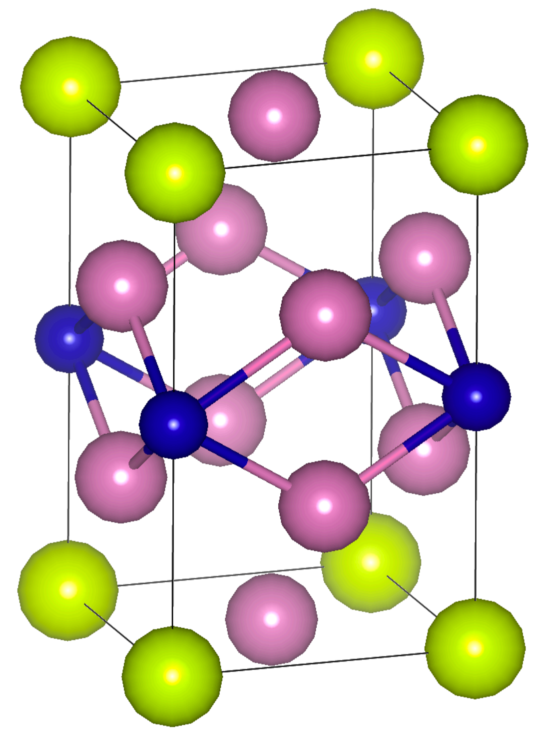

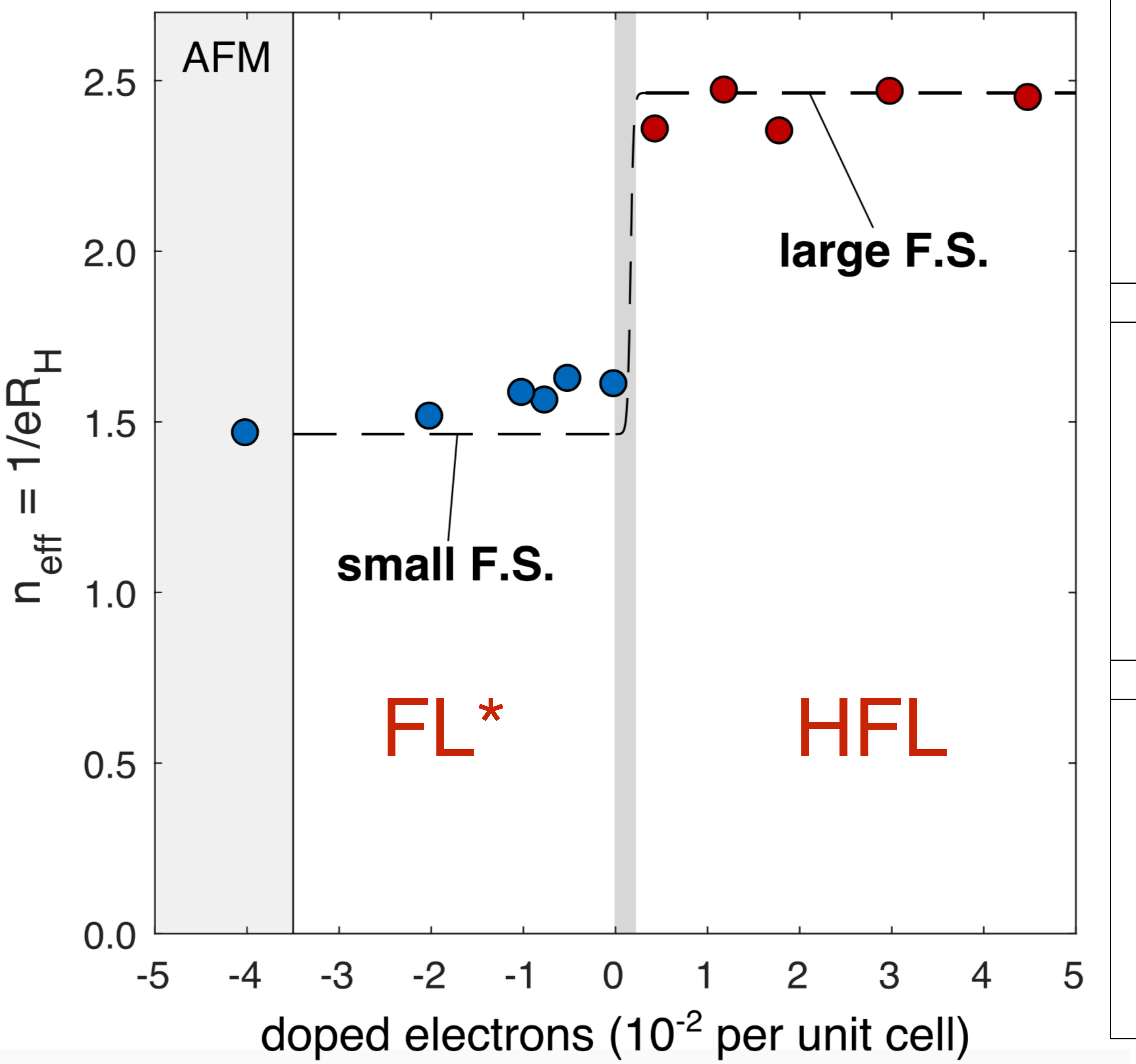

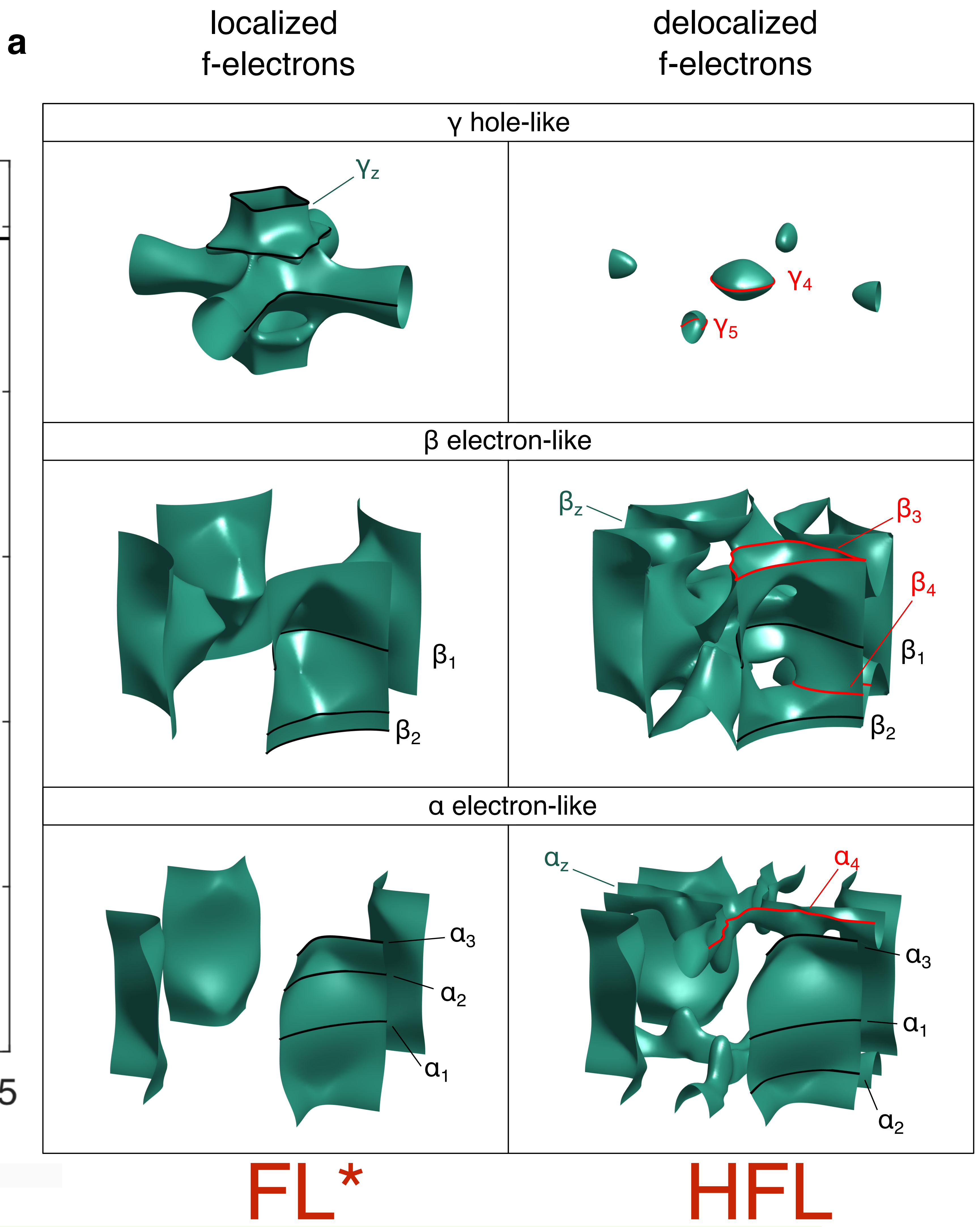

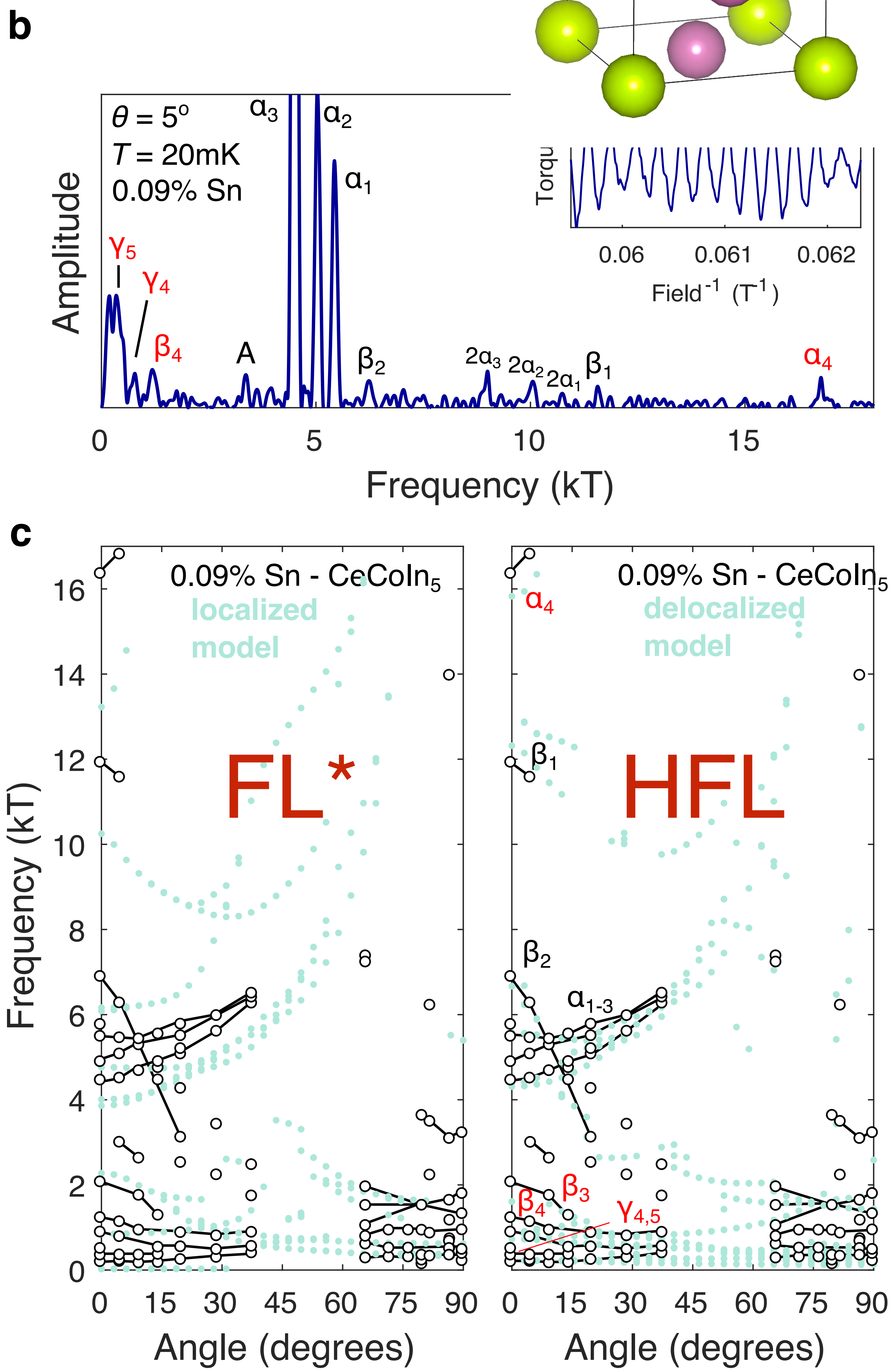

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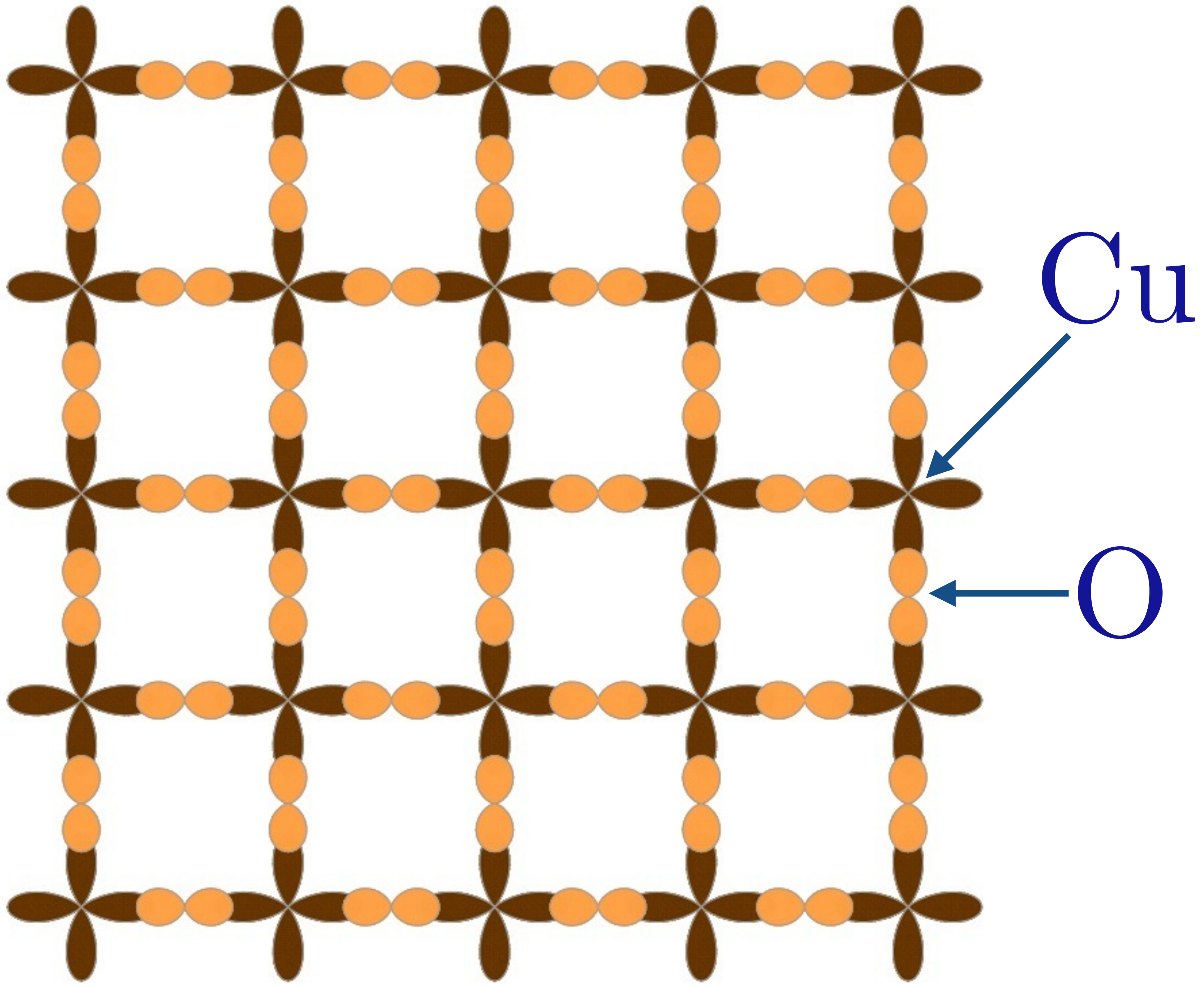
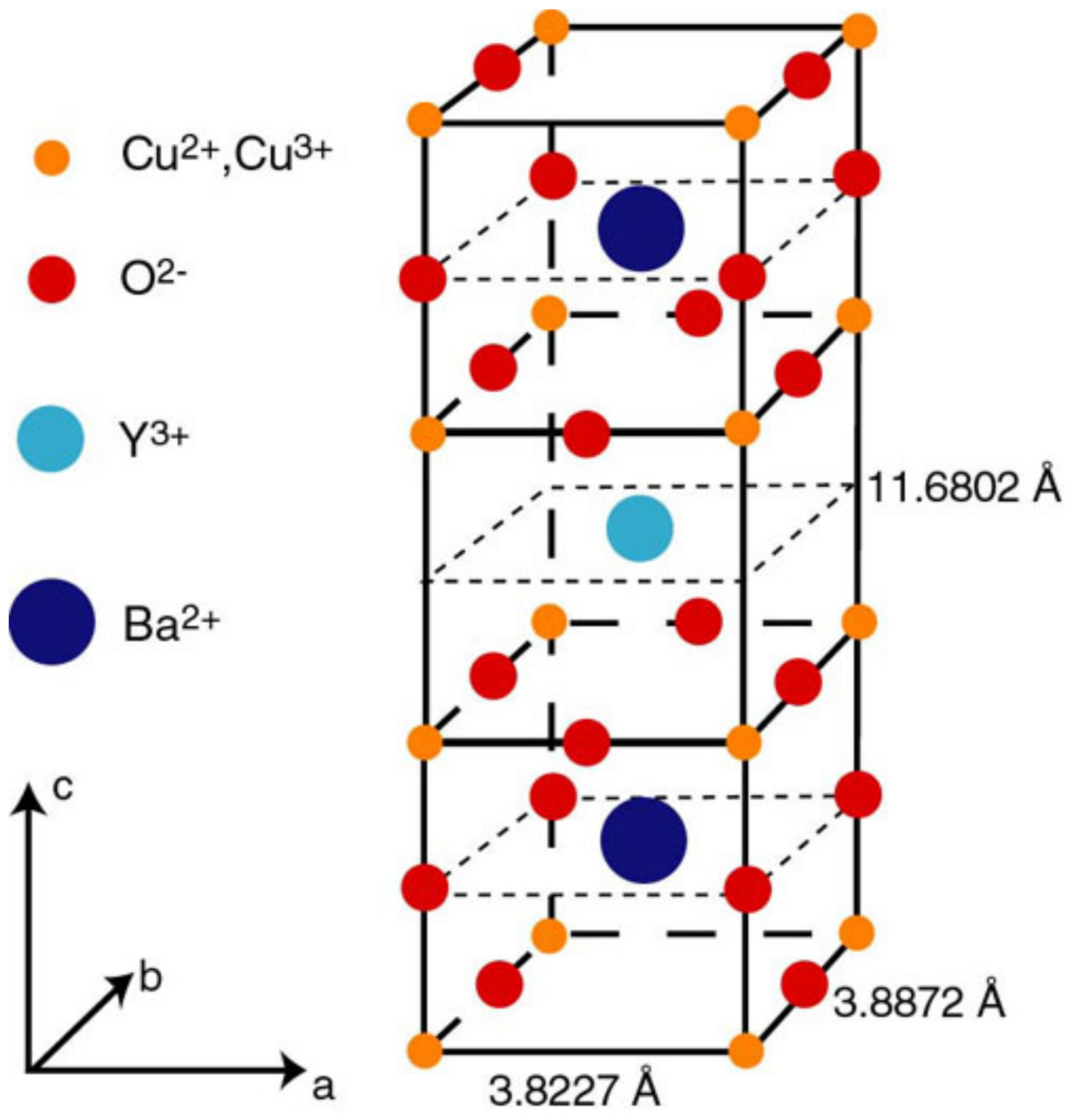
$$\mathcal{H}_H = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c^{\dagger}_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

