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

Condensed Matter in the City: Deep Challenges of Quantum Materials

Skye School: Foundations of Quantum Matter

London, July 1, 2021

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Talk online:
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PHYSICS

HARVARD

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

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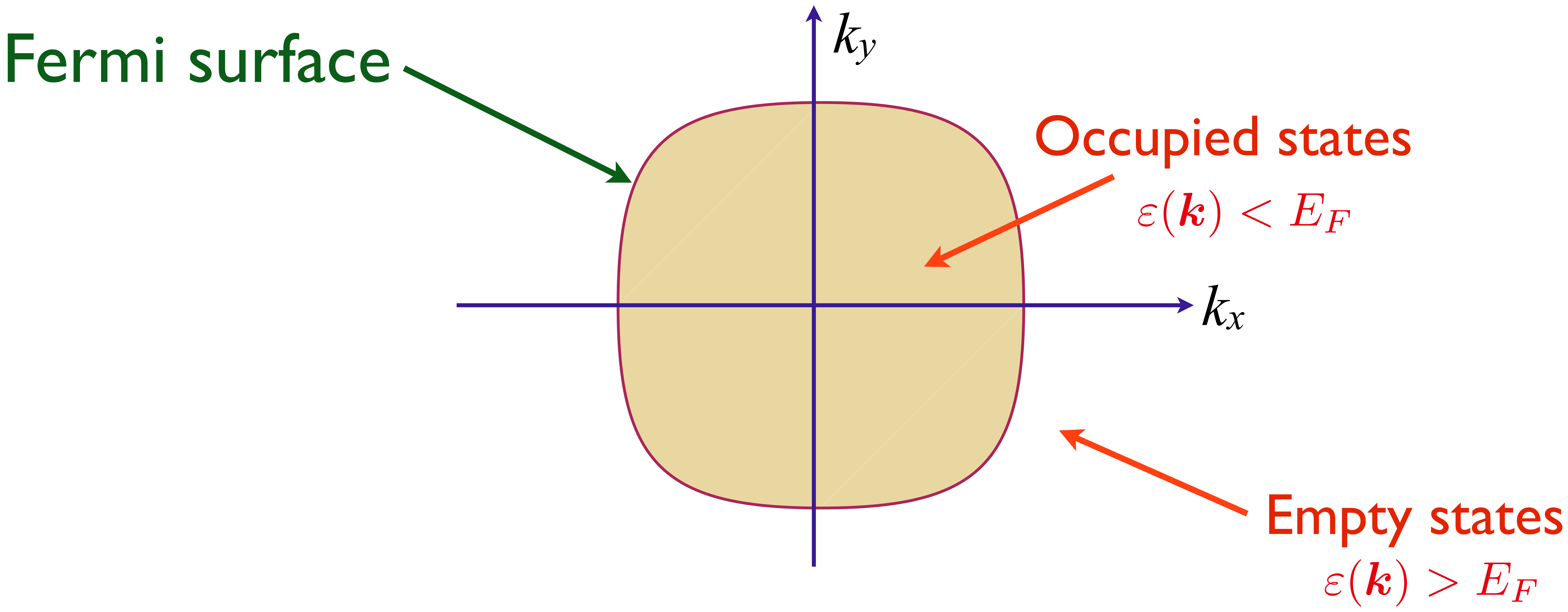
Theory of metals

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



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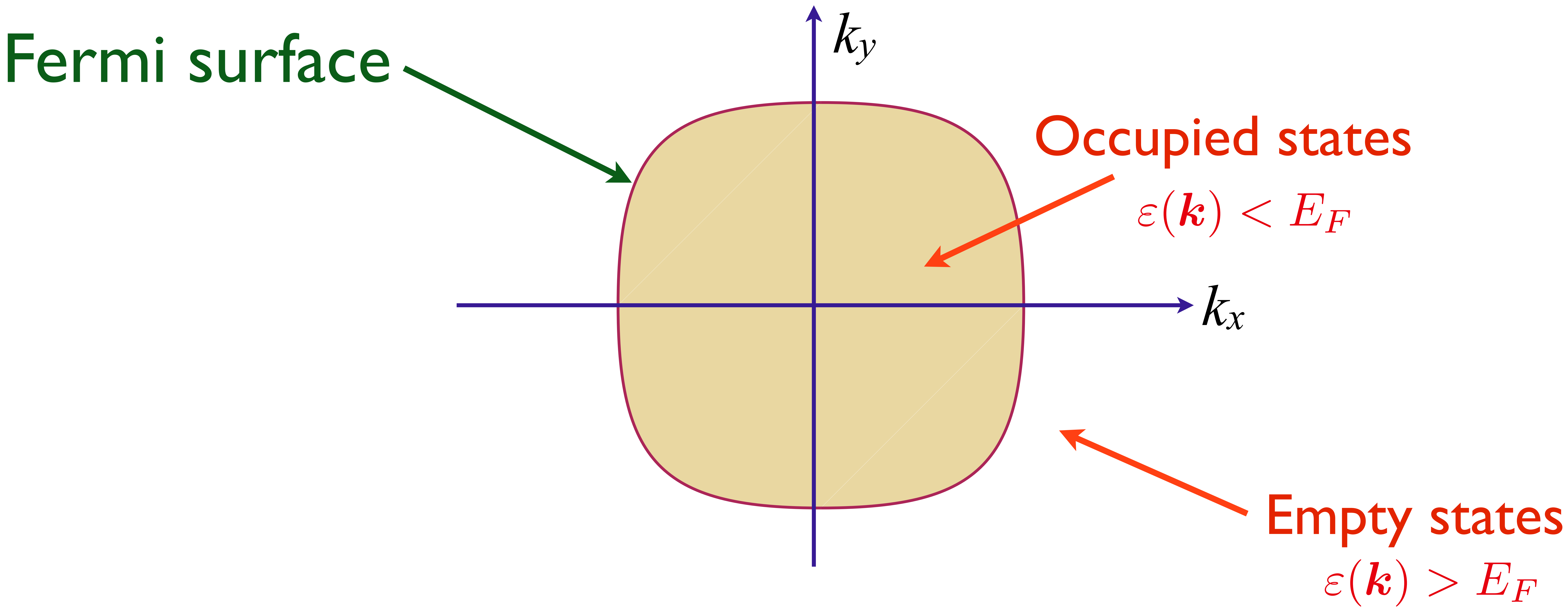

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Luttinger theorem

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$$\mathcal{L}_c = \sum_{\mathbf{p}} c^\dagger_{\mathbf{p}\sigma} \left(\frac{\partial}{\partial \tau} + \varepsilon^0_{\mathbf{p}} - \mu \right) c_{\mathbf{p}\sigma} + \text{Interactions},$$

- Continues to hold in the presence of electron-electron interactions, to all orders in perturbation theory.

- Global symmetry: $c_{\mathbf{p}\sigma} \to c_{\mathbf{p}\sigma} e^{i\theta} \quad , \quad c^\dagger_{\mathbf{p}\sigma} \to c^\dagger_{\mathbf{p}\sigma} e^{-i\theta}$

$$\rho_e = \frac{2}{V} \sum_{\mathbf{p}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G(\mathbf{p}, i\omega) e^{i\omega 0^+} \quad , \quad G(\mathbf{p}, i\omega) = \frac{1}{i\omega - \varepsilon^0_{\mathbf{p}} + \mu - \Sigma(\mathbf{p}, i\omega)}$$

$$G(\mathbf{p}, i\omega) = i \frac{\partial}{\partial \omega} \ln \left[G(\mathbf{p}, i\omega) \right] - i G(\mathbf{p}, i\omega) \frac{\partial}{\partial \omega} \Sigma(\mathbf{p}, i\omega)$$

- Frequency integral of first term yields the free particle result.

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- The vanishing of the frequency integral of the second term relies on the existence of a functional, $\Phi_{LW}\left[G(\mathbf{p}, i\omega)\right]$, of the Green's function, called the Luttinger-Wald functional, so that the self energy is its functional derivative

$$\Sigma(\mathbf{p}, i\omega) = \frac{\delta \Phi_{LW}}{\delta G(\mathbf{p}, i\omega)} \quad \text{and} \quad \Phi\left[G(\mathbf{p}, i\omega + i\omega_0)\right] = \Phi\left[G(\mathbf{p}, i\omega)\right]$$

- Note that frequency shift by ω_0 is equivalent to a time-dependent U(1) symmetry transformation $c_{\mathbf{p}} \rightarrow c_{\mathbf{p}} e^{+i\omega_0 \tau}$, $c^\dagger_{\mathbf{p}} \rightarrow c^\dagger_{\mathbf{p}} e^{-i\omega_0 \tau}$

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There is a Luttinger constraint associated with every U(1) symmetry, provided the U(1) is not broken in the ground state.

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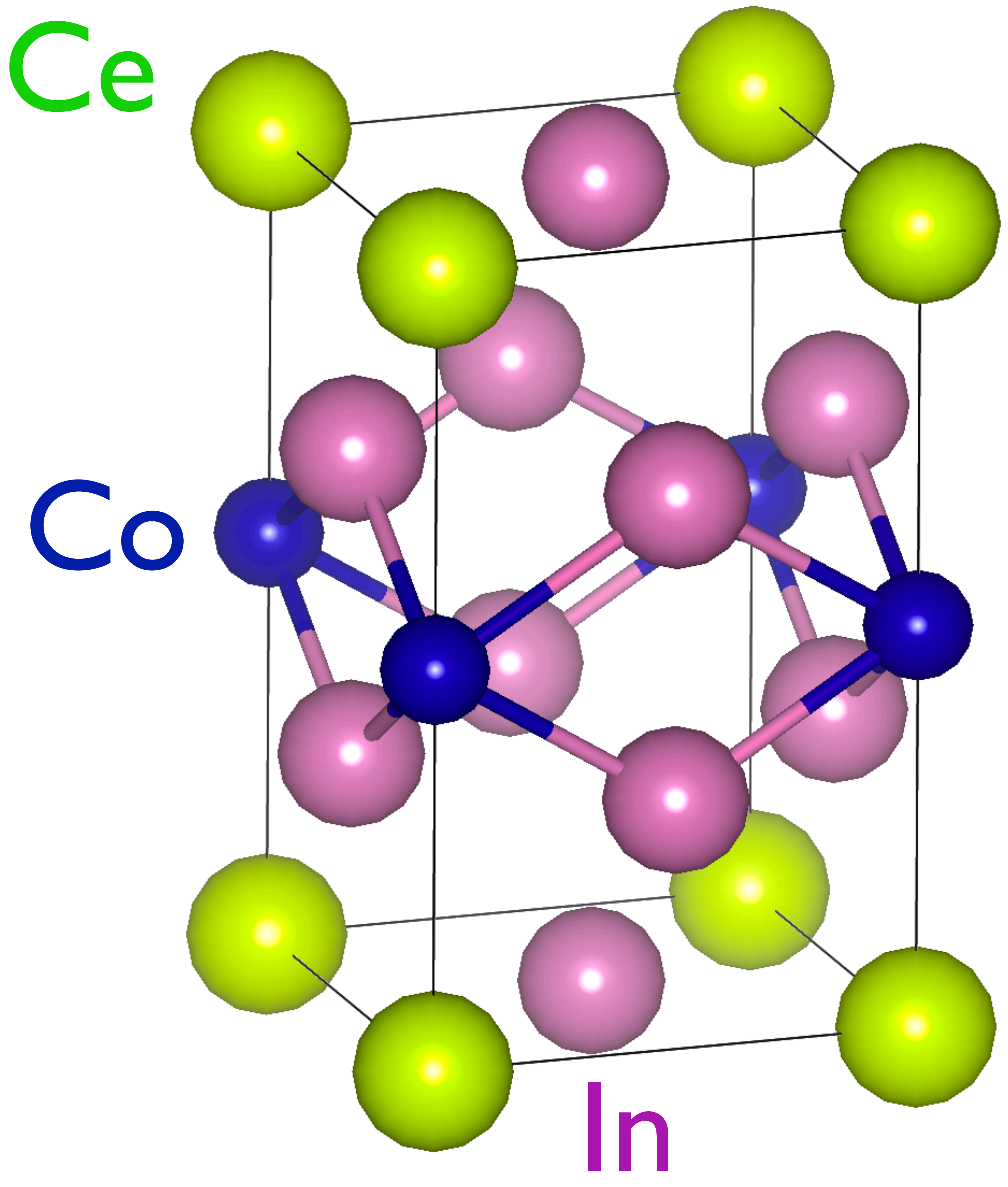