High temperature superconductors



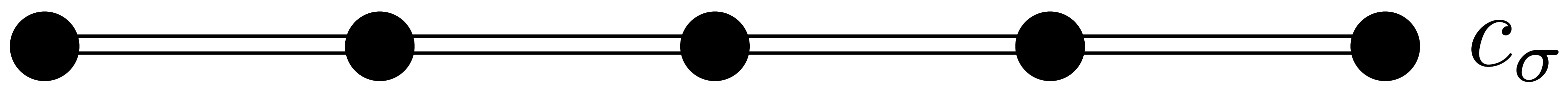
CuO_2 plane



$YBa_2Cu_3O_{6+x}$

$$\mathcal{H}_H = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- The Luttinger theorem implies a FL phase with 'large' Fermi surface of size $1+p$ holes (or $1-p$ electrons) for all U and all p.



density
1+p

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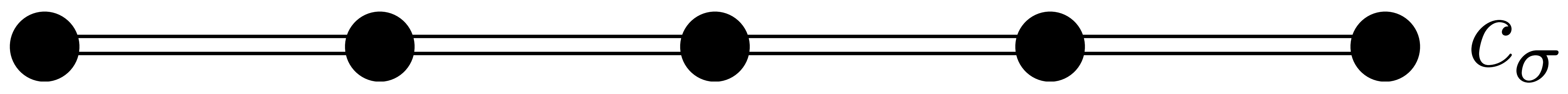
- Vanilla FL theory: Luttinger theorem applies as $p \to 0$ with wavefunction $|\text{Vanilla}\rangle = [\text{Project out sites with 2 } c\text{'s}] \bowtie |\text{Slater determinant of } c\rangle$



density
1+p

P.W. Anderson, P.A. Lee, M. Randeria, T. M. Rice, N. Trivedi, and F. C. Zhang, Journal of Physics Condensed Matter **16**, R755 (2004)

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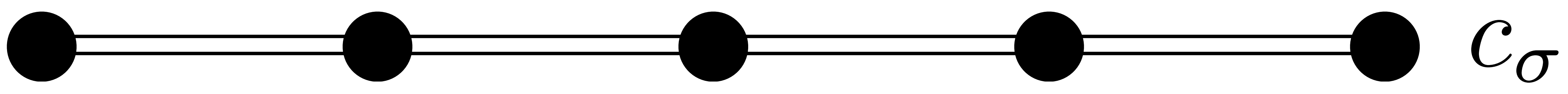
- The main effect of the projection is a 'Brinkman-Rice' enhancement of the quasiparticle mass as $p \to 0$, with $m^*/m \sim 1/p$.



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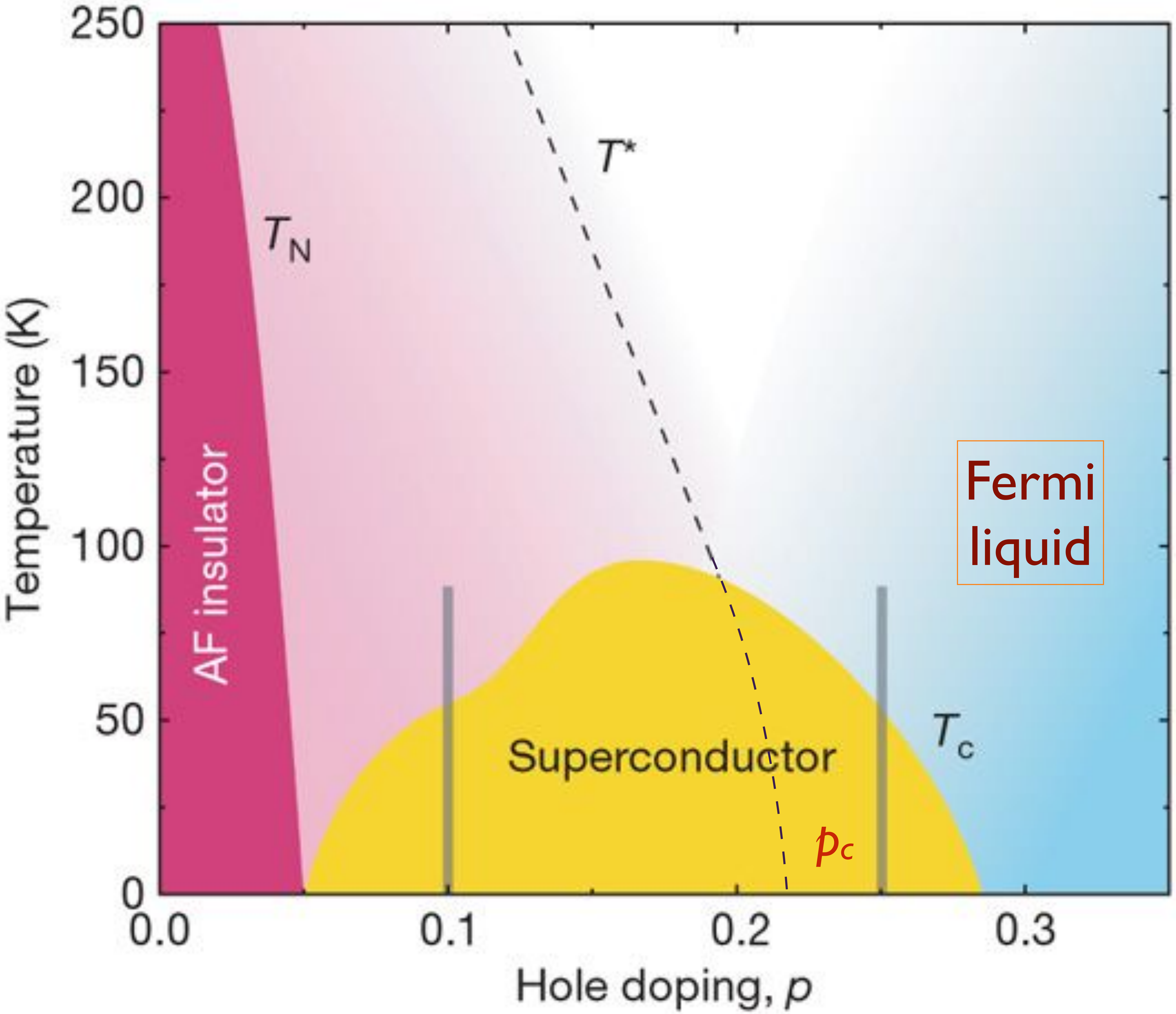
250
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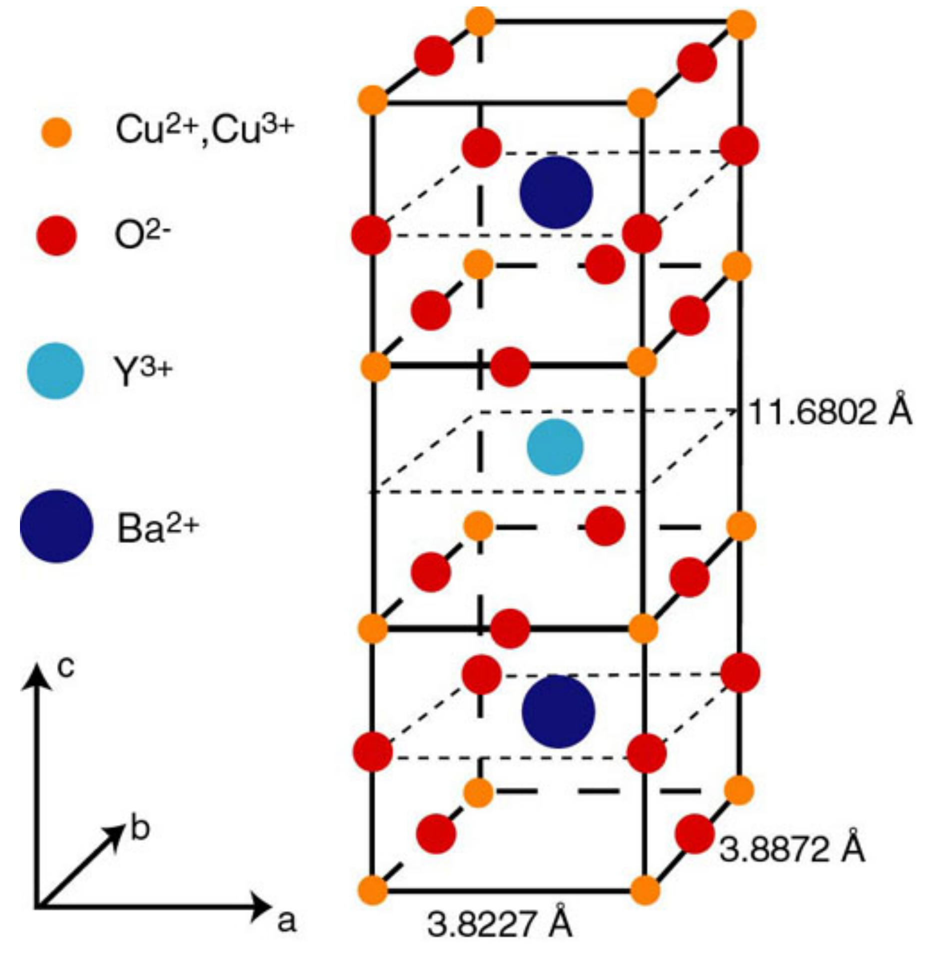
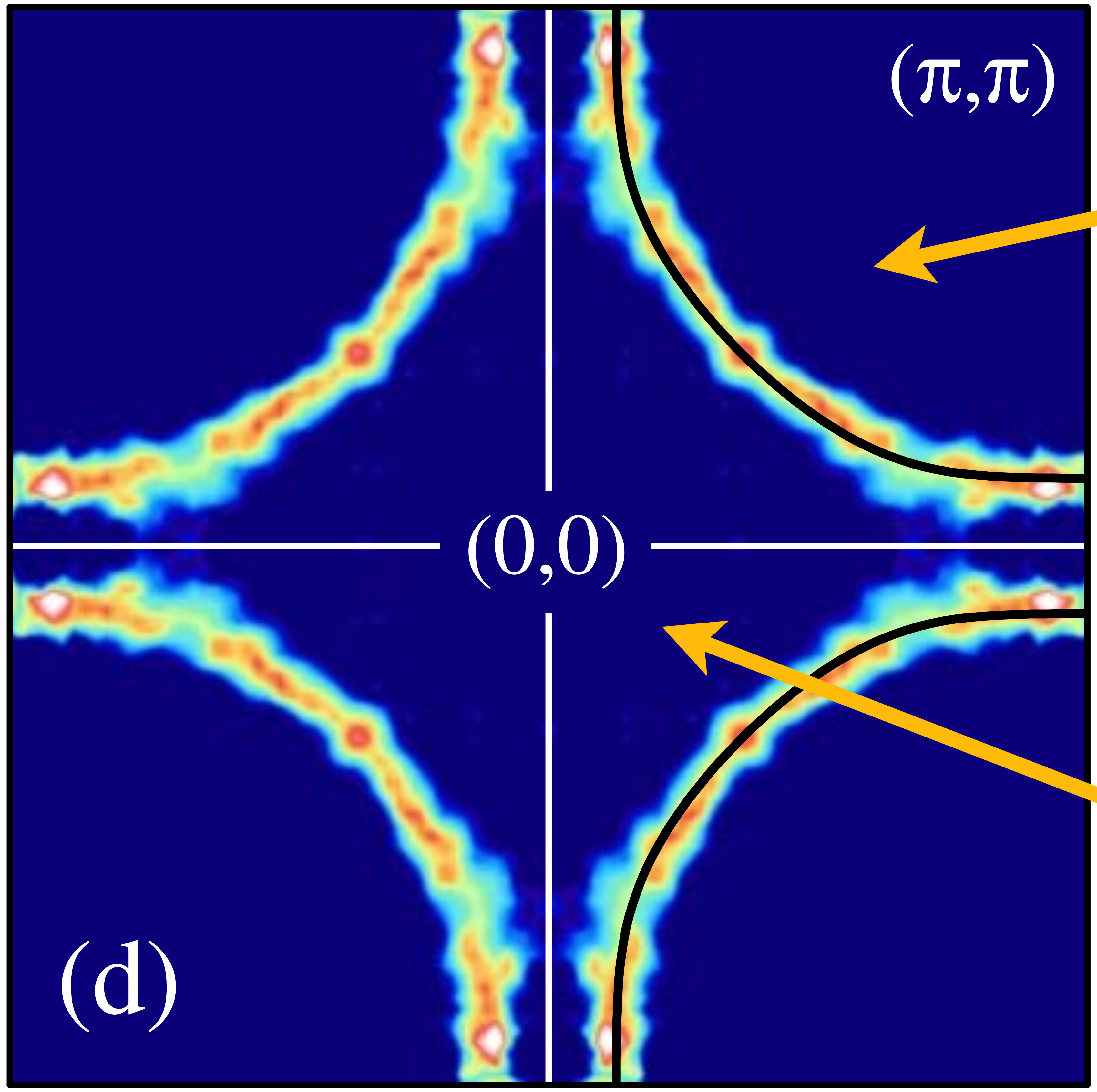
Temperature (K)
Hole doping, p
AF insulator
T_N
T*
Fermi liquid
Superconductor
T_c
p_c