Strong on-site repulsion *U* only on Ce sites

$CeCoIn_5$

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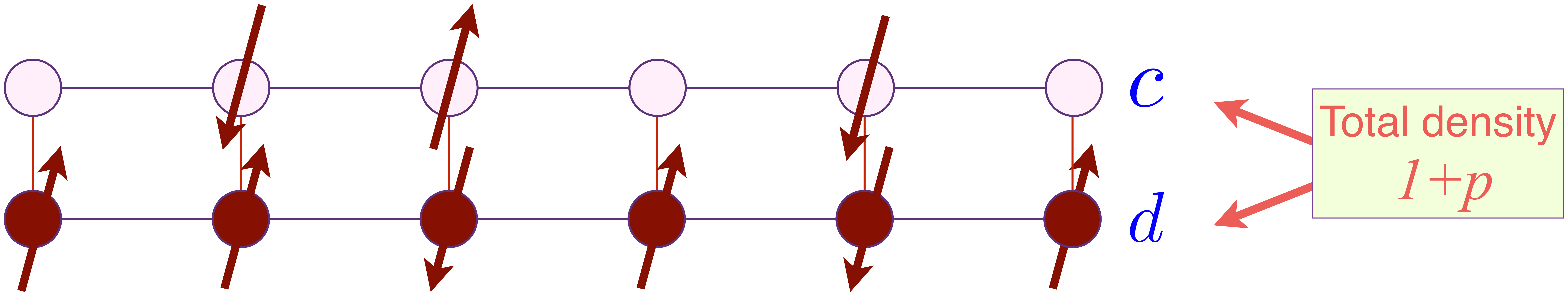

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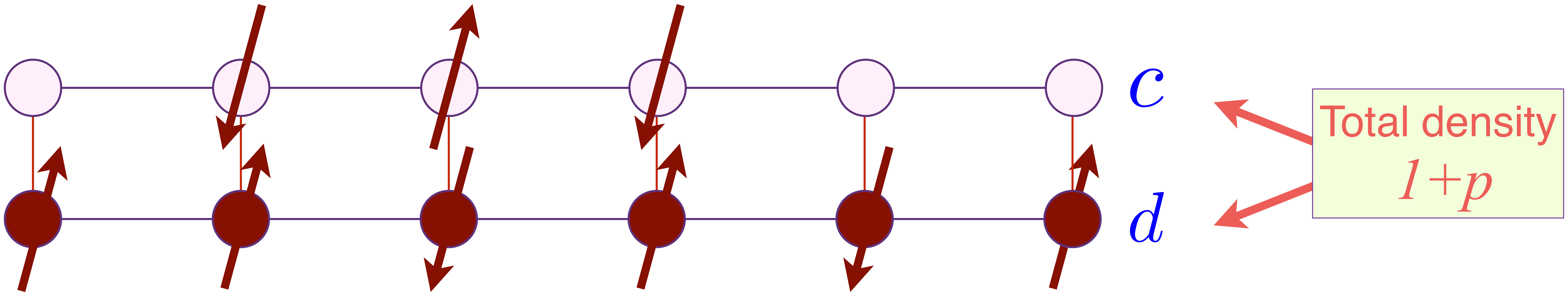

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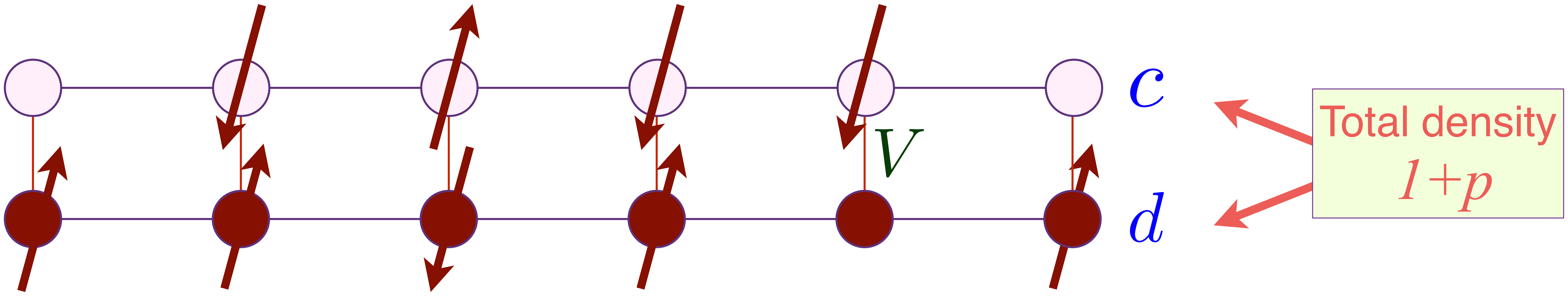

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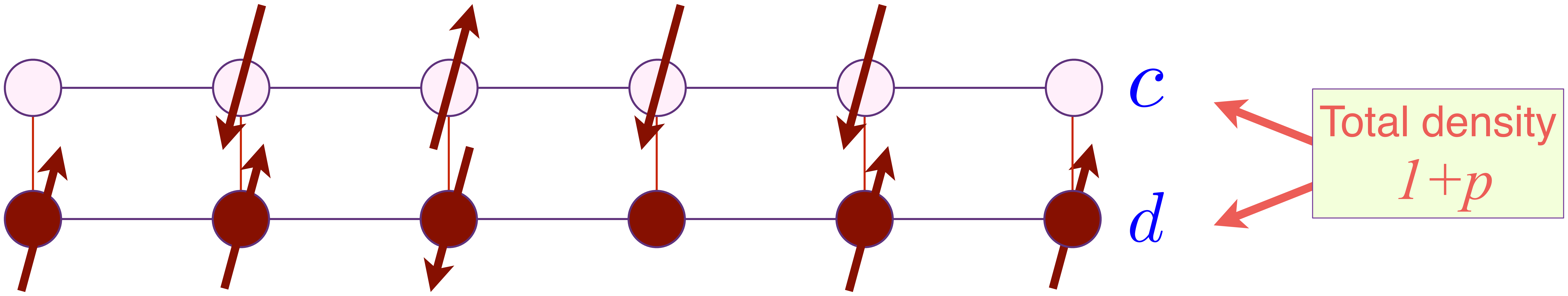

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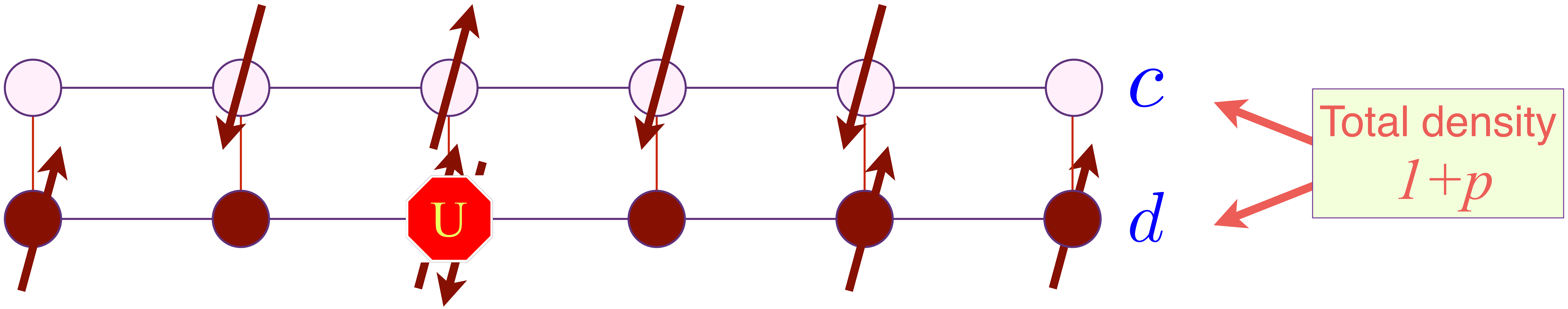

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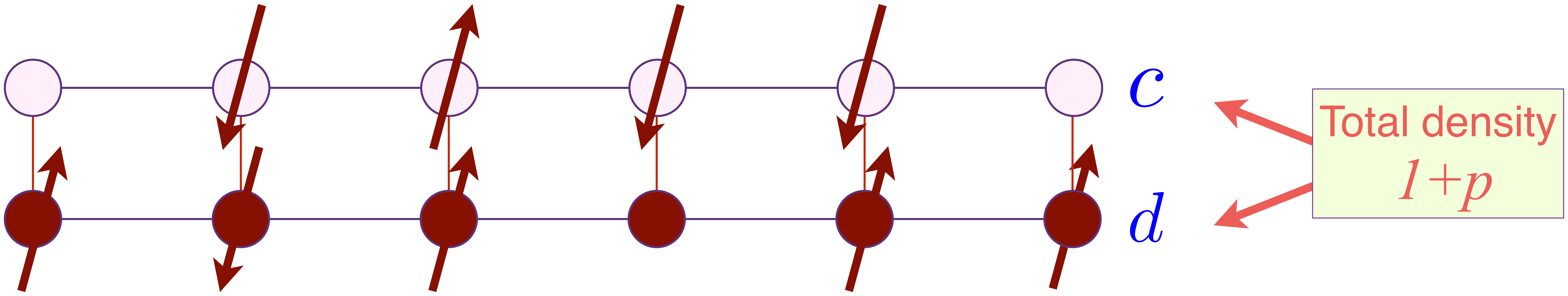