Cu2+,Cu3+
O2-
Y3+
Ba2+
c
b
a
11.6802 Å
3.8872 Å
3.8227 Å

Photoemission at large p



$1+p$ holes

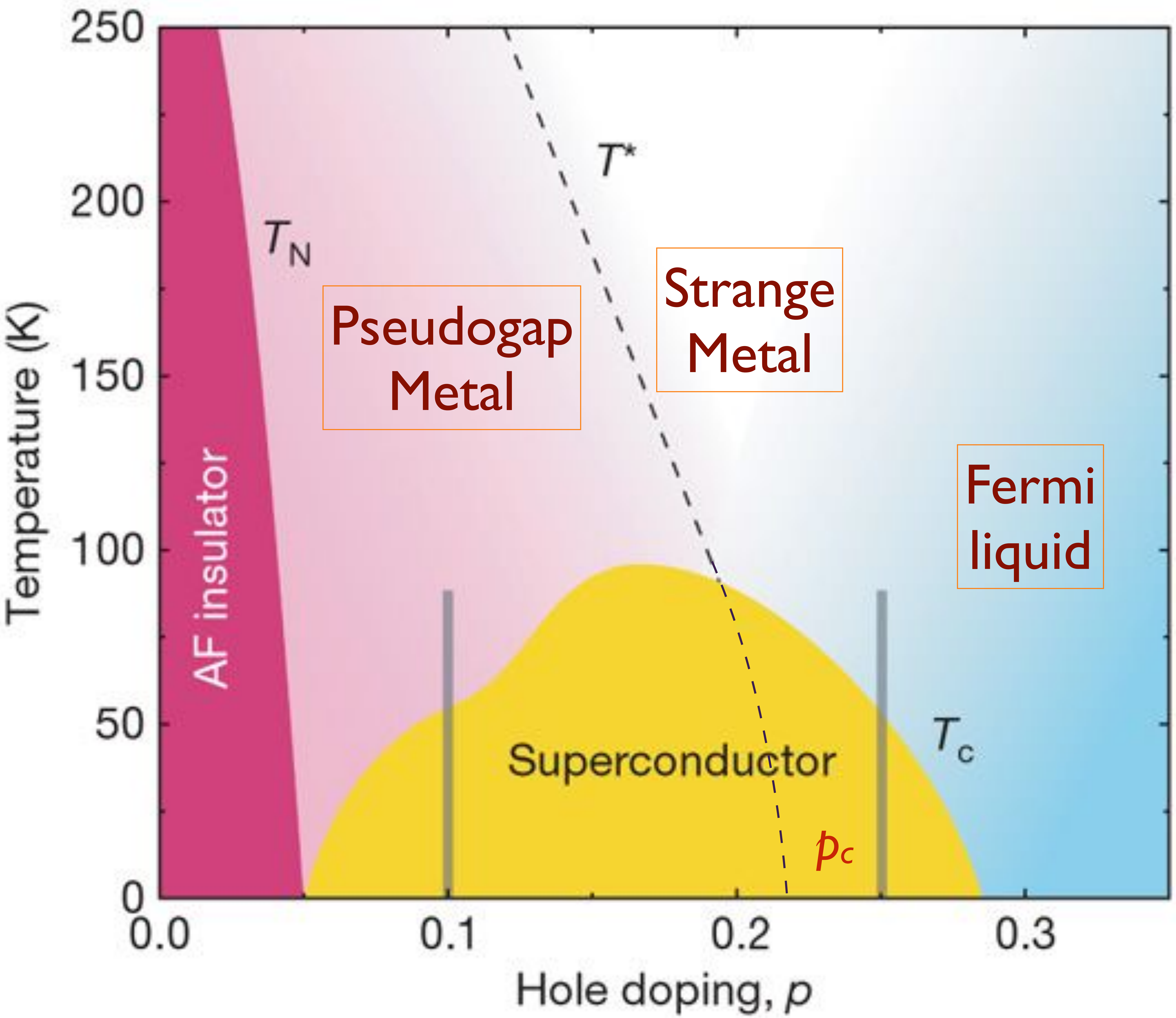
1-p electrons

Overdoped $Tl_2Ba_2CuO_{6+\delta}$
$T_c = 30K$

$1+p$ mobile holes in a filled band

M. Platé, J. D. F. Mottershead, I. S. Elfimov, D. C. Peets, Ruixing Liang, D. A. Bonn, W. N. Hardy, S. Chiuzbaian, M. Falub, M. Shi, L. Patthey, and A. Damascelli, Phys. Rev. Lett. **95**, 077001 (2005)

1. Kondo lattice model: the heavy Fermi liquid (HFL) as the Higgs phase of a U(1) gauge theory
2. Kondo lattice model: the FL* phase — fractionalization, emergent gauge fields, and Luttinger violation
3. Hubbard model: the vanilla FL phase
4. Hubbard model: the FL* phase at small doping p, using ancilla qubits


250
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Temperature (K)
0.0
0.1
0.2
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Hole doping, p
AF insulator
T_N
Pseudogap Metal
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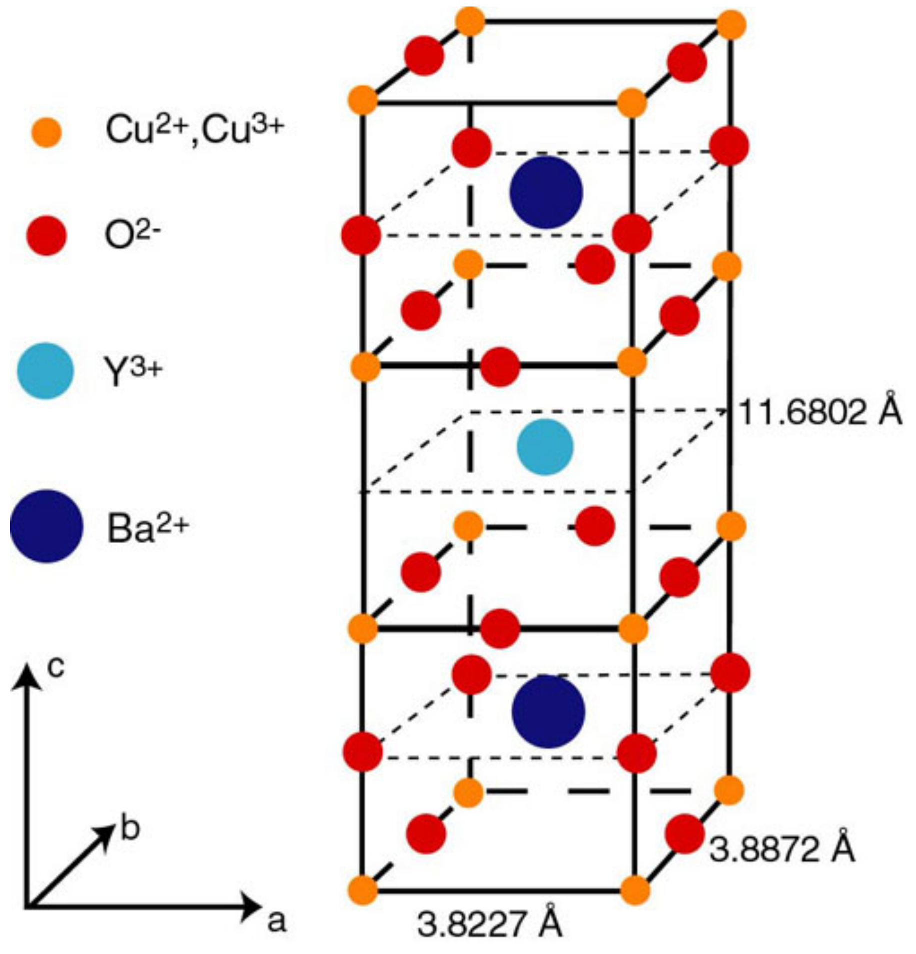
Strange Metal
Fermi liquid
Superconductor
T_c
p_c


Cu^{2+},Cu^{3+}
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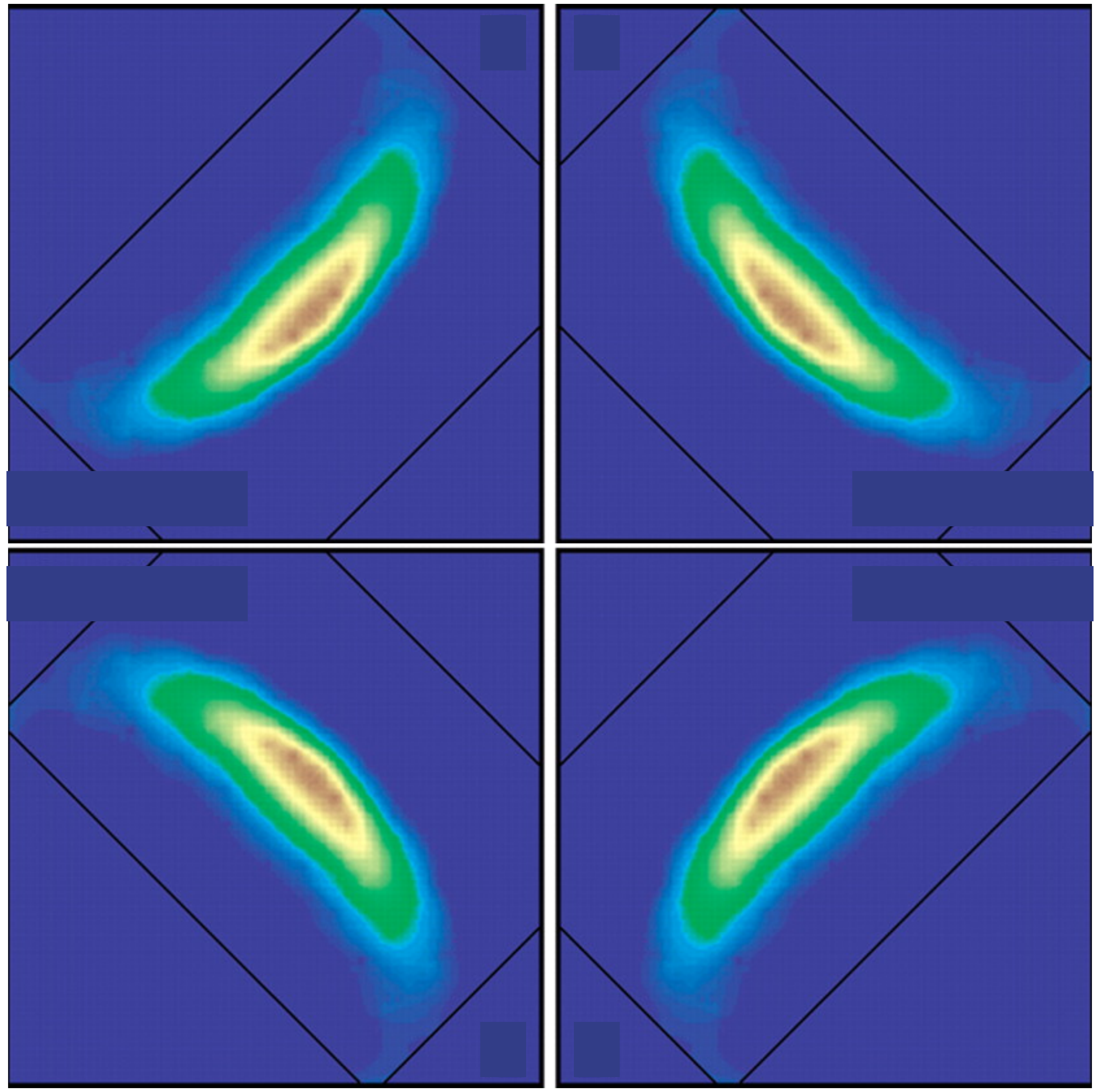


$Ca_{2-x}Na_xCuO_2Cl_2$
at $x = 0.10$

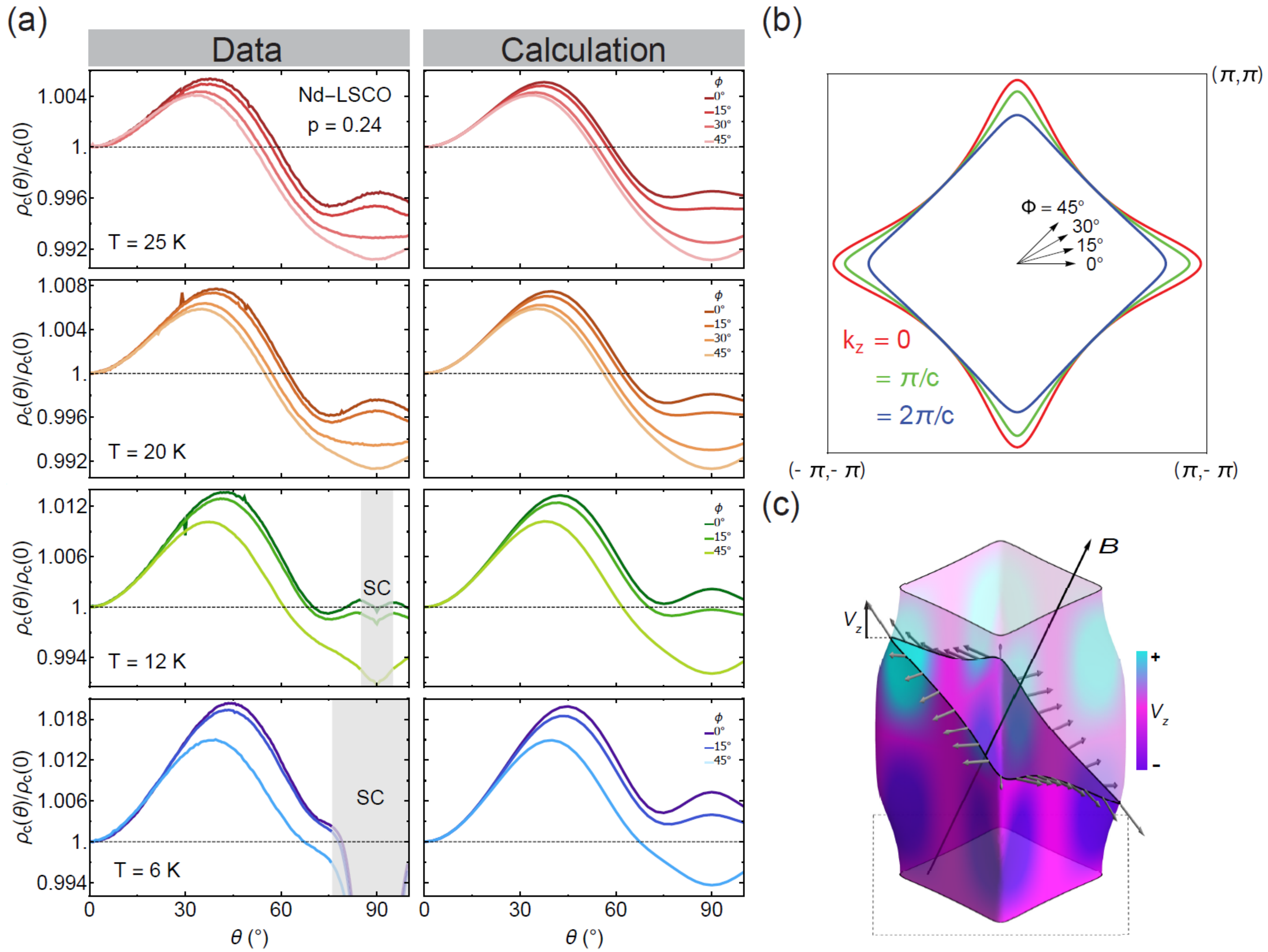
"Fermi arcs"

Kyle M. Shen, F. Ronning, D. H. Lu, F. Baumberger, N. J. C. Ingle, W. S. Lee, W. Meevasana, Y. Kohsaka, M. Azuma, M. Takano, H. Takagi, Z.-X. Shen, Science **307**, 901 (2005)

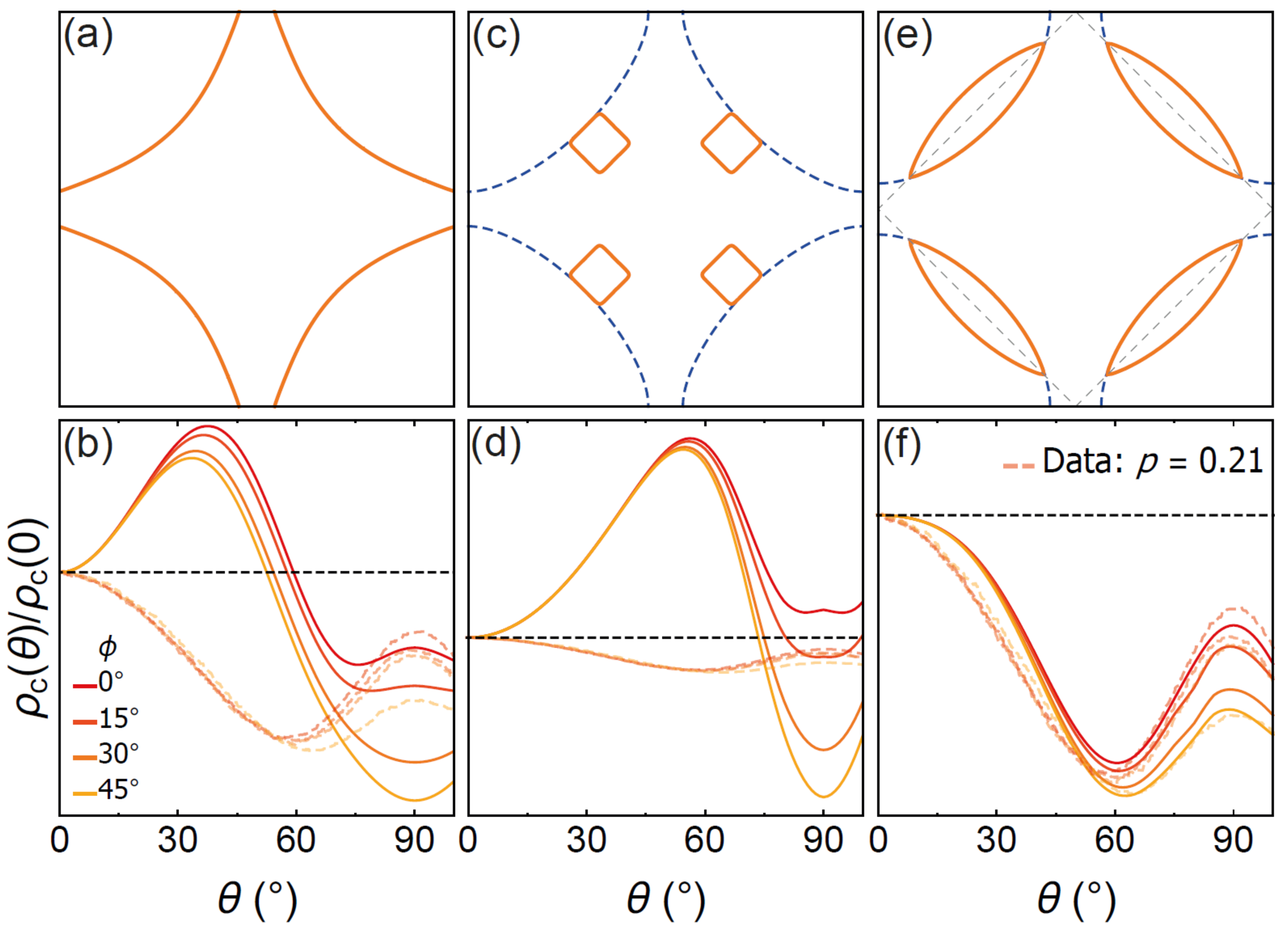
Fermi surface transformation at the pseudogap critical point of a cuprate superconductor