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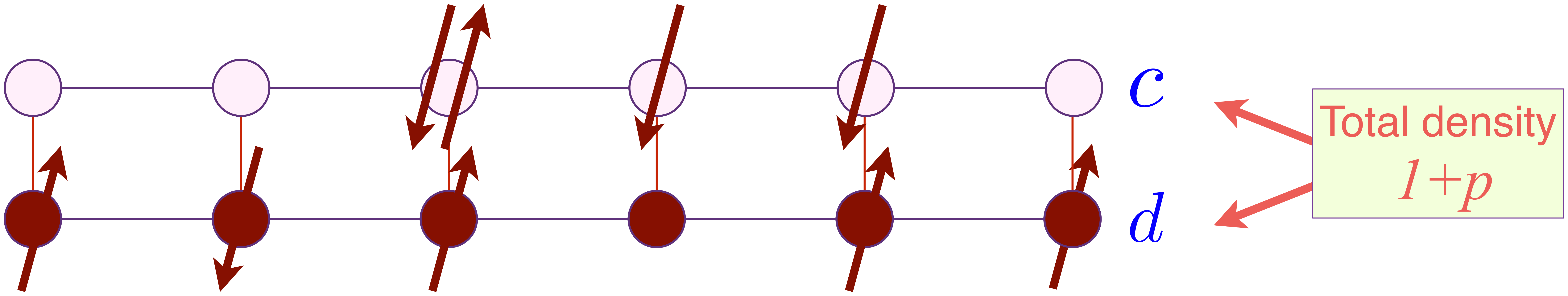

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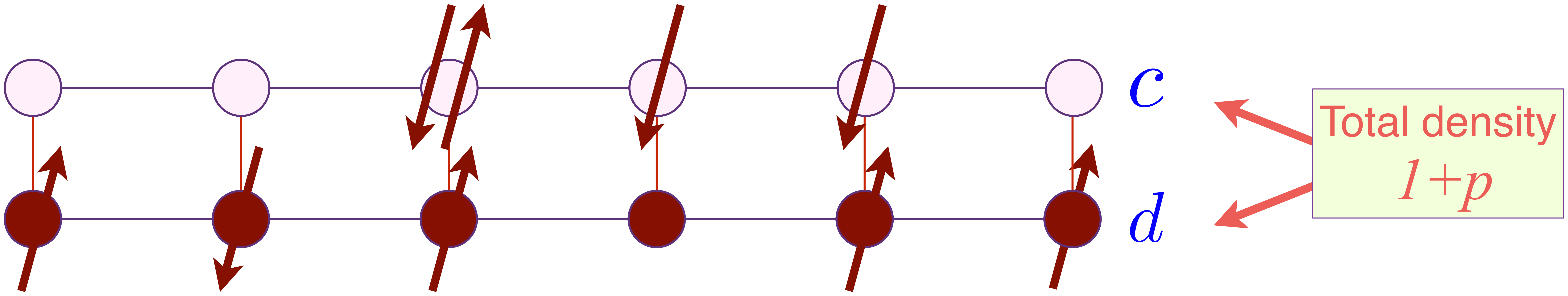

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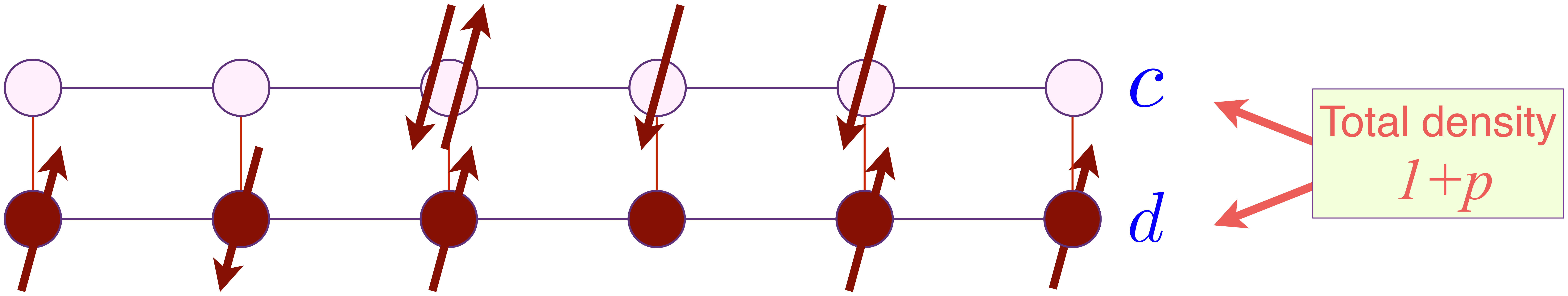

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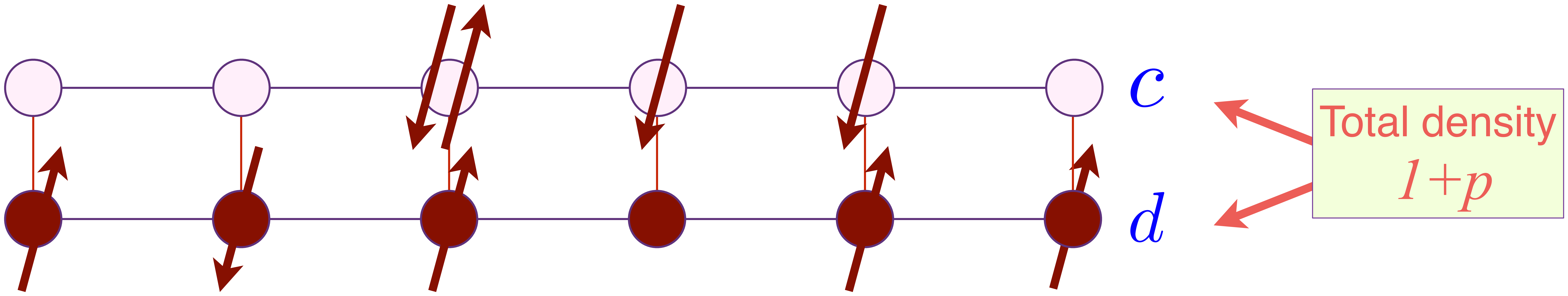
- No fundamental change in the ground state as $U \to \infty$, apart from a large effective mass renormalization of quasiparticles $m^*/m \sim \exp(c_1 U)$. This yields the theory of a heavy fermi liquid (HFL), which has been applied with success to f-electron intermetallics.

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



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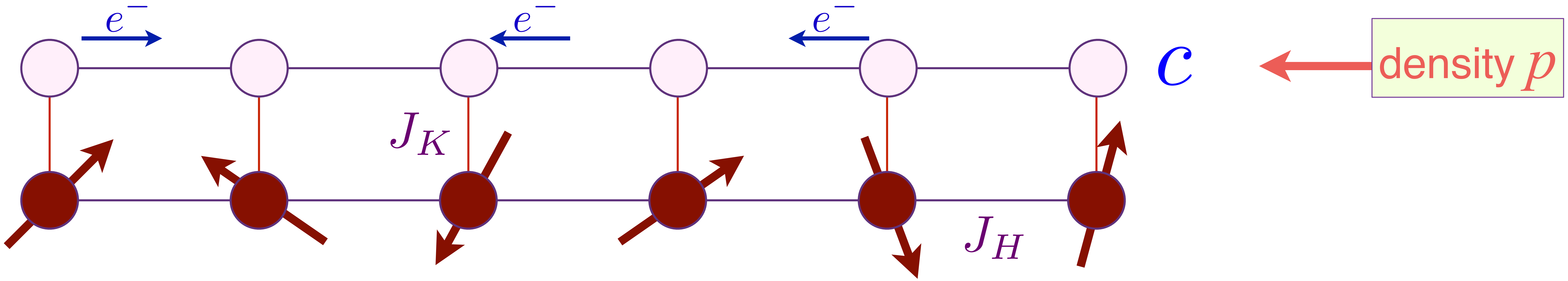
- Obtained from $\mathcal{H}_{AL}$ by a Schrieffer-Wolff canonical transformation with $J_K \sim V^2/U$ and $J_H \sim t_d^2/U$. Now the d-band consists only of spin degrees of freedom, or ‘qubits’.

Kondo lattice



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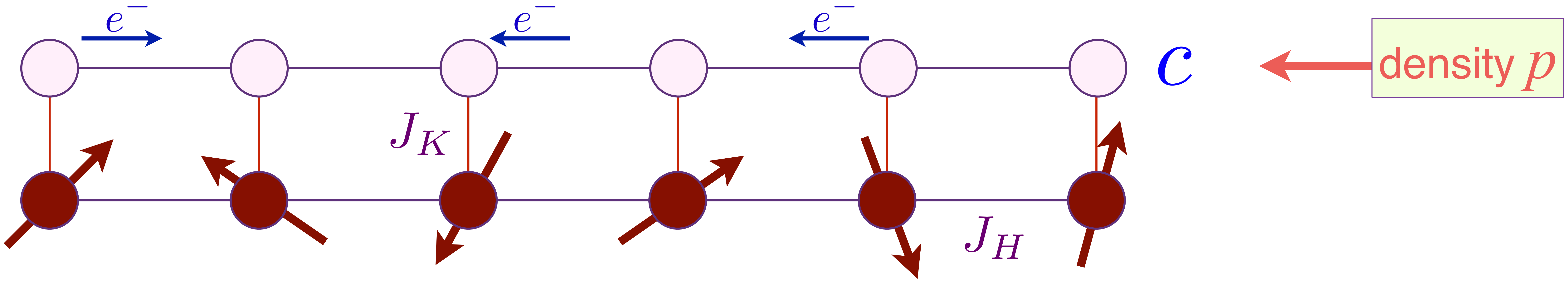