Yawen Fang, Gaël Grissonnanche, Anaëlle Legros, Simon Verret, Francis Laliberté, Clément Collignon, Amirreza Ataei, Maxime Dion, Jianshi Zhou, David Graf, M. J. Lawler, Paul Goddard, Louis Taillefer, and B. J. Ramshaw, arXiv:2004.01725

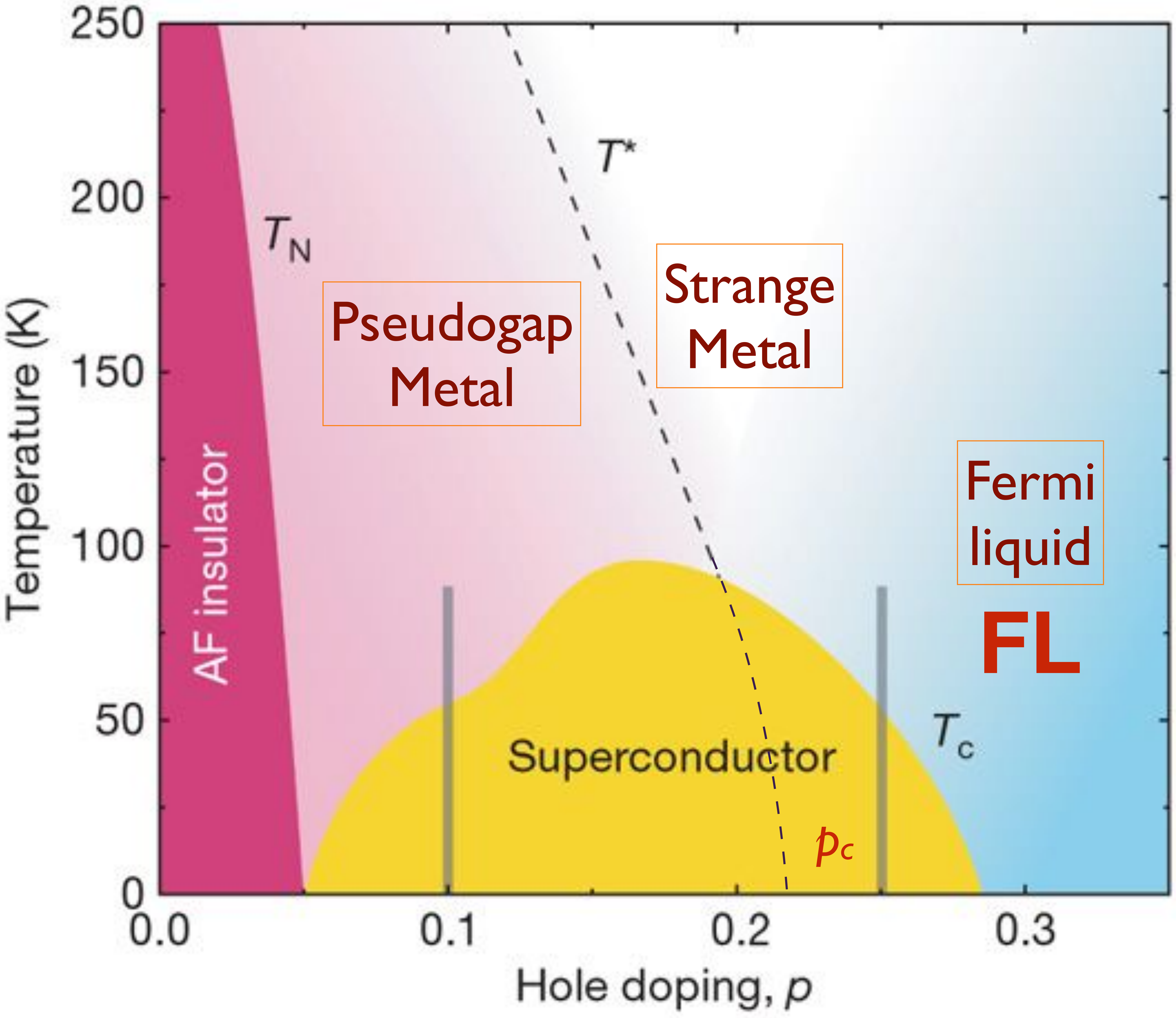
We use angle-dependent magnetoresistance (ADMR) to measure the Fermi surface of the cuprate $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$. Above the critical doping p*—outside of the pseudogap phase—we find a Fermi surface that is in quantitative agreement with angle-resolved photoemission. Below p*, however, the ADMR is qualitatively different, revealing a clear change in Fermi surface topology. We find that our data is most consistent with a Fermi surface that has been reconstructed by a Q = (π,π) wavevector. While static Q = (π,π) antiferromagnetism is not found at these dopings, our results suggest that this wavevector is a fundamental organizing principle of the pseudogap phase.



$p > p_c$ Large Fermi surface



$p < p_c$ Reconstructed Fermi surface



250
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Hole doping, p
AF insulator
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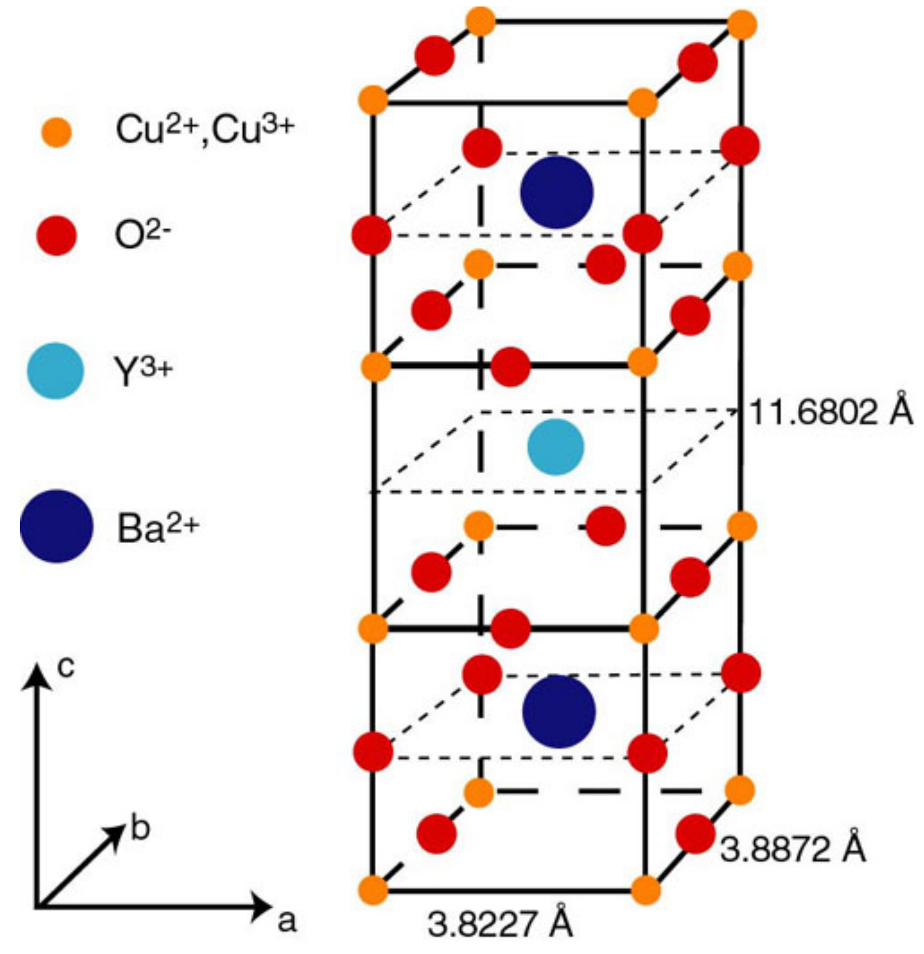

Cu^{2+},Cu^{3+}
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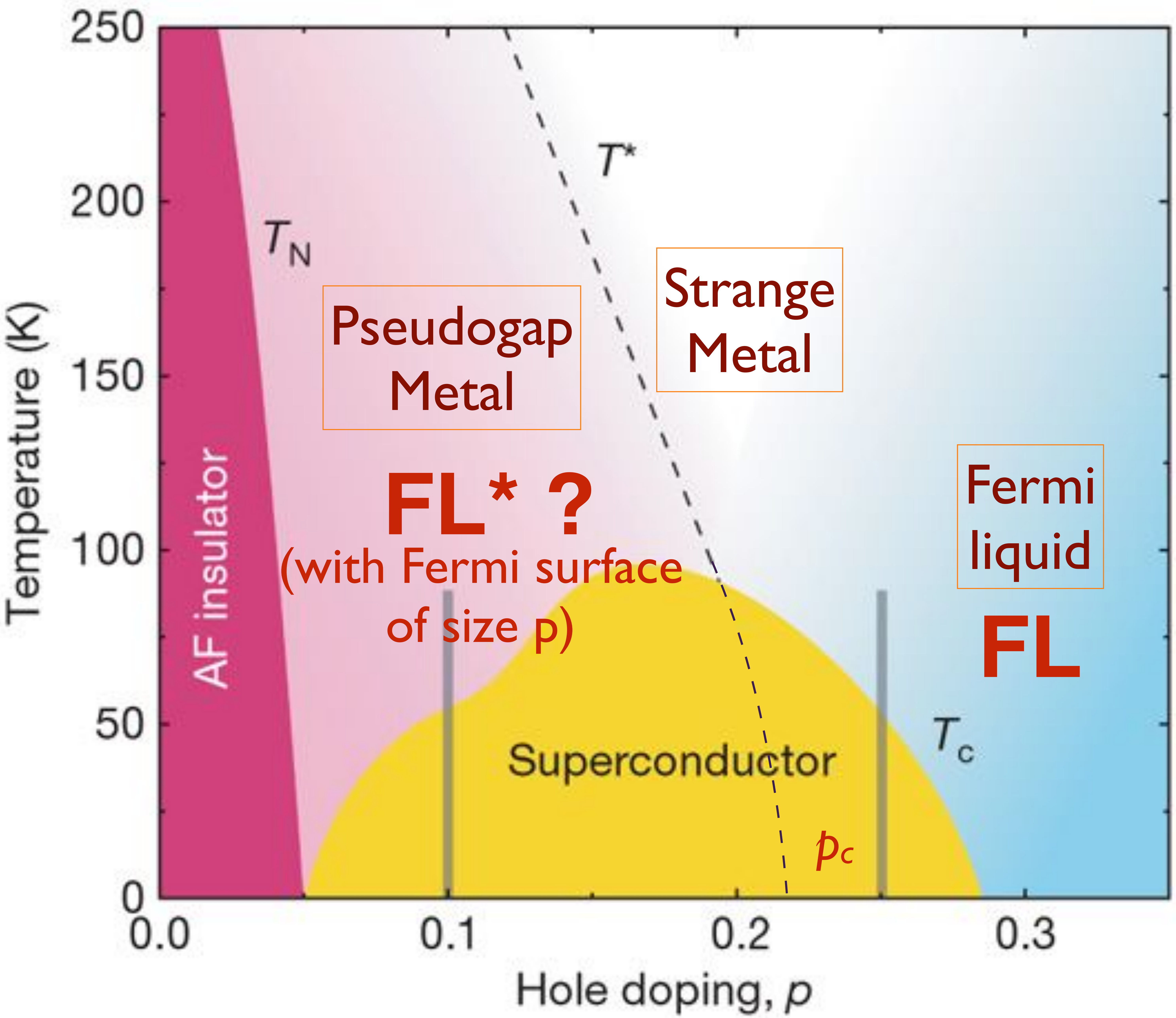
250
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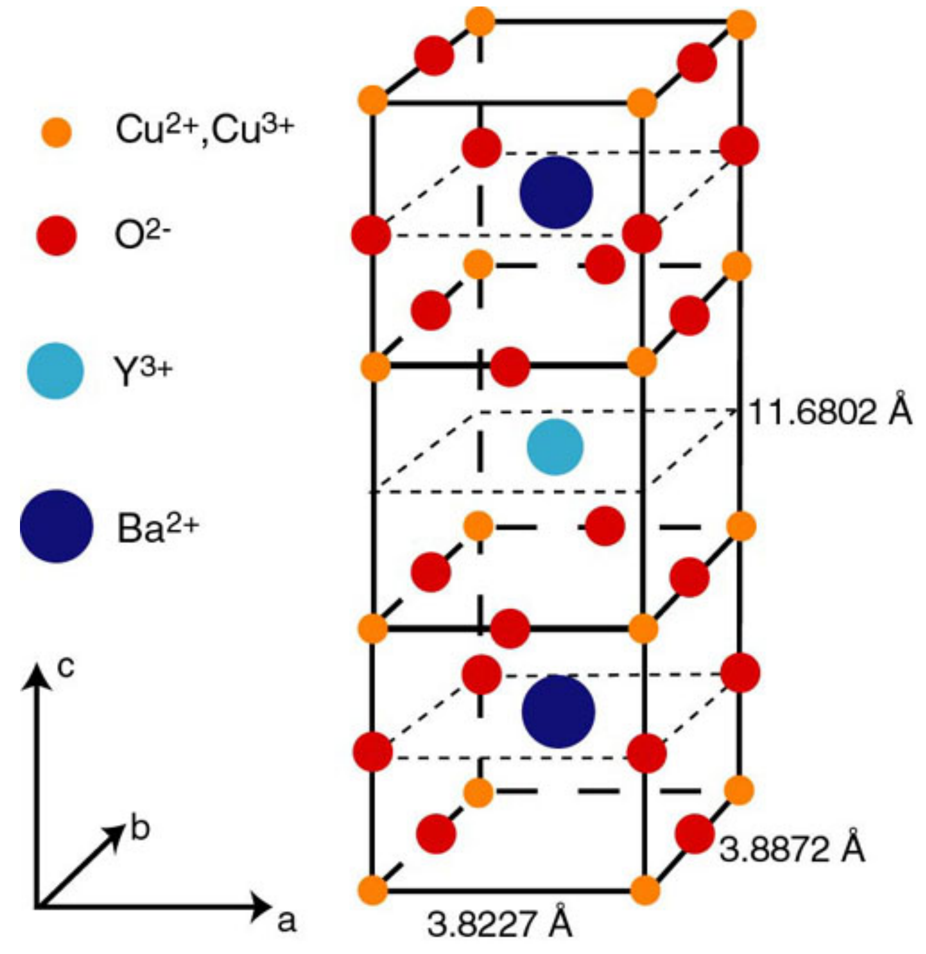
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The pseudogap metal ≈ FL* (these papers fractionalize the mobile electron)

X.-G. Wen and P. A. Lee, "Theory of Underdoped Cuprates," Phys. Rev. Lett. **76**, 503 (1996), arXiv:cond-mat/9506065 [cond-mat].

J.-W. Mei, S. Kawasaki, G.-Q. Zheng, Z.-Y. Weng, and X.-G. Wen, "Luttinger-volume violating Fermi liquid in the pseudogap phase of the cuprate superconductors," Phys. Rev. B **85**, 134519 (2012), arXiv:1109.0406 [cond-mat.supr-con].

K.-Y. Yang, T. M. Rice, and F.-C. Zhang, "Phenomenological theory of the pseudogap state," Phys. Rev. B **73**, 174501 (2006), arXiv:cond-mat/0602164 [cond-mat.supr-con].

N. J. Robinson, P. D. Johnson, T. M. Rice, and A. M. Tsvelik, "Anomalies in the pseudogap phase of the cuprates: competing ground states and the role of umklapp scattering," Reports on Progress in Physics **82**, 126501 (2019), arXiv:1906.09005 [cond-mat.supr-con].

J. Feldmeier, S. Huber, and M. Punk, "Exact solution of a two-species quantum dimer model for pseudogap metals," Phys. Rev. Lett. **120**, 187001 (2018), arXiv:1712.01854 [cond-mat.str-el].

B. Verheijden, Y. Zhao, and M. Punk, "Solvable lattice models for metals with Z_2 topological order," SciPost Physics **7**, 074 (2019), arXiv:1908.00103 [cond-mat.str-el].

J. Brunkert and M. Punk, "Slave-boson description of pseudogap metals in t-J models," Physical Review Research **2**, 043019 (2020), arXiv:2002.04041 [cond-mat.str-el].

The pseudogap metal = FL* (these papers fractionalize the mobile electron)

Quantum phases of the Shraiman-Siggia model by S. Sachdev Physical Review B **49**, 6770 (1994).

R. K. Kaul, Y. B. Kim, S. Sachdev, and T. Senthil, "Algebraic charge liquids," Nature Physics **4**, 28 (2008), arXiv:0706.2187 [cond-mat.str-el].

Y. Qi and S. Sachdev, "Effective theory of Fermi pockets in fluctuating antiferromagnets," Phys. Rev. B **81**, 115129 (2010), arXiv:0912.0943 [cond-mat.str-el].