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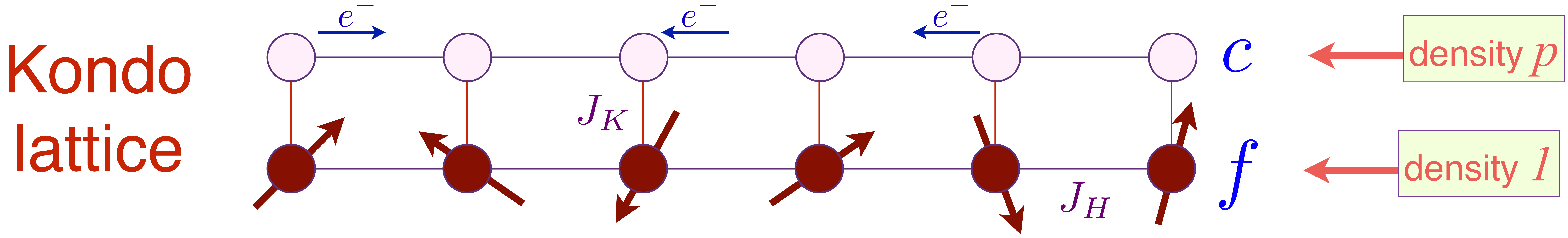
Varma, Yafet, Coleman, Read, Newns, Millis, P.A. Lee, Auerbach, Levin



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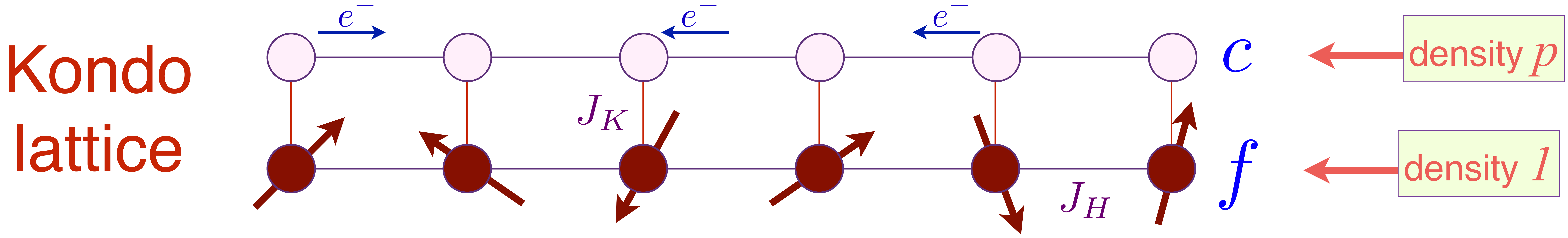
- Variational wavefunction for HFL with 'large' Fermi surface of size $1 + p$: $|\text{HFL}\rangle = [\text{Projection onto one } f \text{ per site}] \bowtie |\text{Slater determinant of } (c, f)\rangle$

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



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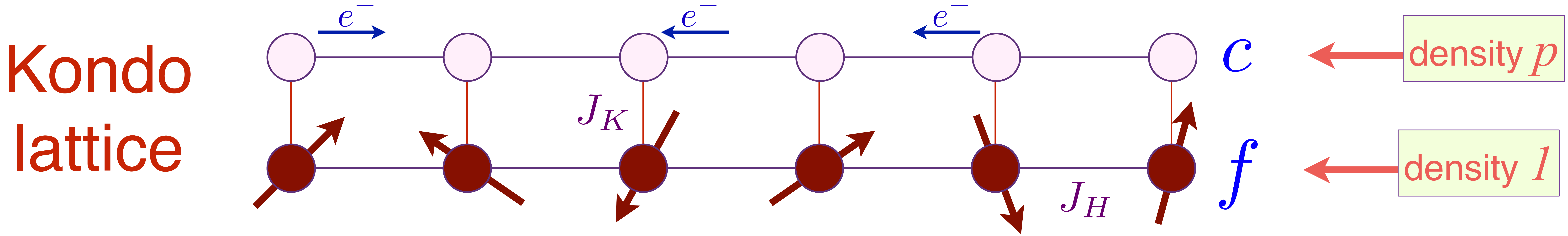

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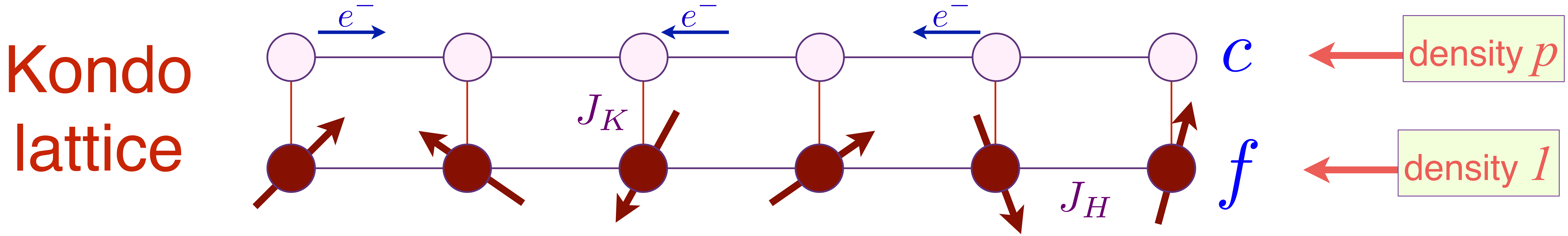

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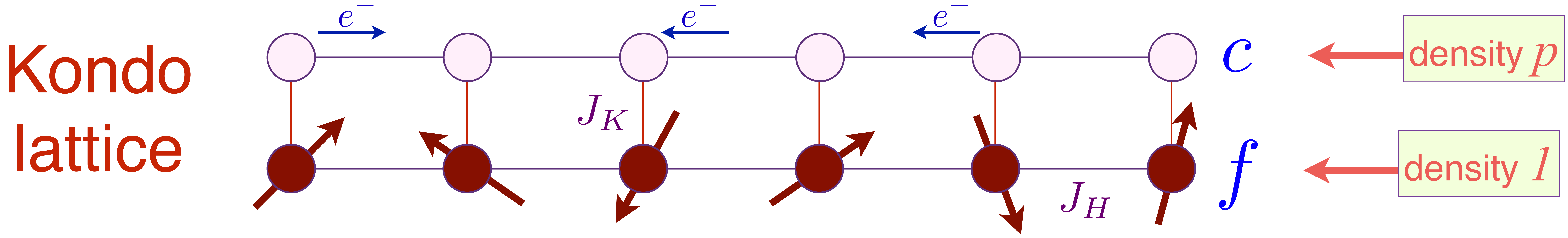

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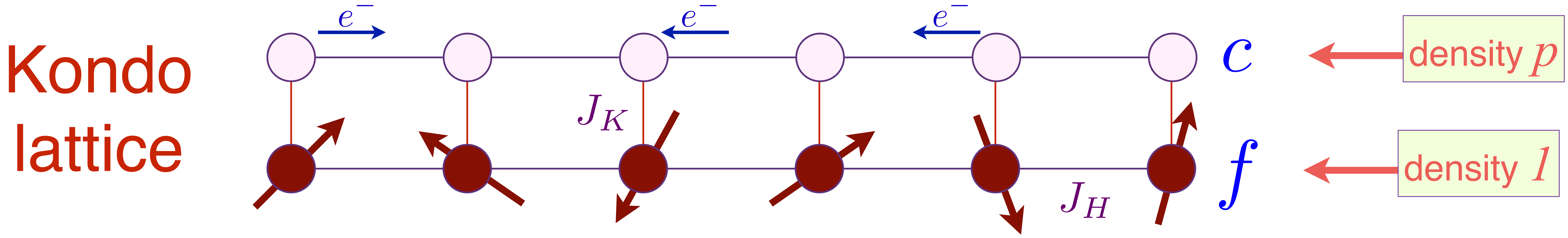

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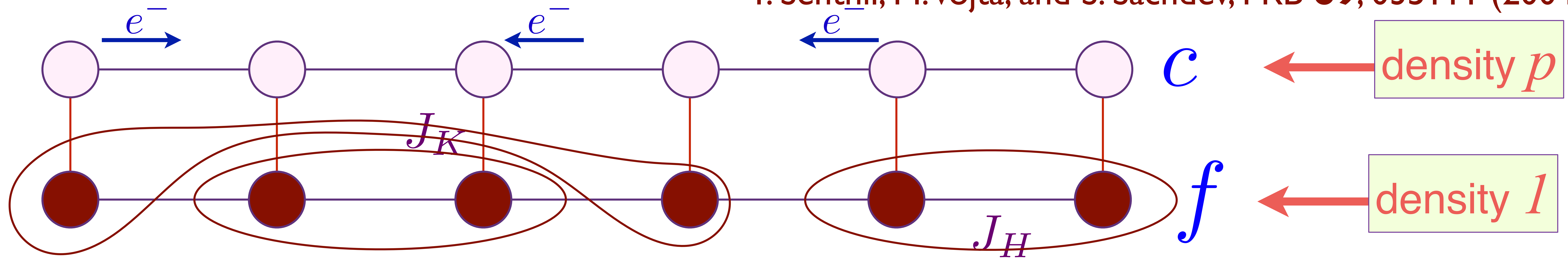
- FL*: The $\mathrm{U}(1)_{\mathrm{gauge}} \times \mathrm{U}(1)$ symmetry is unbroken (or broken to $\mathbb{Z}_{2,\mathrm{gauge}} \times \mathrm{U}(1)$).

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

Kondo lattice



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

- FL*: The $\mathrm{U}(1)_{\mathrm{gauge}} \times \mathrm{U}(1)$ symmetry is unbroken (or broken to $\mathbb{Z}_{2,\mathrm{gauge}} \times \mathrm{U}(1)$).
- The unbroken gauge symmetry requires the presence of fractionalized spinons and emergent gauge fields *i.e.* a spin-liquid sector.

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

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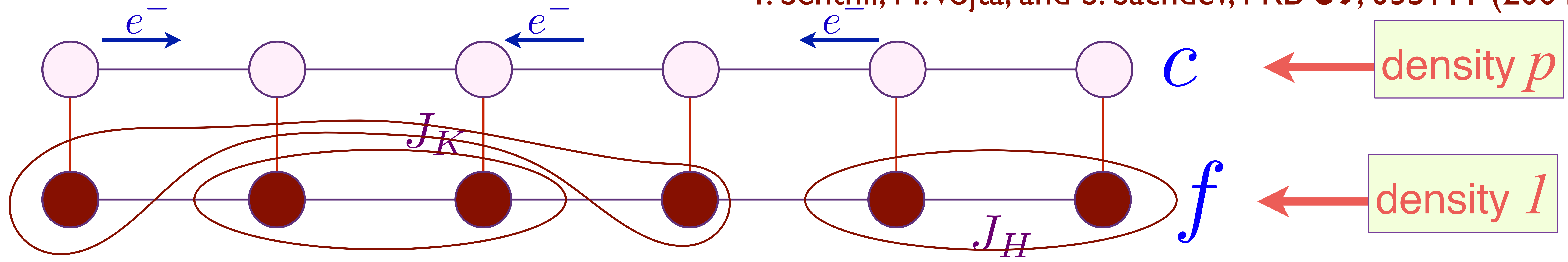

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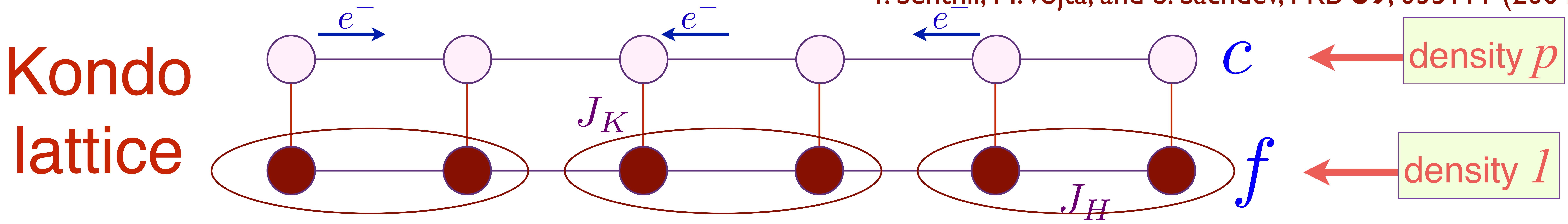

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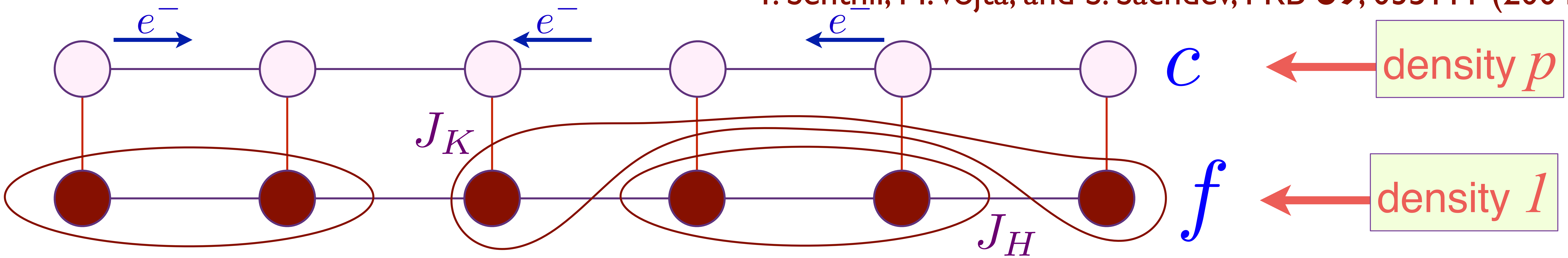

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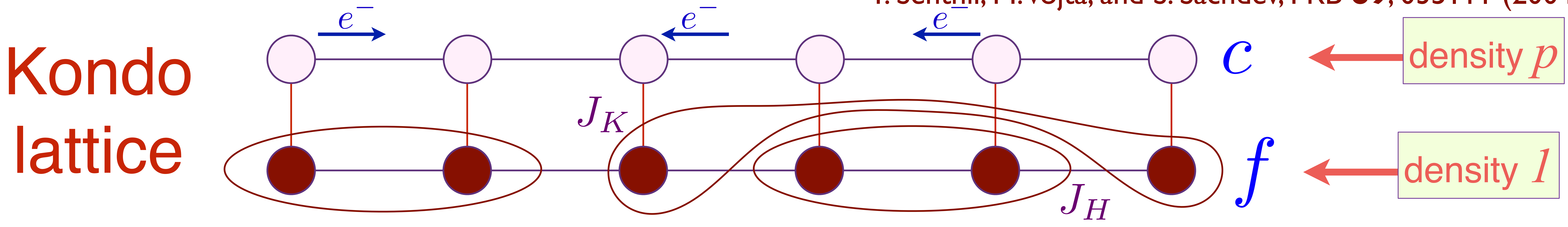

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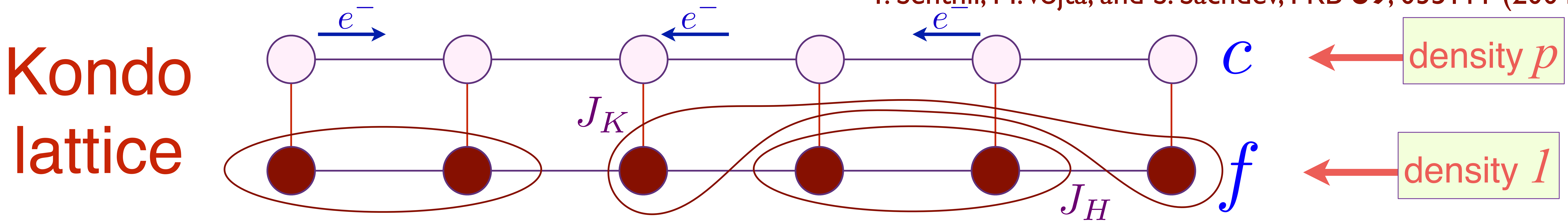
- The Luttinger arguments applied to $\mathrm{U}(1)_{\mathrm{gauge}}$ lead to 'symmetry enriched topological (SET)' or 'symmetry fractionalization' constraints on the spin liquid sector.

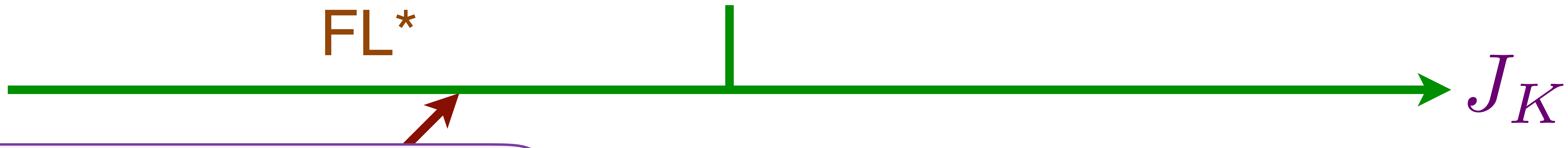
P. Bonderson, M. Cheng, K. Patel, E. Plamadeala, arXiv:1601.07902

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



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

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

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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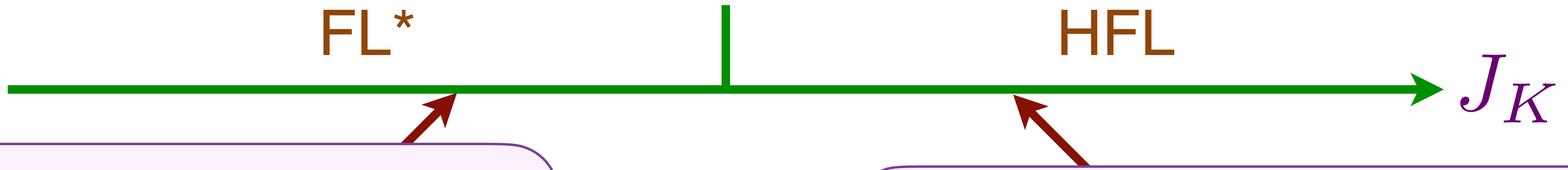

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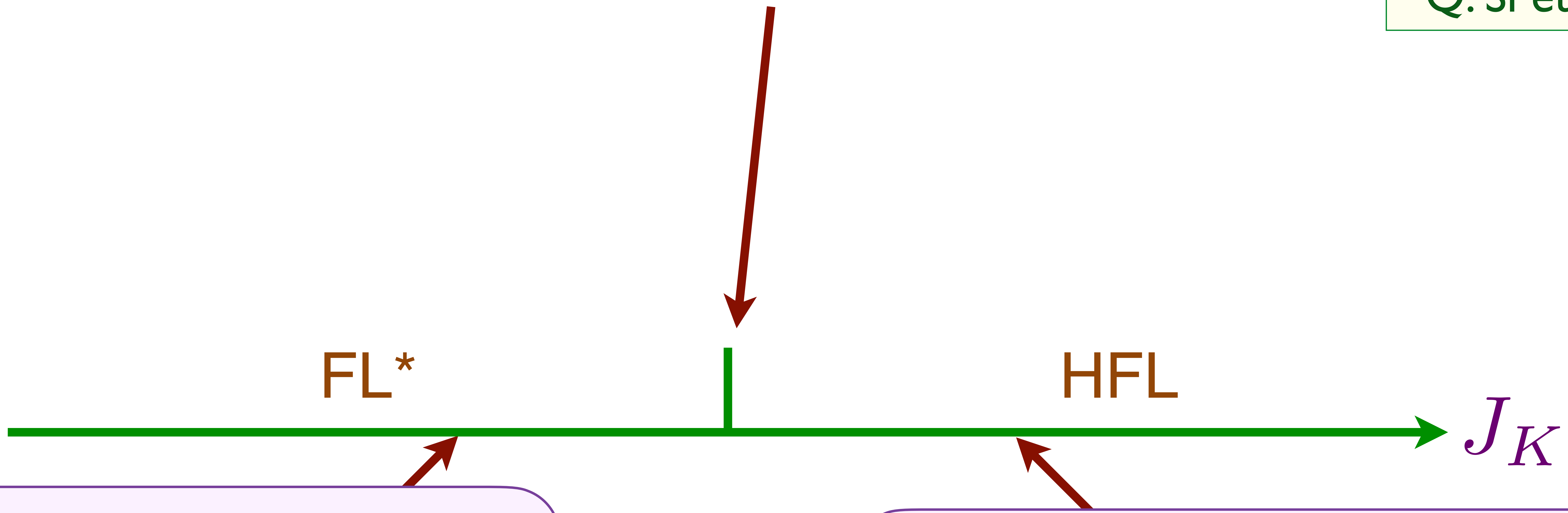
A. Sengupta (2000)
Q. Si et al. (2001)