E. G. Moon and S. Sachdev, "Underdoped cuprates as fractionalized Fermi liquids: Transition to superconductivity," Phys. Rev. B **83**, 224508 (2011), arXiv:1010.4567 [cond-mat.str-el].

M. Punk and S. Sachdev, "Fermi surface reconstruction in hole-doped t-J models without long-range antiferromagnetic order," Phys. Rev. B **85**, 195123 (2012), arXiv:1202.4023 [cond-mat.str-el].

M. Punk, A. Allais, and S. Sachdev, "A quantum dimer model for the pseudogap metal," Proc. Nat. Acad. Sci. **112**, 9552 (2015), arXiv:1501.00978 [cond-mat.str-el].

M. S. Scheurer, S. Chatterjee, W. Wu, M. Ferrero, A. Georges, and S. Sachdev, "Topological order in the pseudogap metal," Proc. Nat. Acad. Sci. **115**, E3665 (2018), arXiv:1711.09925 [cond-mat.str-el].

S. Sachdev, H. D. Scammell, M. S. Scheurer, and G. Tarnopolsky, "Gauge theory for the cuprates near optimal doping," Phys. Rev. B **99**, 054516 (2019), arXiv:1811.04930 [cond-mat.str-el].

S. Sachdev, "Topological order, emergent gauge fields, and Fermi surface reconstruction," Rep. Prog. Phys. **82**, 014001 (2019), arXiv:1801.01125 [cond-mat.str-el].

The pseudogap metal = FL*

Main lesson from the Kondo lattice

Do not fractionalize the mobile electron, $c_{i\sigma} \neq f_{i\sigma} b^\dagger$.

The pseudogap metal = FL*

Main lesson from the Kondo lattice

Do not fractionalize the mobile electron, $c_{i\sigma} \neq f_{i\sigma} b^\dagger$.

We avoid this particular fractionalization because the excitations around the small Fermi surface carry spin-1/2 and charge e, just like the bare electron: so it is cumbersome to fractionalize all the electrons (which occurs on energy scale J), and then undo the fractionalization for a small density of them by forming bound states of spinons and holons (which occurs on an energy scale t). In particular, no complete theory of this bound state formation has yet been presented.

Yahui Zhang

arXiv: 2001.09159
arXiv: 2006.01140
arXiv: 2103.05009

Maria Tikhanovskaya

Alexander Nikolaenko

Paramagnon theory of the Hubbard model

$$H = -\sum_{i<j} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) - \mu \sum_i c^\dagger_{i\sigma} c_{i\sigma}$$

We use the operator equation (valid on each site i):

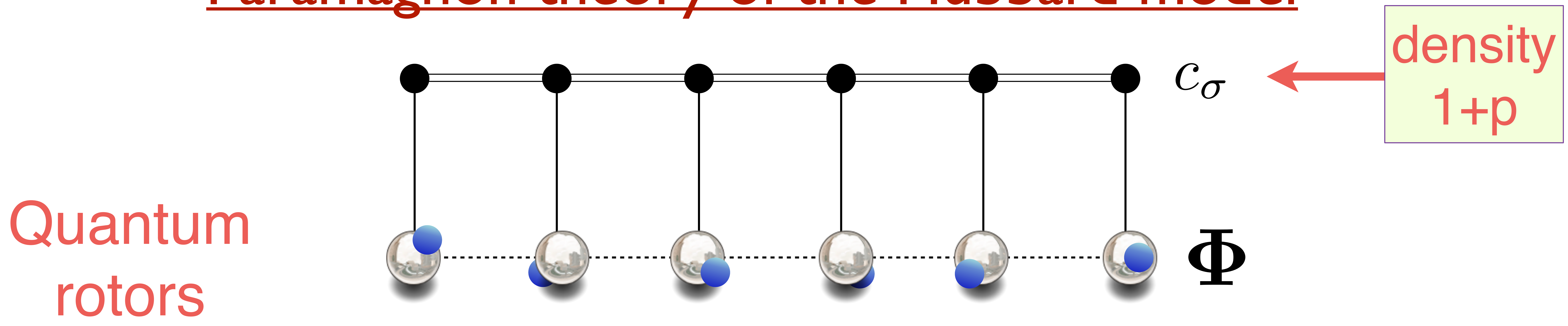
$$U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) = -\frac{2U}{3}\boldsymbol{S}^2 + \frac{U}{4}$$

Then we decouple the interaction via

$$\exp\left(\frac{2U}{3}\sum_i \int d\tau \boldsymbol{S}_i^2\right) = \int \mathcal{D}\boldsymbol{\Phi}_i(\tau) \exp\left(-\sum_i \int d\tau \left[\frac{3}{8U}\boldsymbol{\Phi}_i^2 - \boldsymbol{\Phi}_i \cdot c^\dagger_{i\sigma} \frac{\boldsymbol{\tau}_{\sigma\sigma'}}{2} c_{i\sigma'}\right]\right)$$

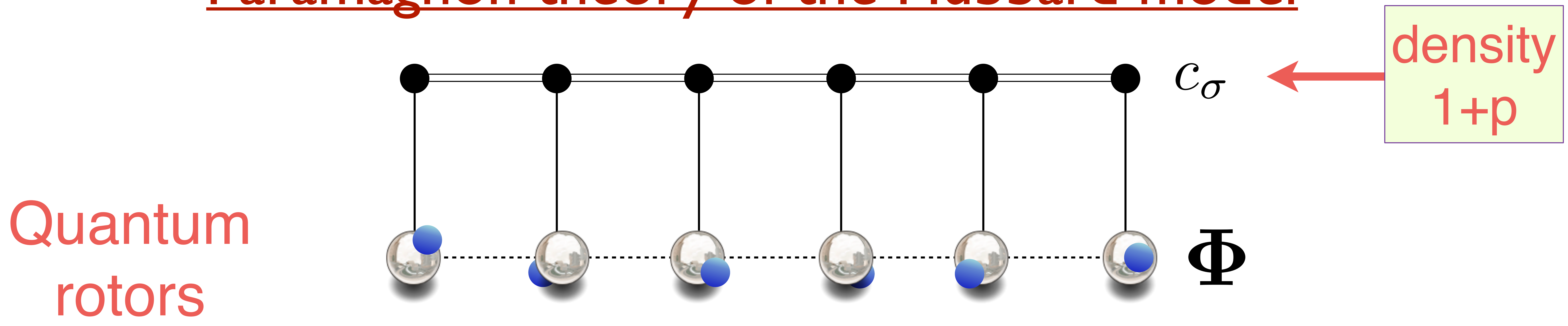
This yields the 'Hertz-Millis' theory for a 'paramagnon quantum rotor' $\boldsymbol{\Phi}_i$ coupled to otherwise free fermions $c_{i\sigma}$.

Paramagnon theory of the Hubbard model



$$\mathcal{H}_{\rm rotor} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c_{\mathbf{p}\sigma}^{\dagger} c_{\mathbf{p}\sigma} + \sum_i \left[\widetilde{t} \, \boldsymbol{L}_i^2 + \frac{3}{8U} \mathbf{\Phi}_i^2 \right] - \sum_i c_{i\sigma}^{\dagger} \frac{\boldsymbol{\tau}_{\sigma\sigma'}}{2} c_{i\sigma'} \cdot \mathbf{\Phi}_i$$

Paramagnon theory of the Hubbard model



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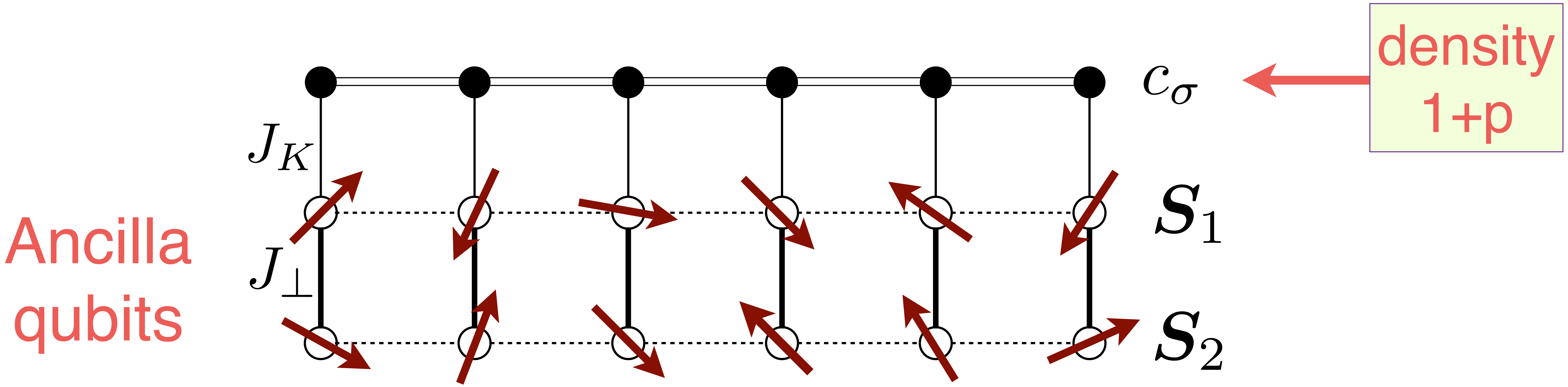
Key idea:

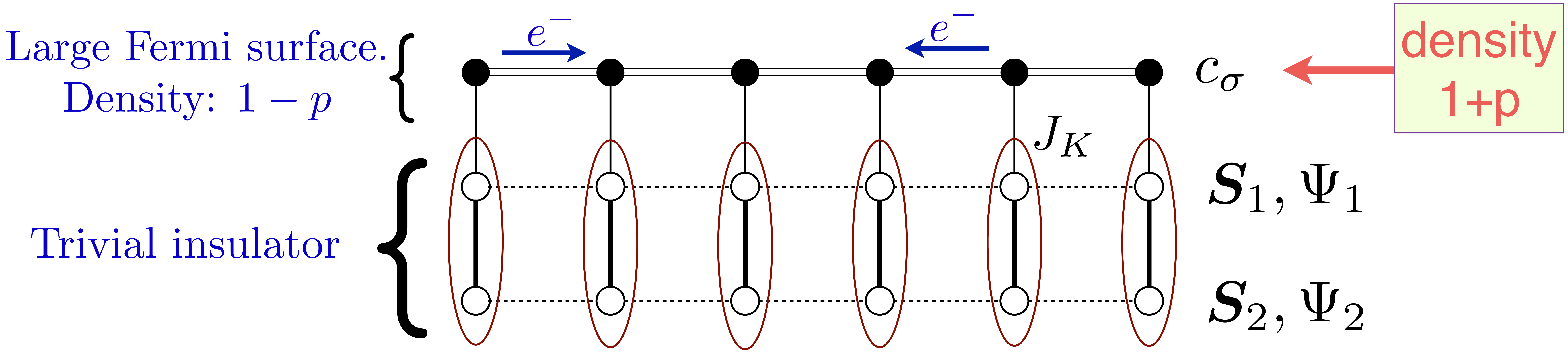
Fractionalize the 'paramagnon rotor' $\boldsymbol{\Phi}_i$
into 2 "ancilla qubits",
$S = 1/2$ spins $\boldsymbol{S}_{1i}$ and $\boldsymbol{S}_{2i}$ on each site,
and don't fractionalize the mobile electron $c_{i\sigma}$.

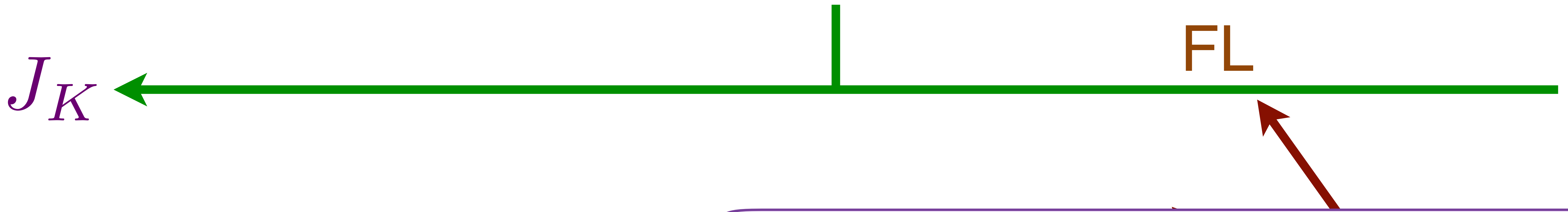
Ancilla theory of the Hubbard model



$$\mathcal{H}_{\rm ancilla} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma} + \sum_i \left[J_K \, c^\dagger_{i\sigma} \frac{\boldsymbol{\tau}_{\sigma\sigma'}}{2} c_{i\sigma'} \cdot \boldsymbol{S}_{1i} + J_\perp \, \boldsymbol{S}_{1i} \cdot \boldsymbol{S}_{2i} \right] + \sum_{\langle ij \rangle} \left[J_1 \, \boldsymbol{S}_{1i} \cdot \boldsymbol{S}_{1j} + J_2 \, \boldsymbol{S}_{2i} \cdot \boldsymbol{S}_{2j} \right]$$

Ancilla theory of the Hubbard model

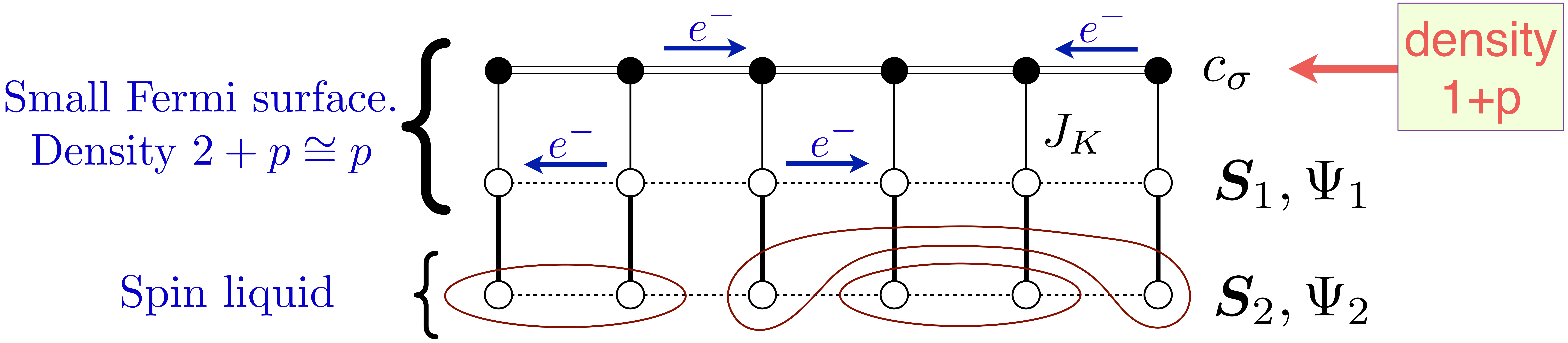


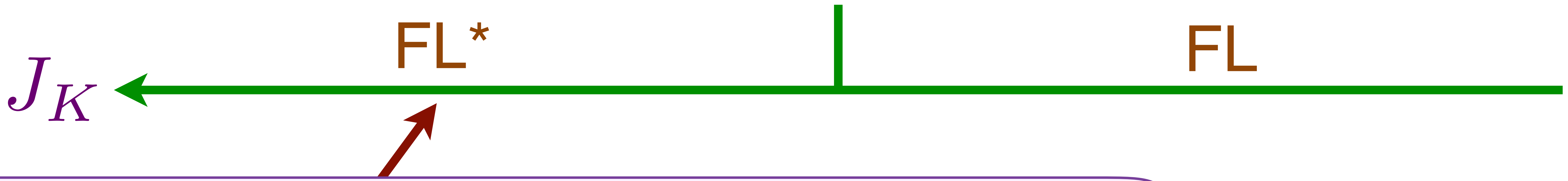


Large Fermi surface of size $1+p$

$|\mathrm{FL}\rangle = |\text{Rung singlets of } \Psi_1, \Psi_2\rangle$
$\otimes\ |\text{Slater determinant of } c\rangle$