Kondo-breakdown transition



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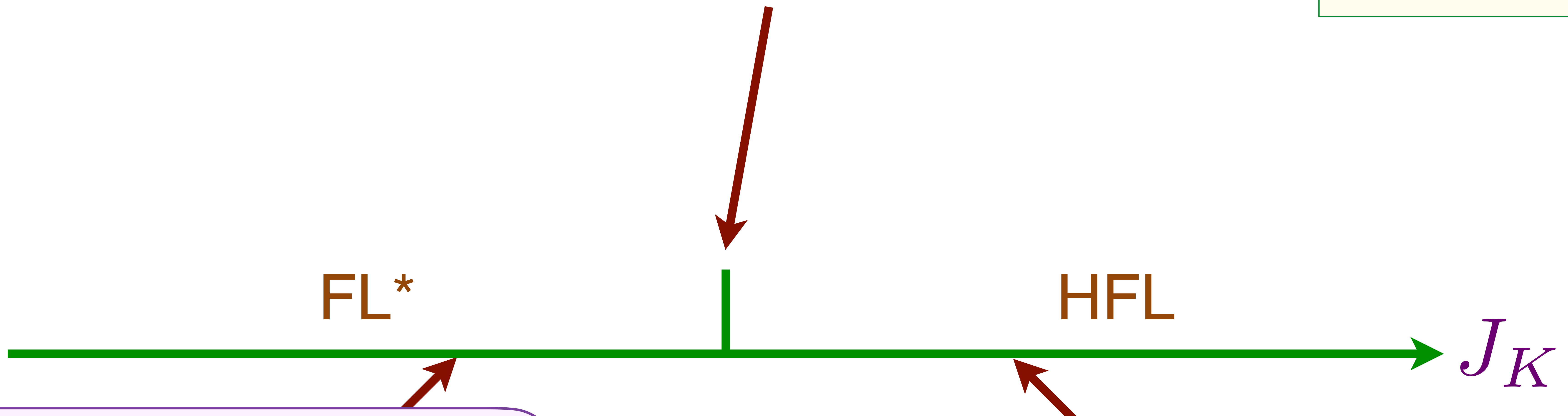
Kondo-breakdown transition
'Selective Mott' transition

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



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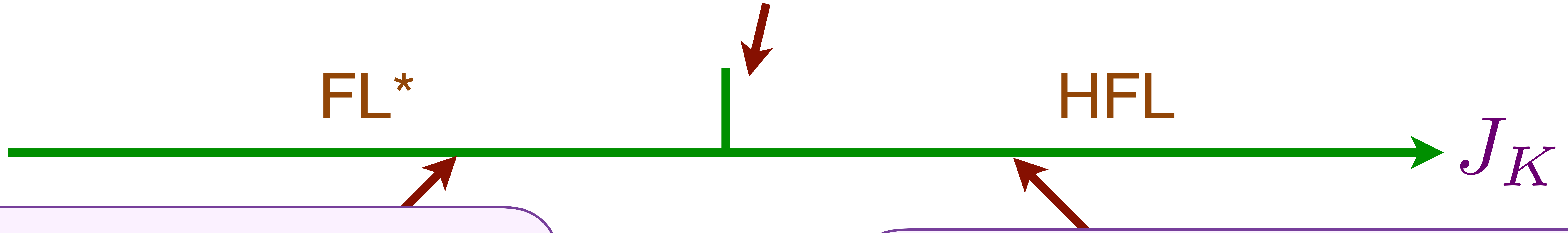
T. Senthil, M. Vojta, and S. Sachdev, PRB **69**, 035111 (2004)

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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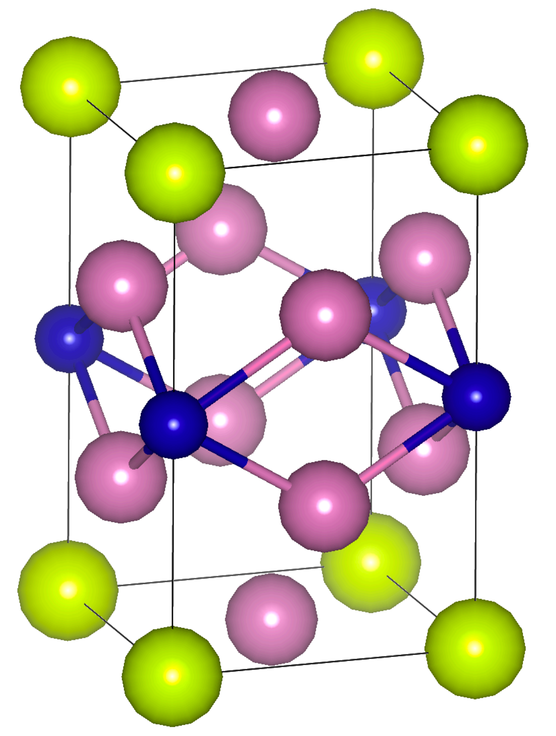
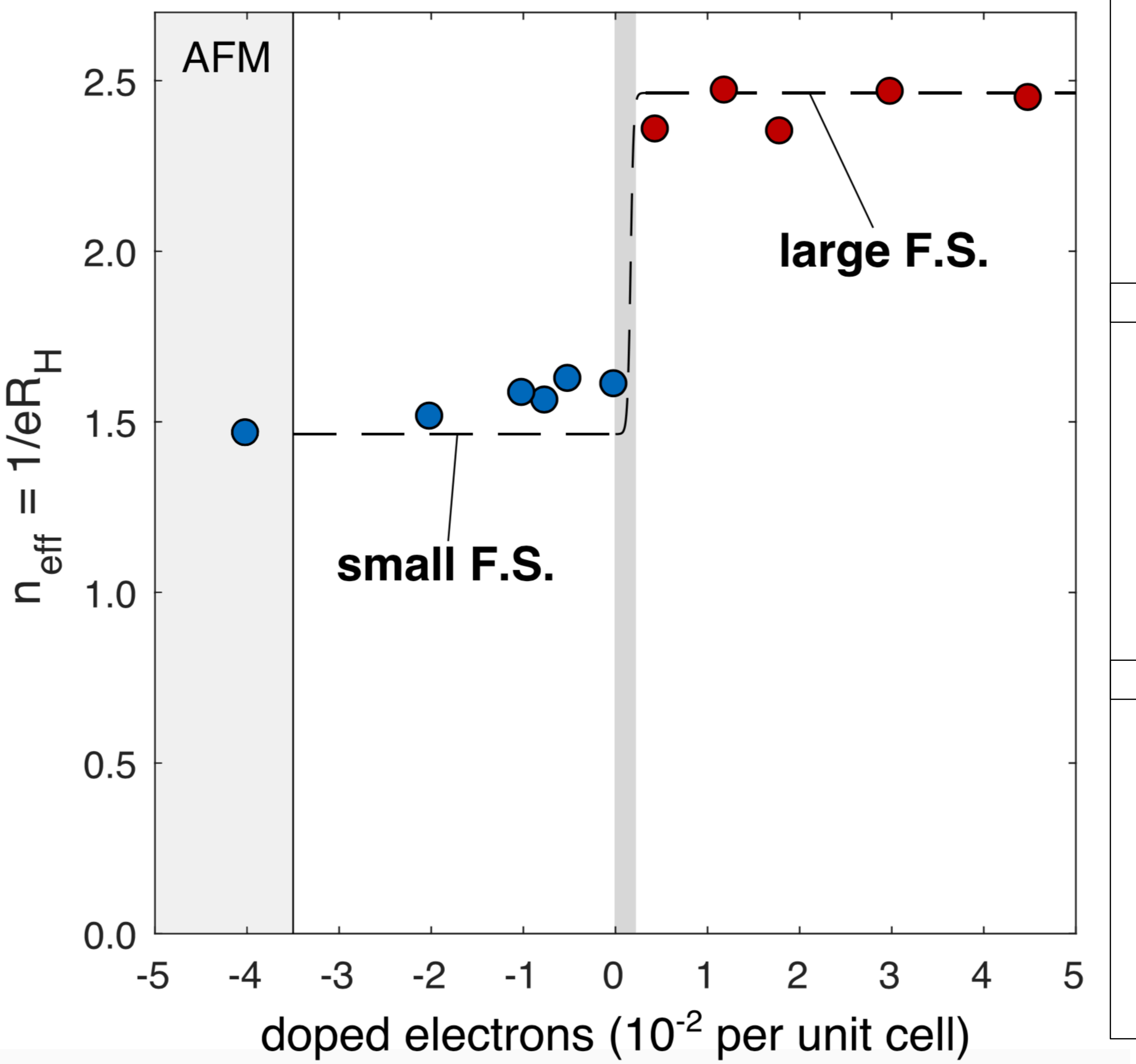
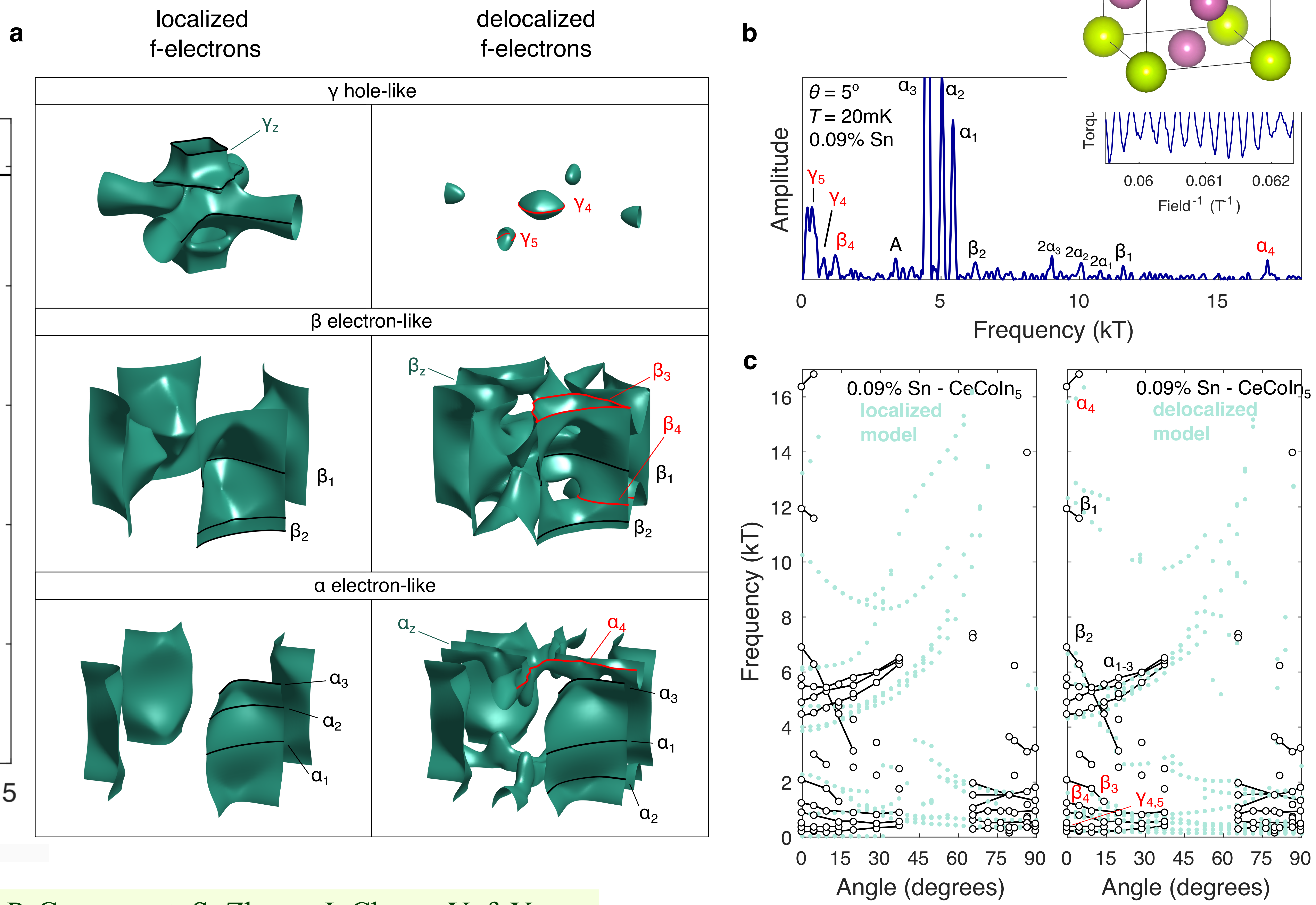


arXiv:2011.12951





See also H. Zhao, J. Zhang, M. Lyu, S. Bachus, Y. Tokiwa, P. Gegenwart, S. Zhang, J. Cheng, Y.-f. Yang, G. Chen, Y. Isikawa, Q. Si, F. Steglich, and P. Sun, Nature Physics 15, 1261 (2019) for CePdAl

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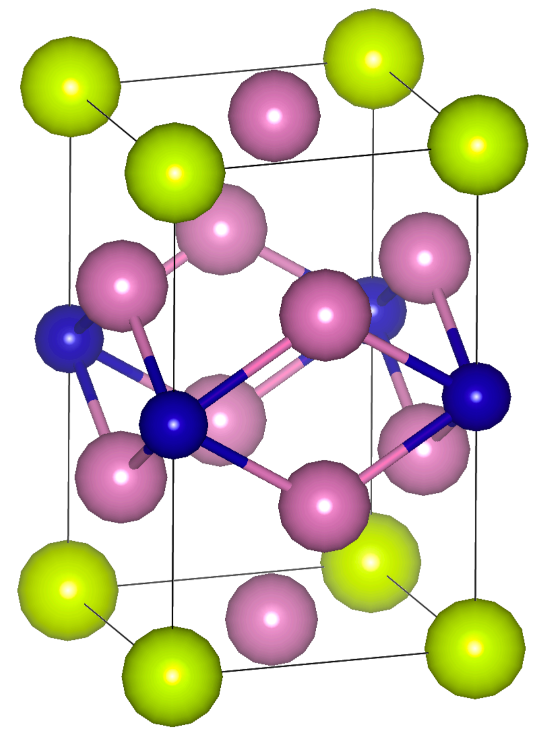
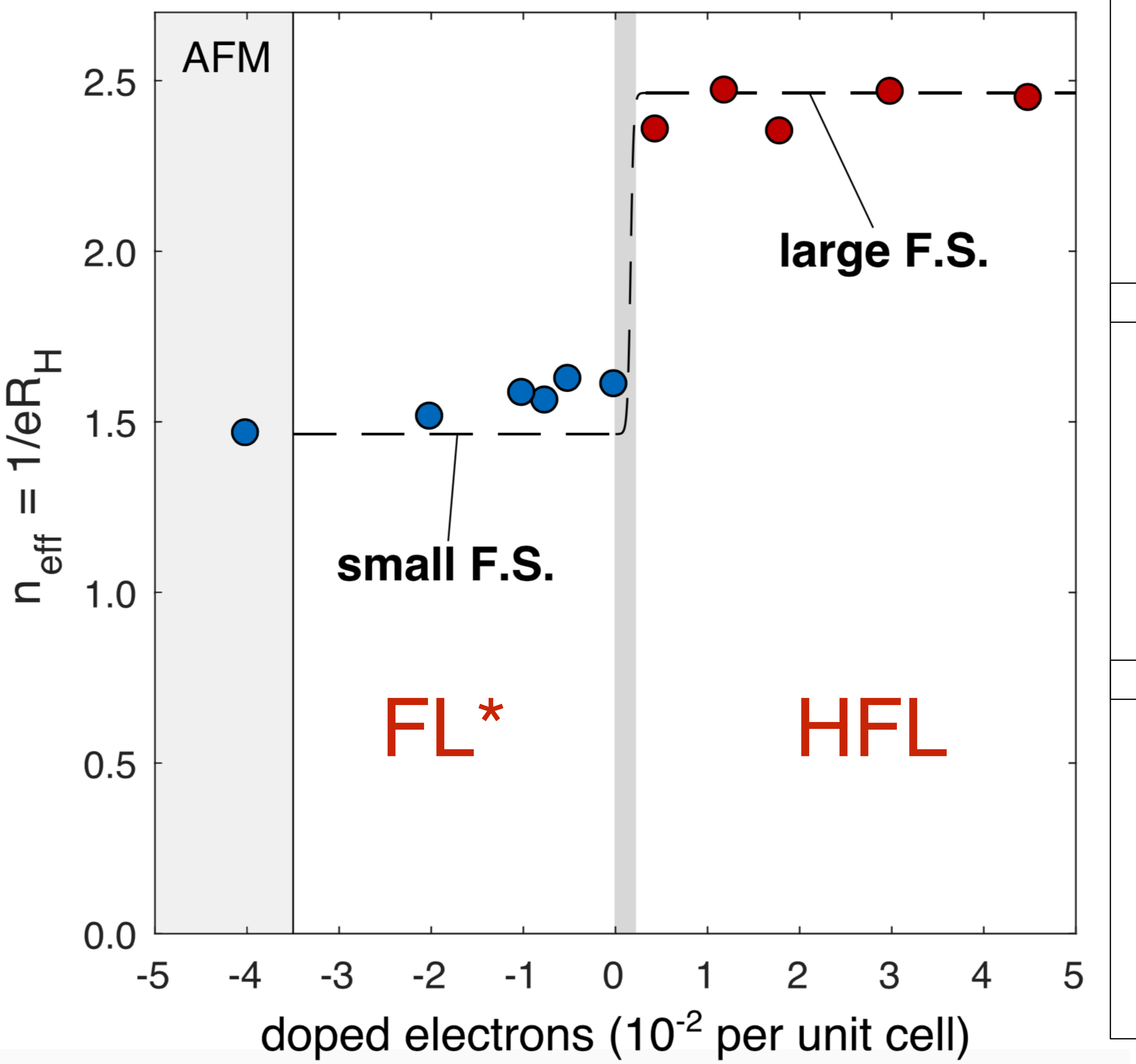
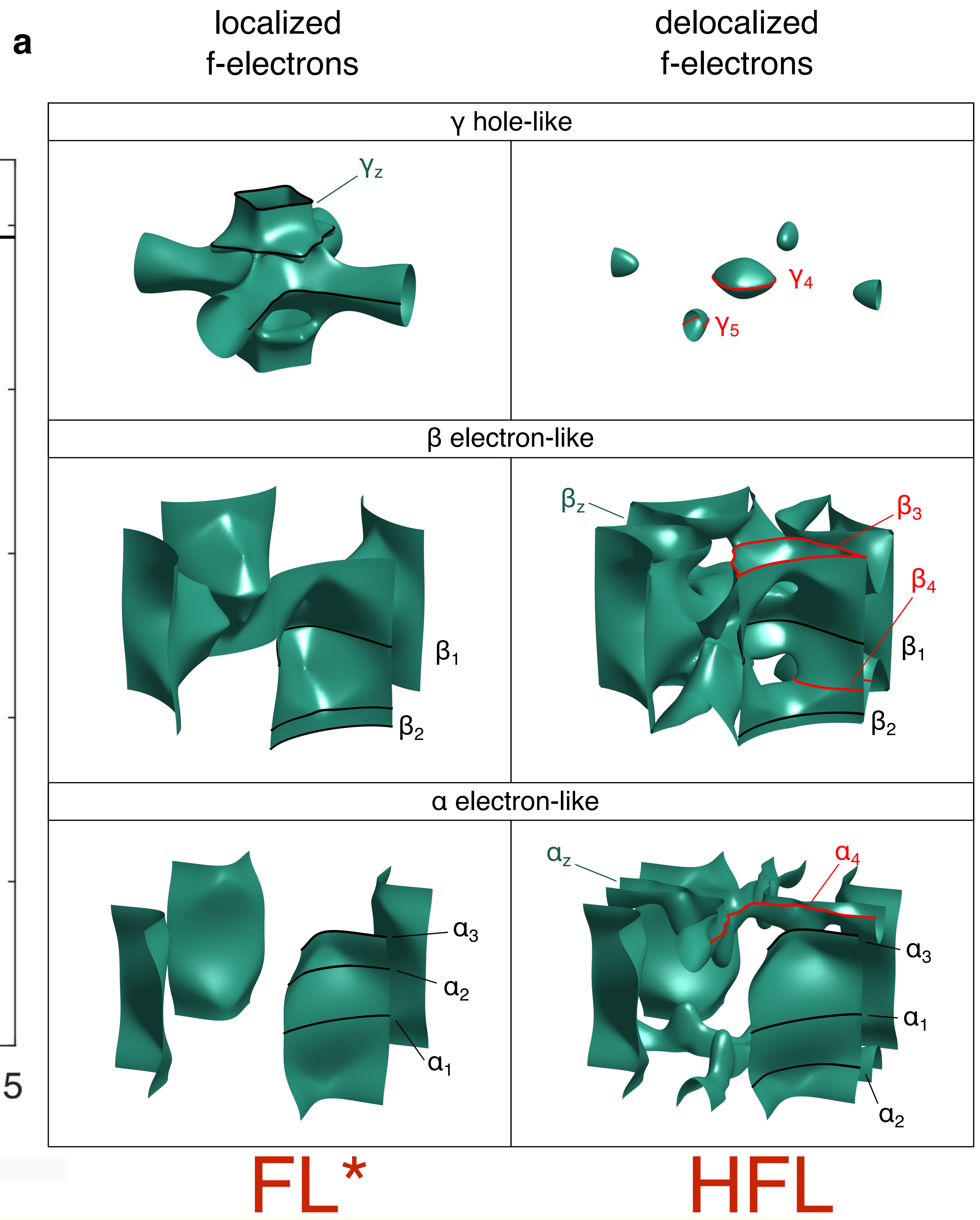
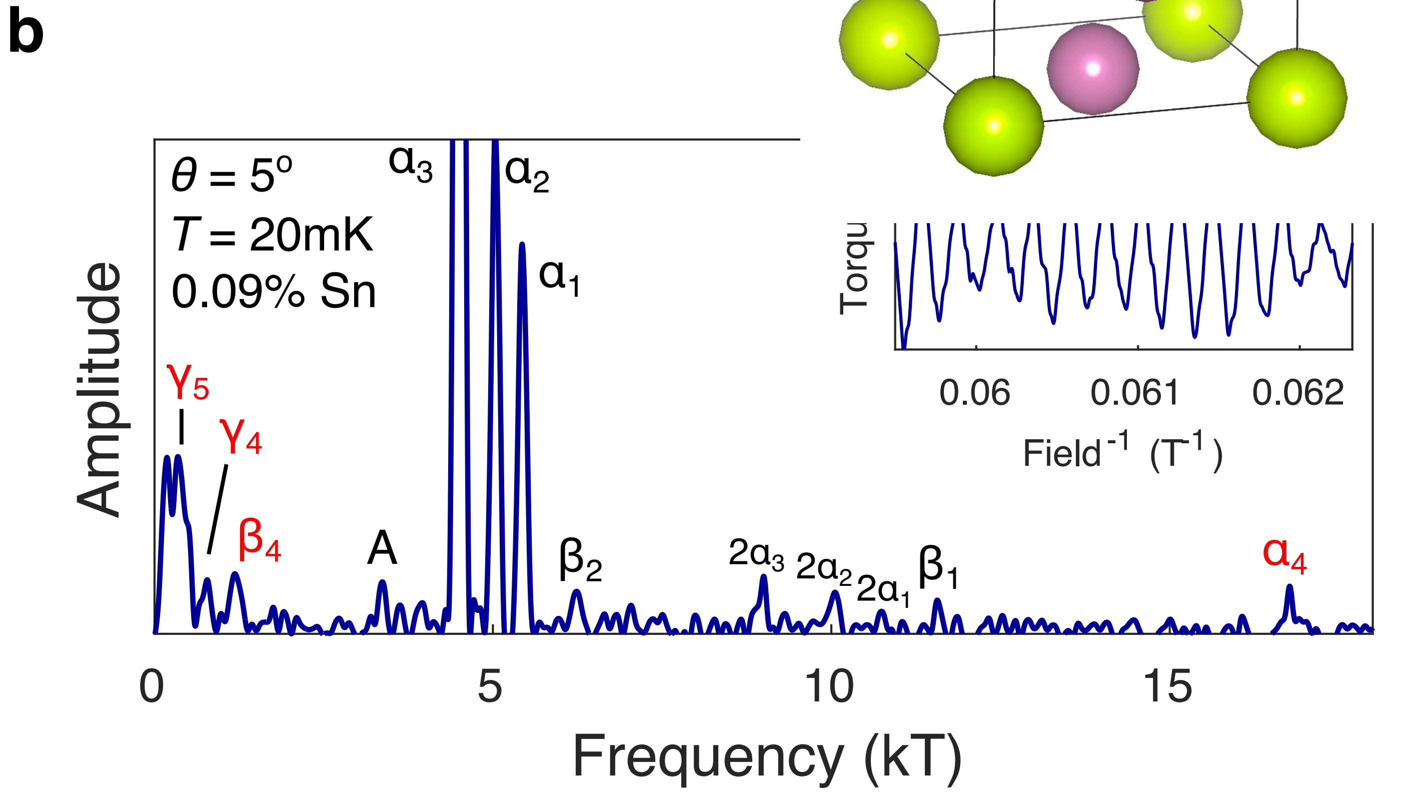
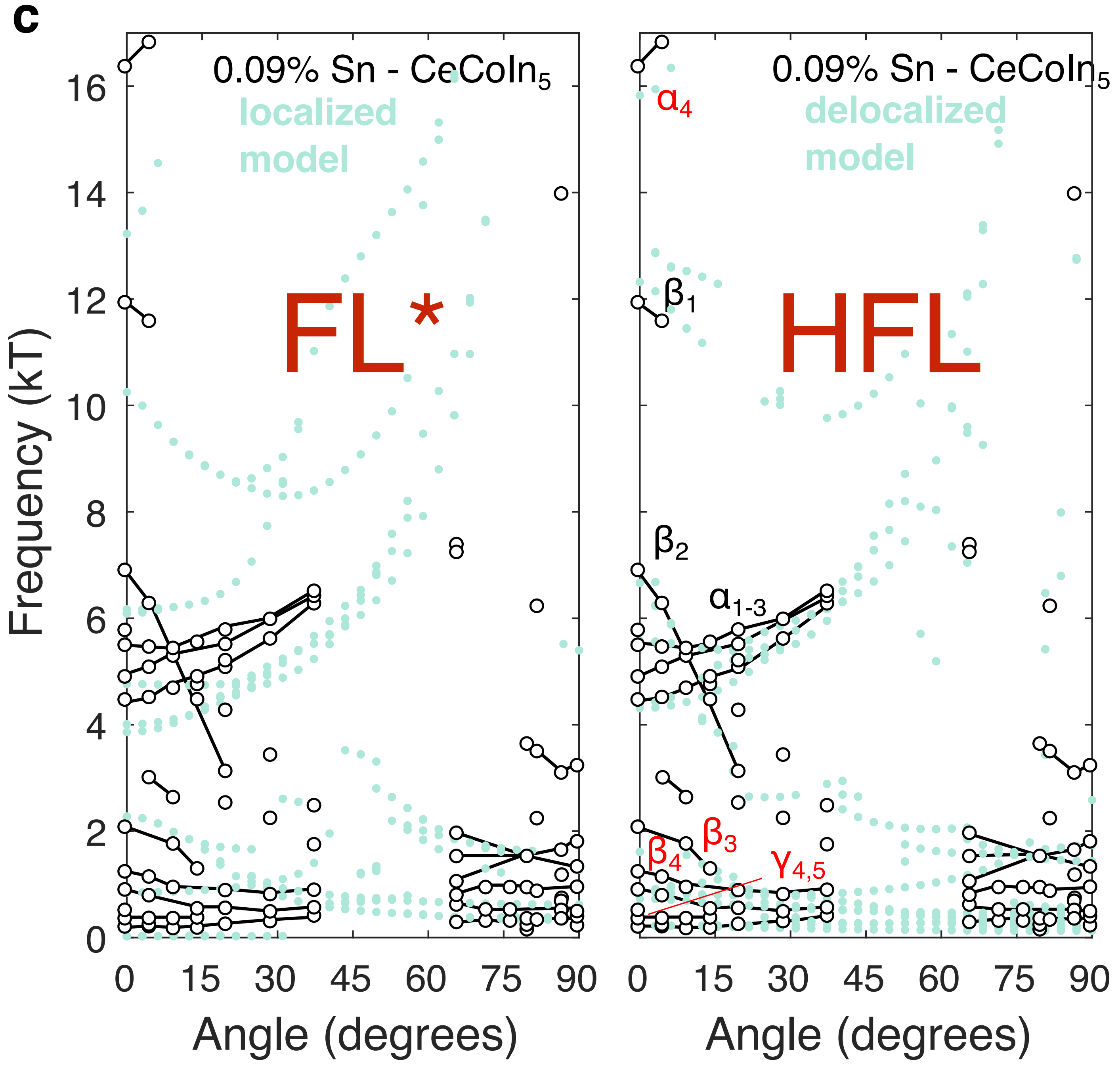