Ancilla theory of the Hubbard model

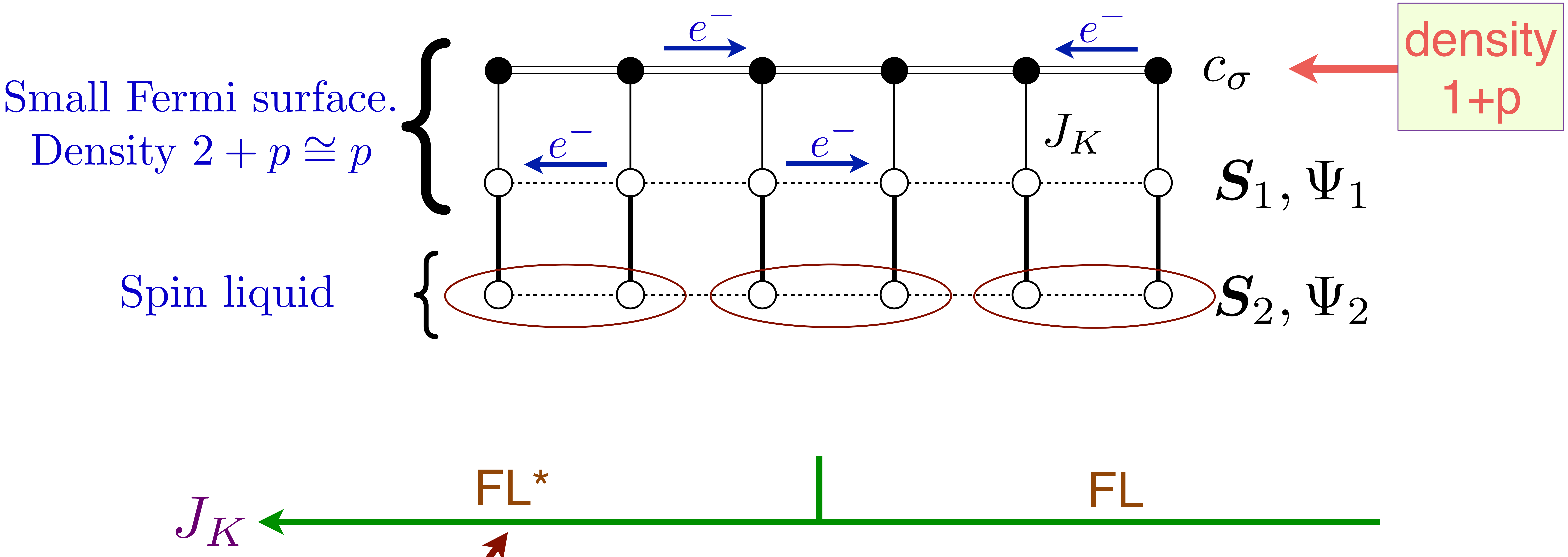




Small Fermi surface of size p

$$|\mathrm{FL}*\rangle = [\text{Projection onto rung singlets of } \Psi_1, \Psi_2]$$
$$\bowtie |\text{Slater determinant of } (c, \Psi_1)\rangle$$
$$\otimes |\text{Slater determinant of } \Psi_2\rangle$$

Ancilla theory of the Hubbard model



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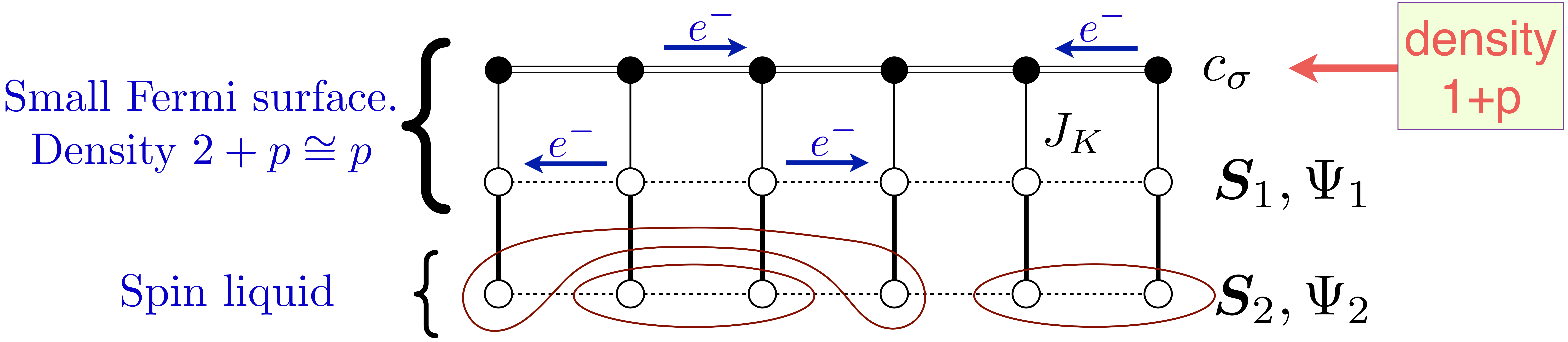
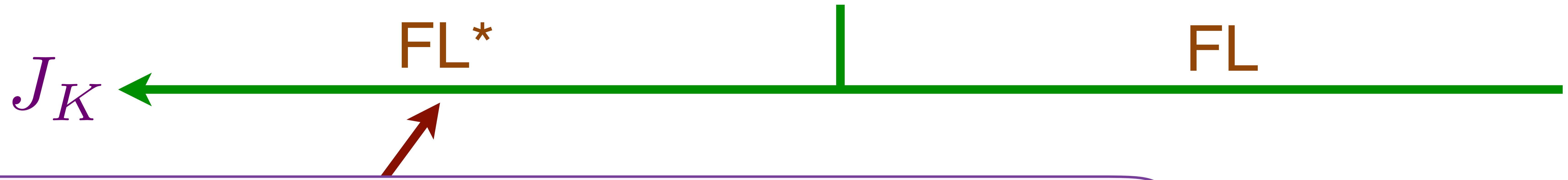
Ancilla theory of the Hubbard model





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$(\mathrm{SU}(2)_1 \times \mathrm{SU}(2)_2 \times \mathrm{SU}(2)_S)/\mathbb{Z}_2$ gauge theory of **one-band** model

Write fermion operators as 2×2 matrices

$$\mathbf{\Psi} = \begin{pmatrix} \Psi_\uparrow & -\Psi_\downarrow^\dagger \\ \Psi_\downarrow & \Psi_\uparrow^\dagger \end{pmatrix} \quad , \quad \widetilde{\mathbf{\Psi}} = \begin{pmatrix} \widetilde{\Psi}_\uparrow & -\widetilde{\Psi}_\downarrow^\dagger \\ \widetilde{\Psi}_\downarrow & \widetilde{\Psi}_\uparrow^\dagger \end{pmatrix}$$

Constraints $\Psi_\alpha^\dagger \Psi_\alpha = 1$ and $\widetilde{\Psi}_\alpha^\dagger \widetilde{\Psi}_\alpha = 1$ lead to:

P.A. Lee, N. Nagaosa, and X.-G. Wen, RMP **78**, 17 (2006)

$$\mathrm{SU}(2)_1 : \quad \mathbf{\Psi} \to \mathbf{\Psi} U_1 \quad , \quad \widetilde{\mathbf{\Psi}} \to \widetilde{\mathbf{\Psi}}$$

$$\mathrm{SU}(2)_2 : \quad \mathbf{\Psi} \to \mathbf{\Psi} \quad , \quad \widetilde{\mathbf{\Psi}} \to \widetilde{\mathbf{\Psi}} U_2$$

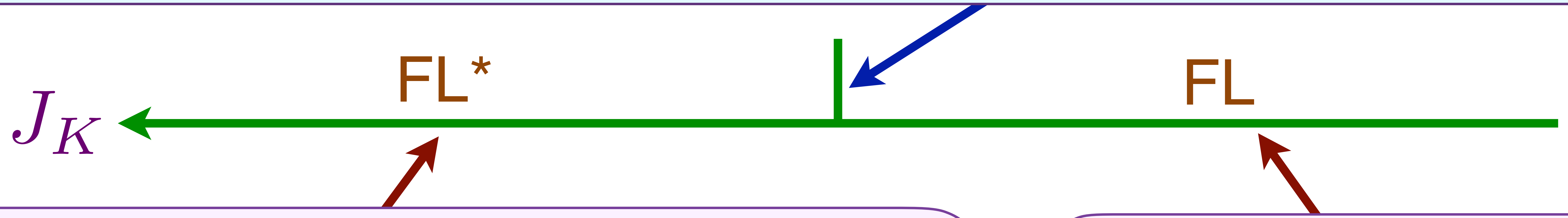
S. Sachdev, M.A. Metlitski, Yang Qi, and Cenke Xu, PRB **80**, 155129 (2009)
S. Sachdev, H. D. Scammell, M. S. Scheurer, and G. Tarnopolsky, PRB **99**, 054516 (2019)

Rung singlet formation $\boldsymbol{S}_1 + \boldsymbol{S}_2 \approx 0$ leads to:

$$\mathrm{SU}(2)_S : \quad \mathbf{\Psi} \to U_S \mathbf{\Psi} \quad , \quad \widetilde{\mathbf{\Psi}} \to U_S \widetilde{\mathbf{\Psi}}$$

Ancilla theory of the Hubbard model

- Deconfined criticality of a $(\mathrm{SU}(2)_S \times \mathrm{U}(1)_1)/Z_2$ gauge theory.
- 'Hybridization-Higgs' boson $\sim C_\sigma^\dagger \Psi_a$ which condenses on the FL* side (in Kondo lattice, Higgs boson was condensed on the FL side).
- Gauge-charged 'ghost' Fermi surface of Ψ_1 fermions.
- Large Fermi surface of c_σ gauge-neutral electrons.



Small Fermi surface of size p

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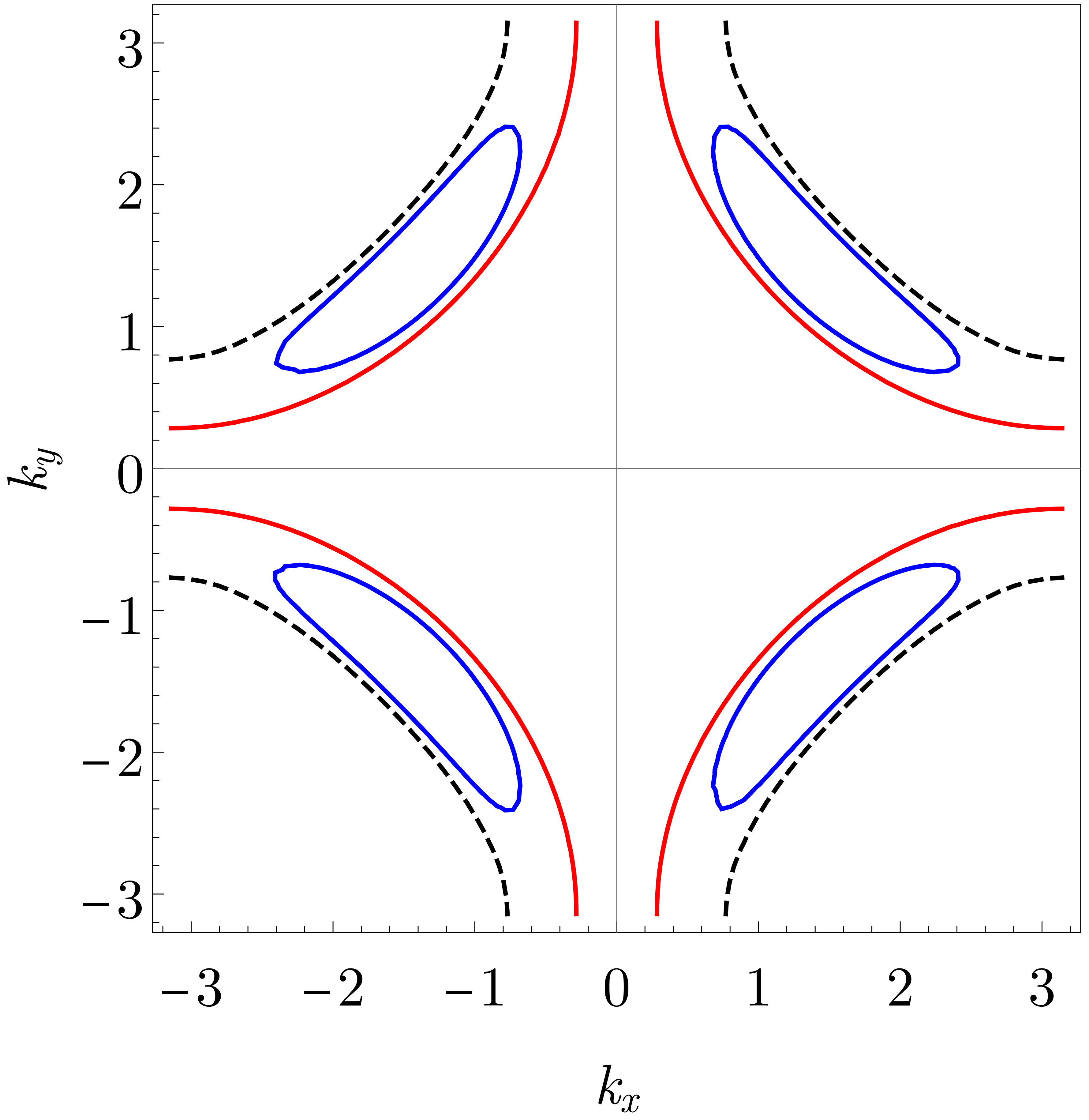
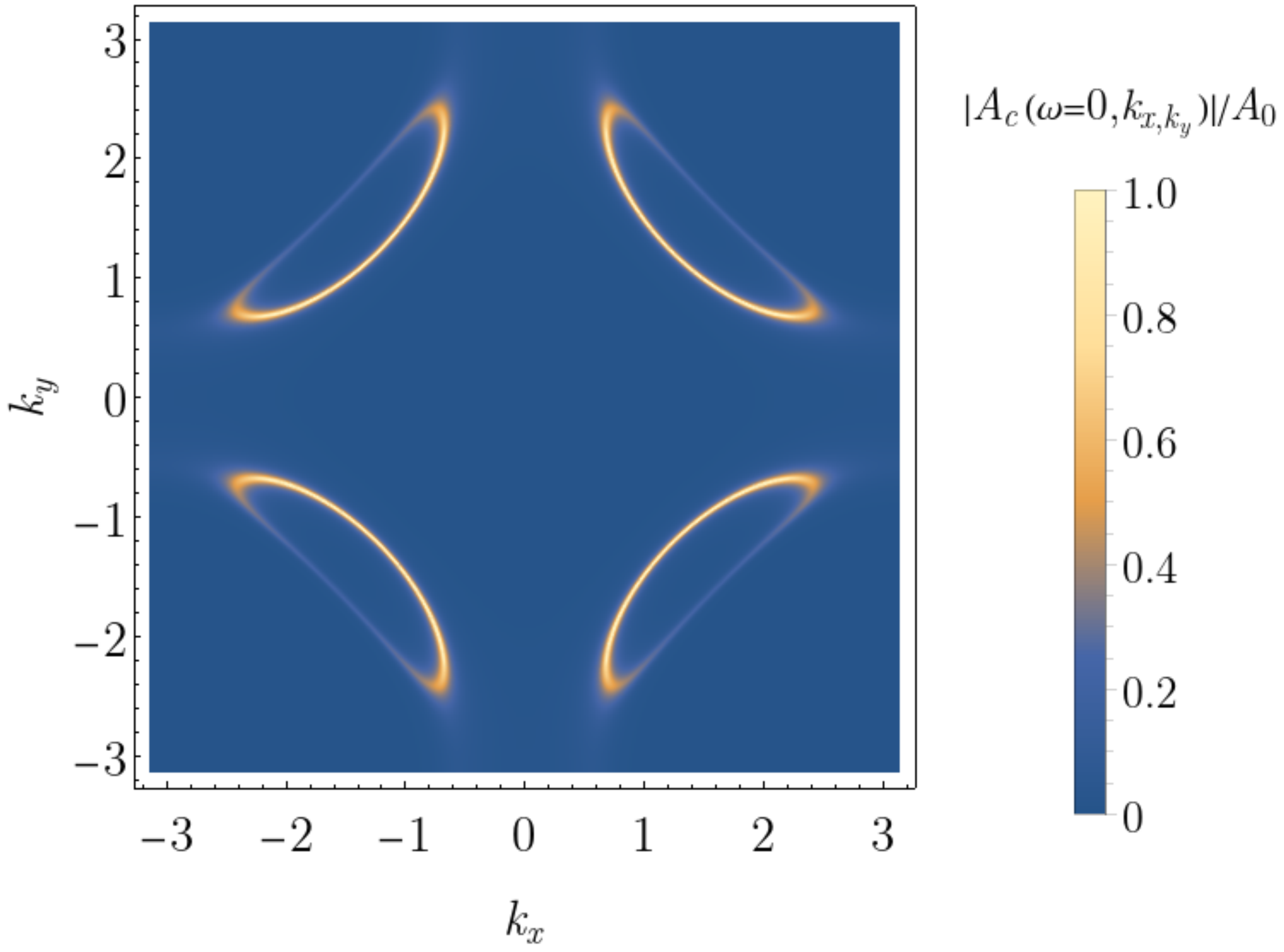
Large Fermi surface of size $1+p$

$$|\mathrm{FL}\rangle = |\text{Rung singlets of } \Psi_1, \Psi_2\rangle \otimes |\text{Slater determinant of } c\rangle$$

FL* in a ***one-band*** model



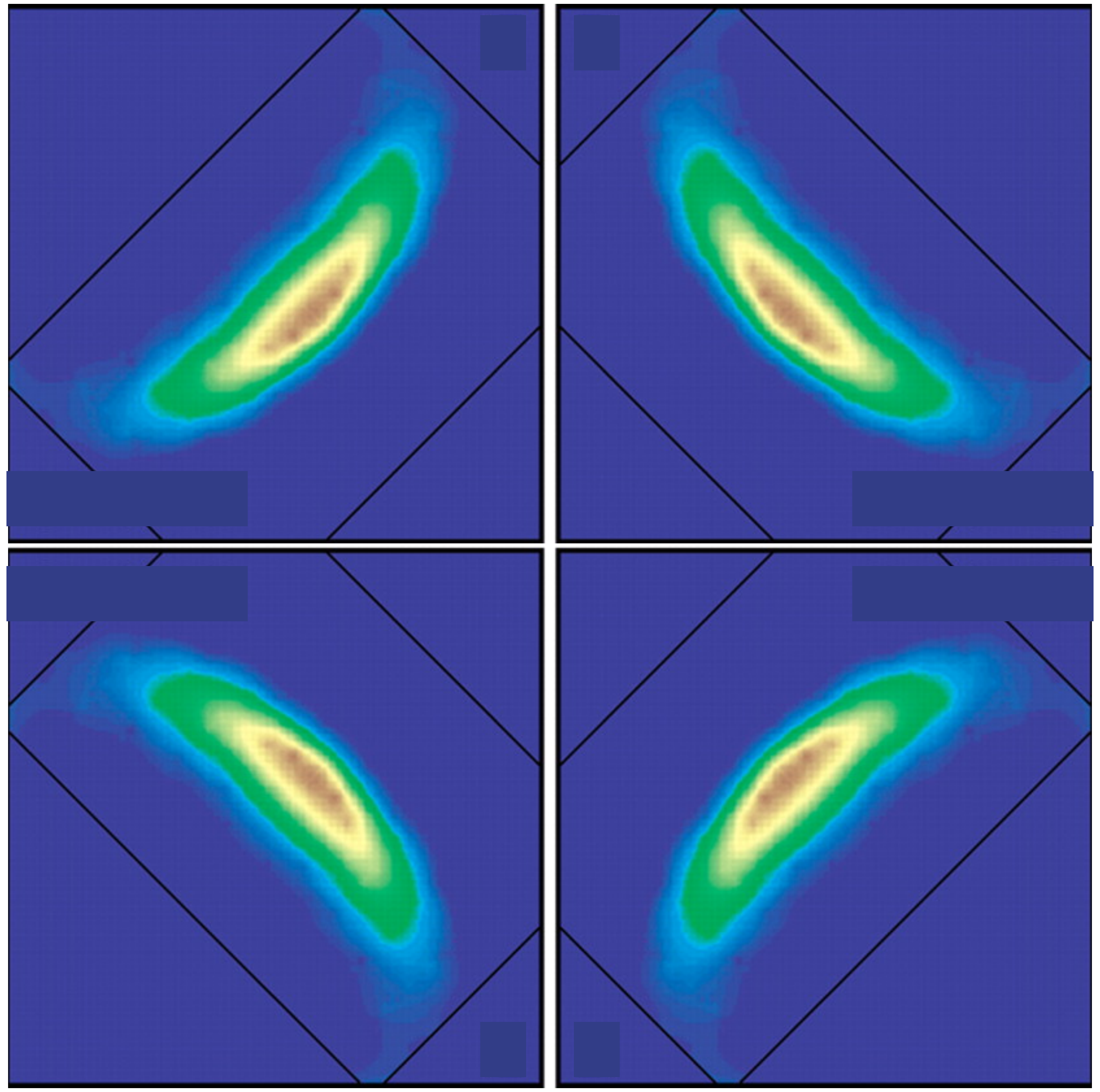
"Fermi arc" spectral functions



Effective Hamiltonian for FL*: $(\mathrm{SU}(2)_1 \times \mathrm{SU}(2)_S)/\mathbb{Z}_2$ fully broken by Higgs condensate Φ:

$$H = -\sum_{i,j} t_{ij} c^\dagger_{i;\alpha} c_{j;\alpha} + \sum_{i,j} t_{1,ij} \Psi^\dagger_{i;\alpha} \Psi_{j;\alpha} + \sum_i \Phi_i (c^\dagger_{i;\alpha} \Psi_{i;\alpha} + \Psi^\dagger_{i;\alpha} c_{i;\alpha})$$

Photoemission at small p



$Ca_{2-x}Na_xCuO_2Cl_2$
at $x = 0.10$

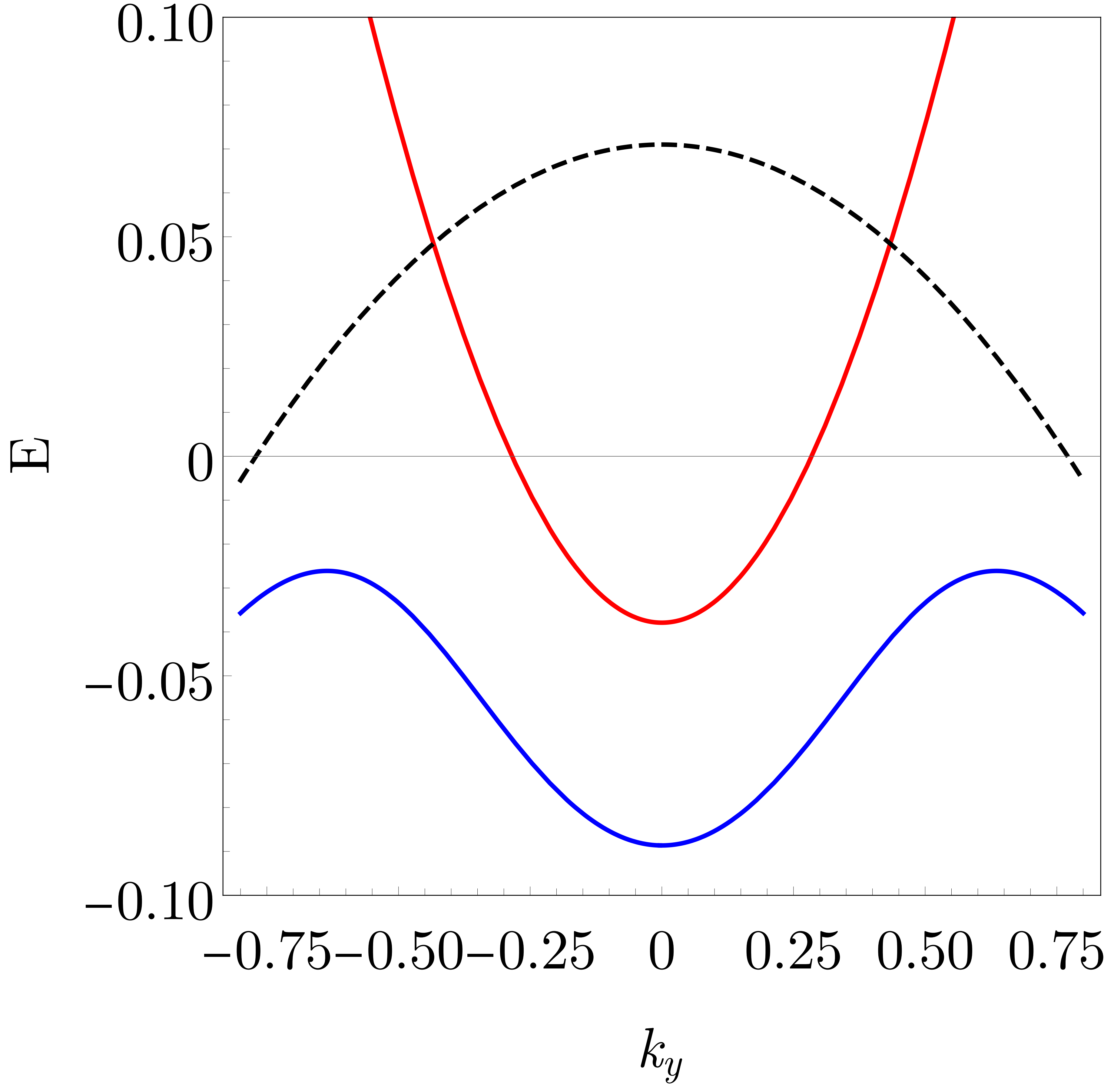
"Fermi arcs"

Kyle M. Shen, F. Ronning, D. H. Lu, F. Baumberger, N. J. C. Ingle, W. S. Lee, W. Meevasana, Y. Kohsaka, M. Azuma, M. Takano, H. Takagi, Z.-X. Shen, Science **307**, 901 (2005)

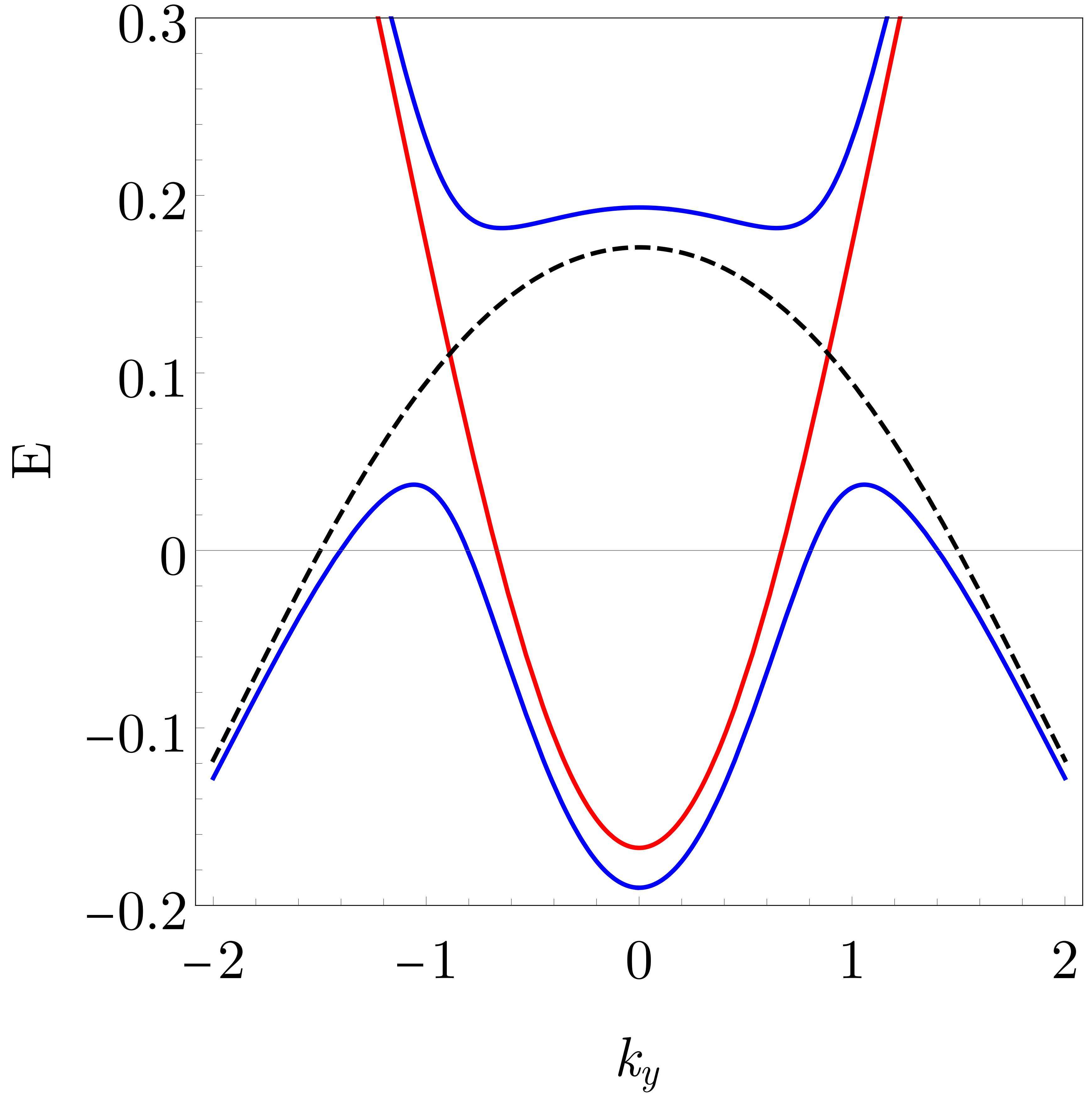
FL* in a ***one-band*** model

Electronic dispersion

Anti-node: $k_x = \pi$



Node: $k_x = 2$



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ARPES experiment

He *et al.*, *Science* **331**, 1579 (2011)

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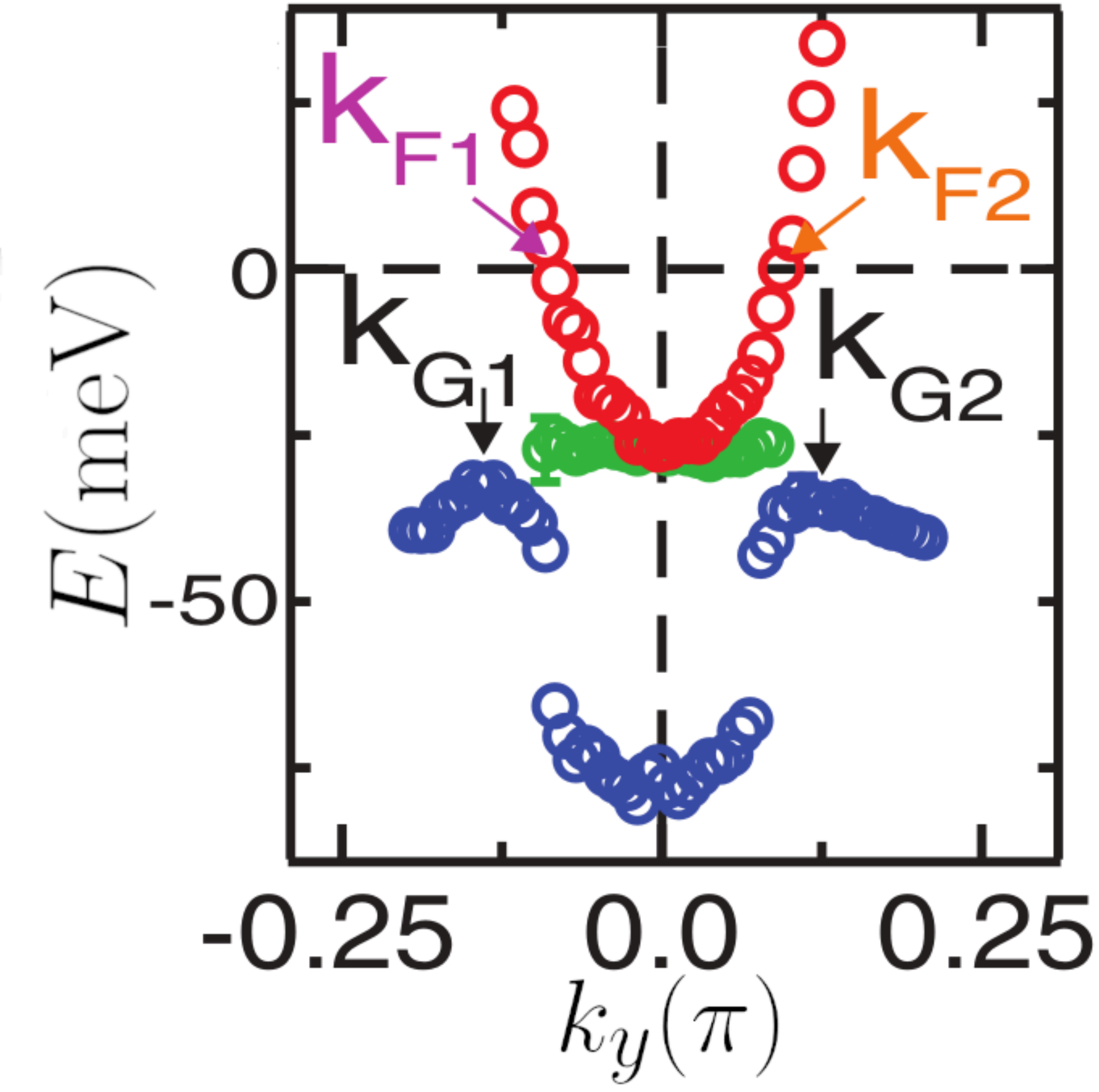

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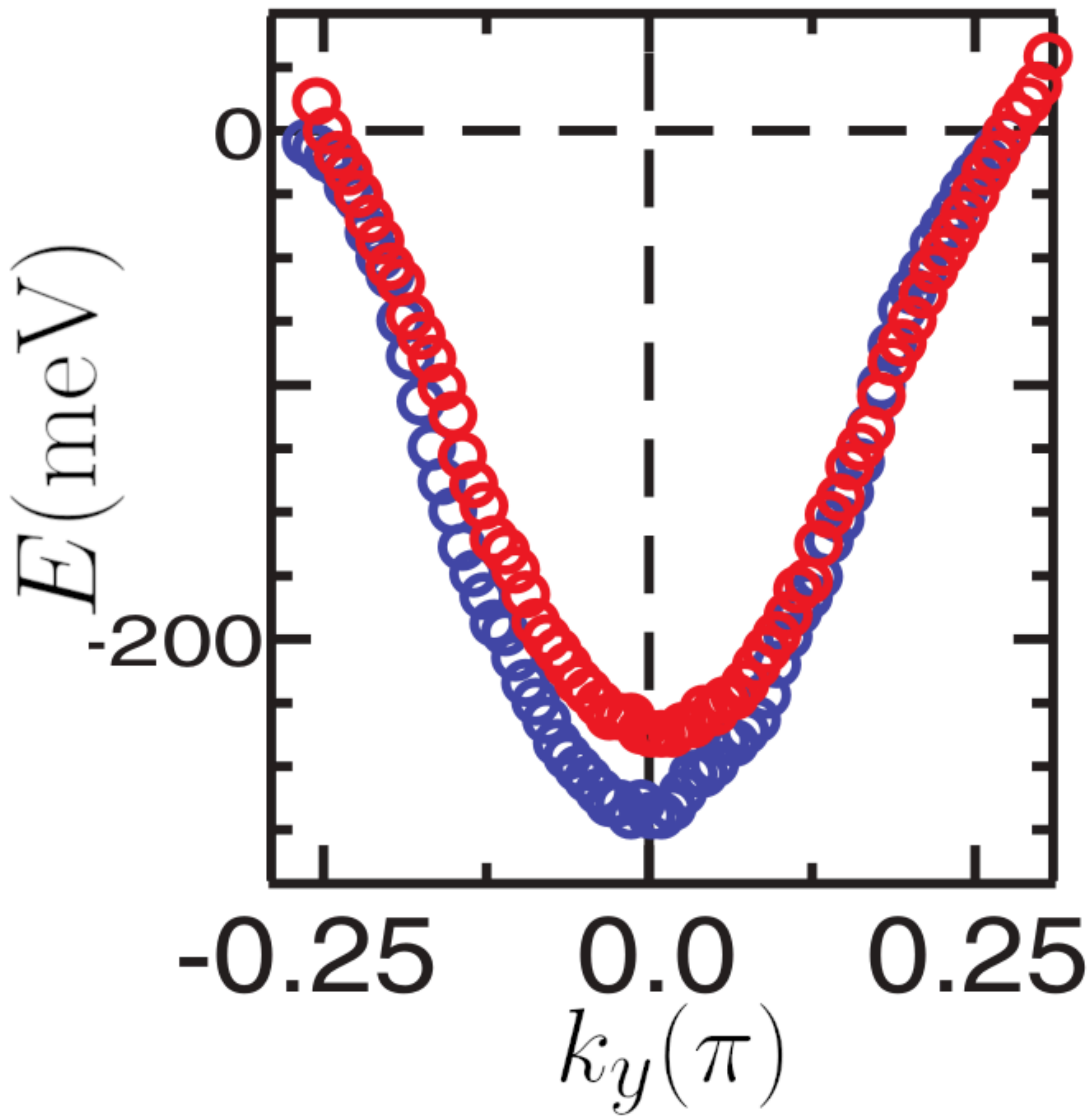
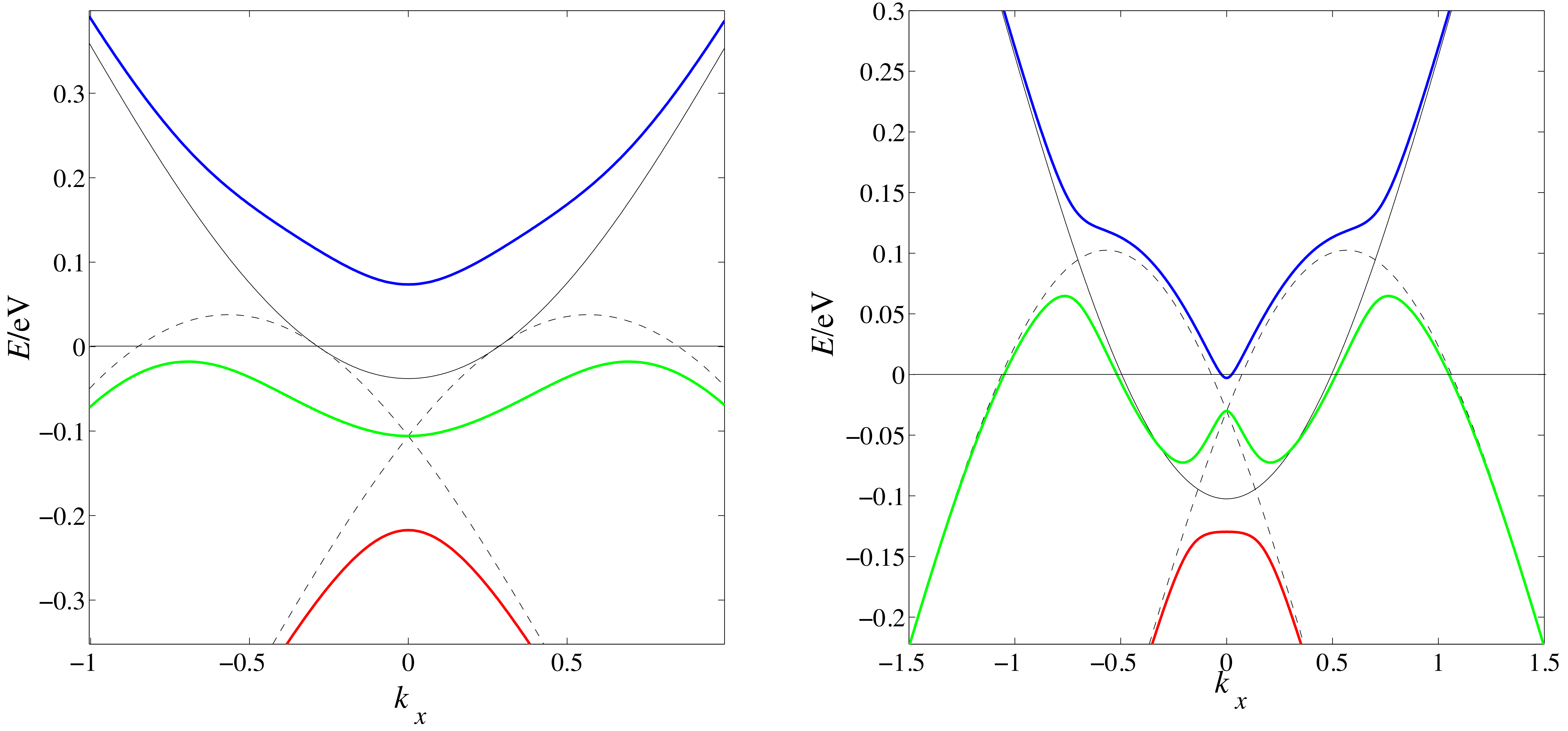


Electronic dispersion in the pseudogap metal

Pair Density Wave

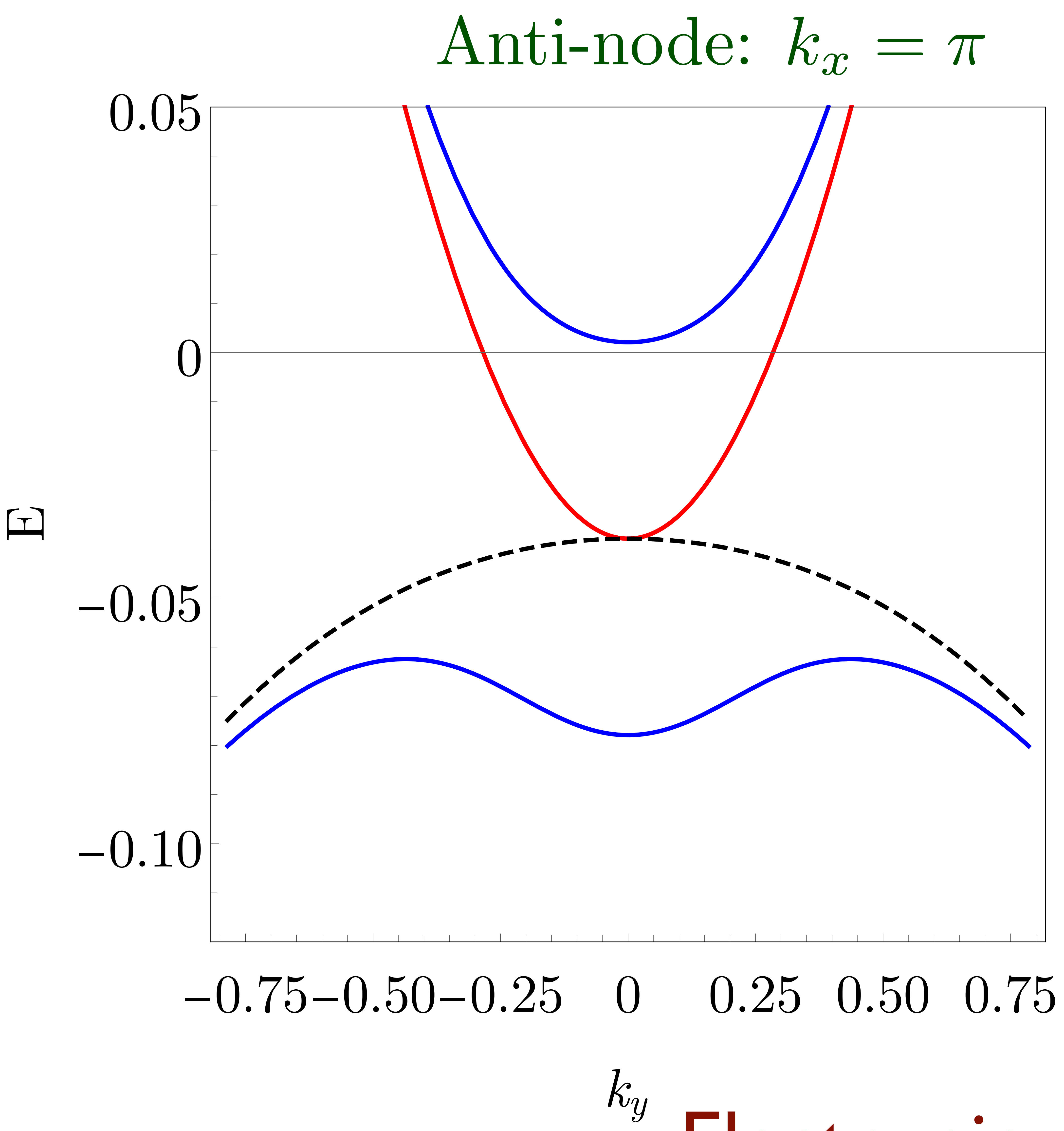
P.A. Lee, PRX **4**, 031017 (2014)

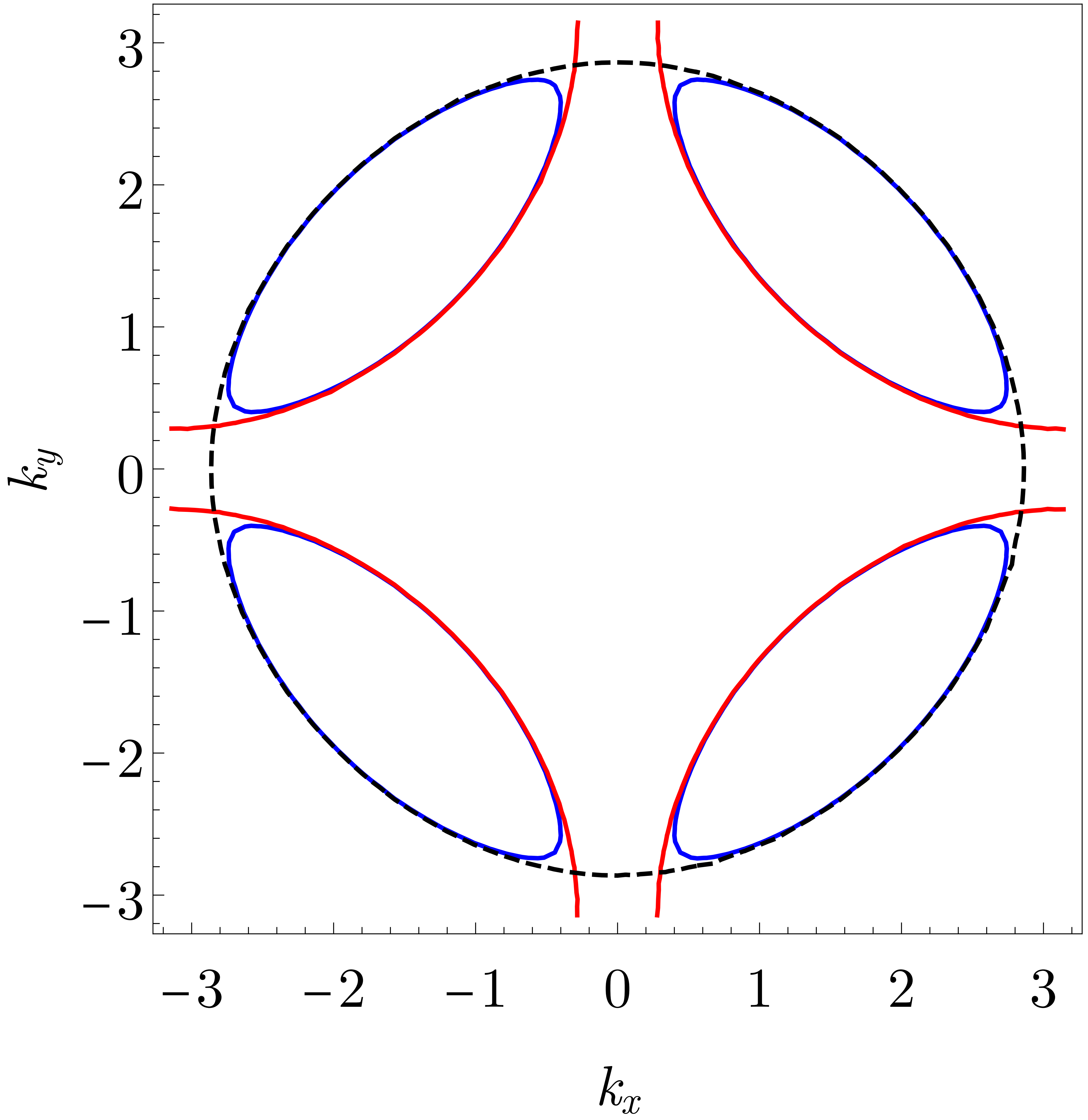
Anti-node: $k_y = \pi$ Node: $k_y = \pi - 1$



Electronic dispersion in the PDW

Spin Density Wave





Electronic dispersion in the SDW

FL*

- Recent evidence for a FL* phase in a Kondo lattice: $CeCoIn_5$ (Maksimovic *et al.*, arXiv:2011.12951, and in CePdAl, Zhao *et al.*, Nature Physics **15**, 1261 (2019). And perhaps YbB_{12} (Liu *et al.* arXiv:2102.09545)?

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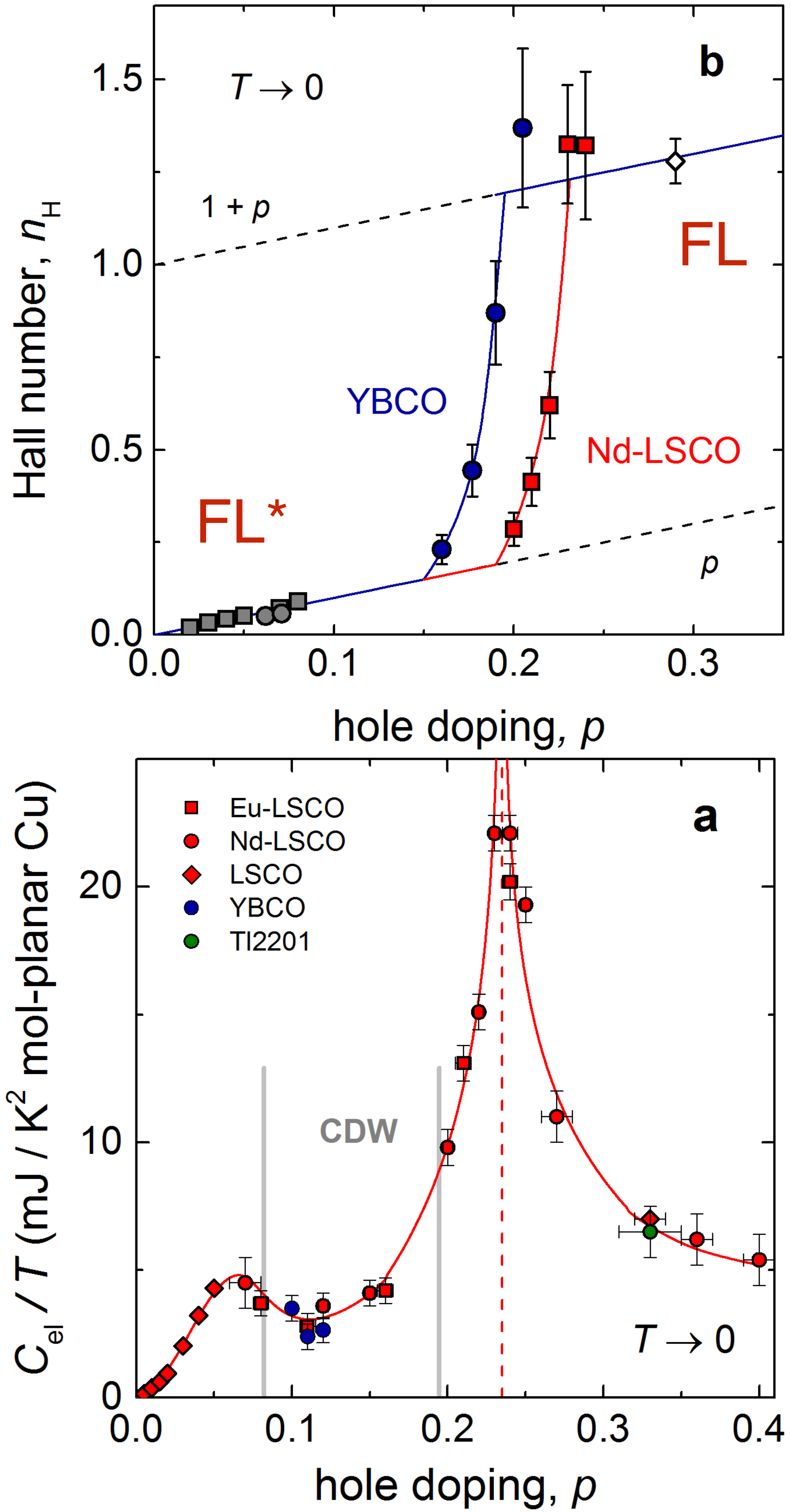
- Theory of FL-FL* transition on a single band Hubbard model: $(\mathrm{SU}(2)\times\mathrm{U}(1))/\mathbb{Z}_2$ gauge theory coupled to hybridization boson, a gauge-neutral *large* Fermi surface of electrons, and a 'ghost' Fermi surface.
  Prediction: critical 'ghost' Fermi surfaces near the transition.

Cuprates



Evidence for
ghost Fermi surfaces
in the
FL*-FL transition
in a
single-band model ?

$CeCoIn_5$