arXiv:2011.12951









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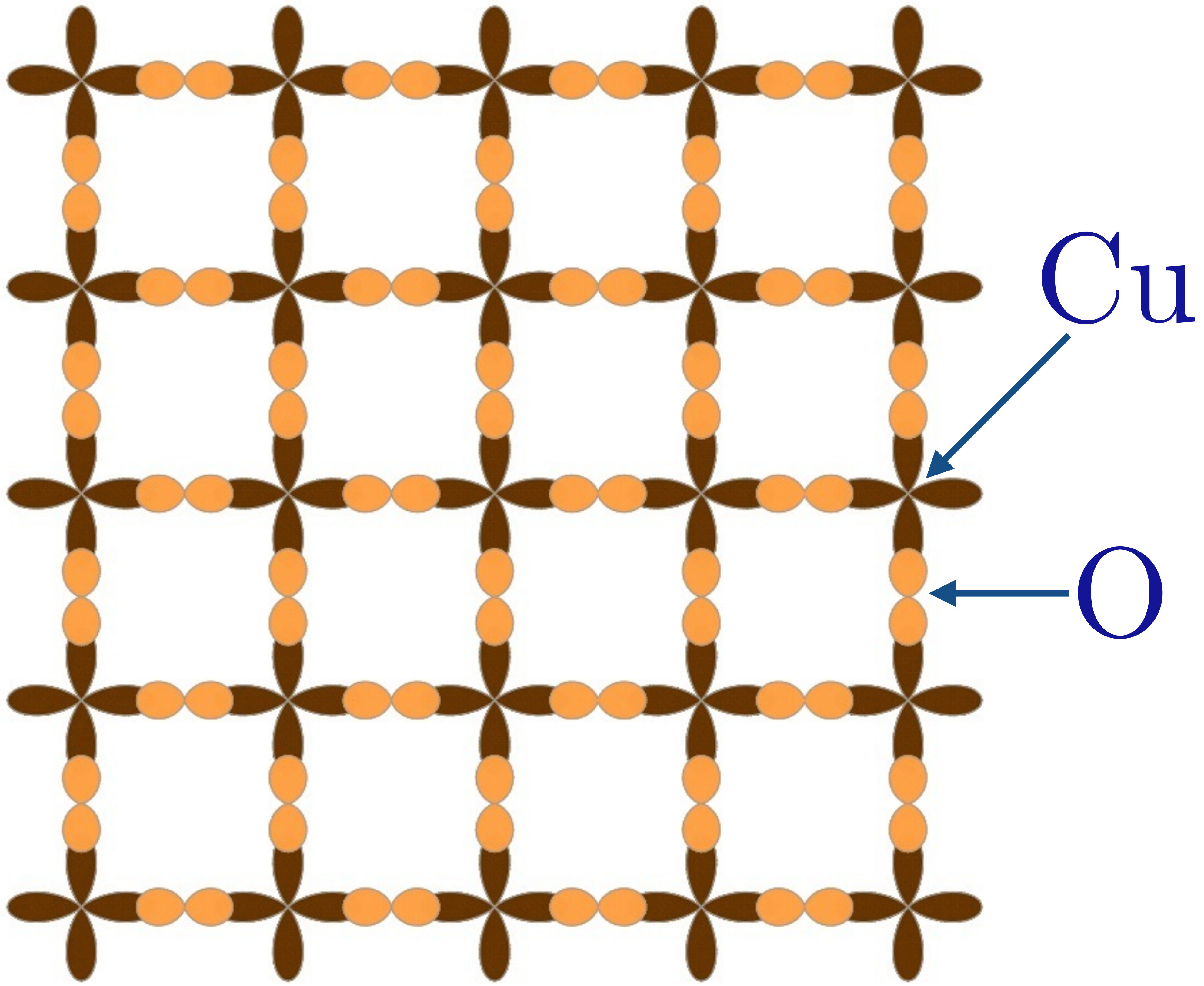
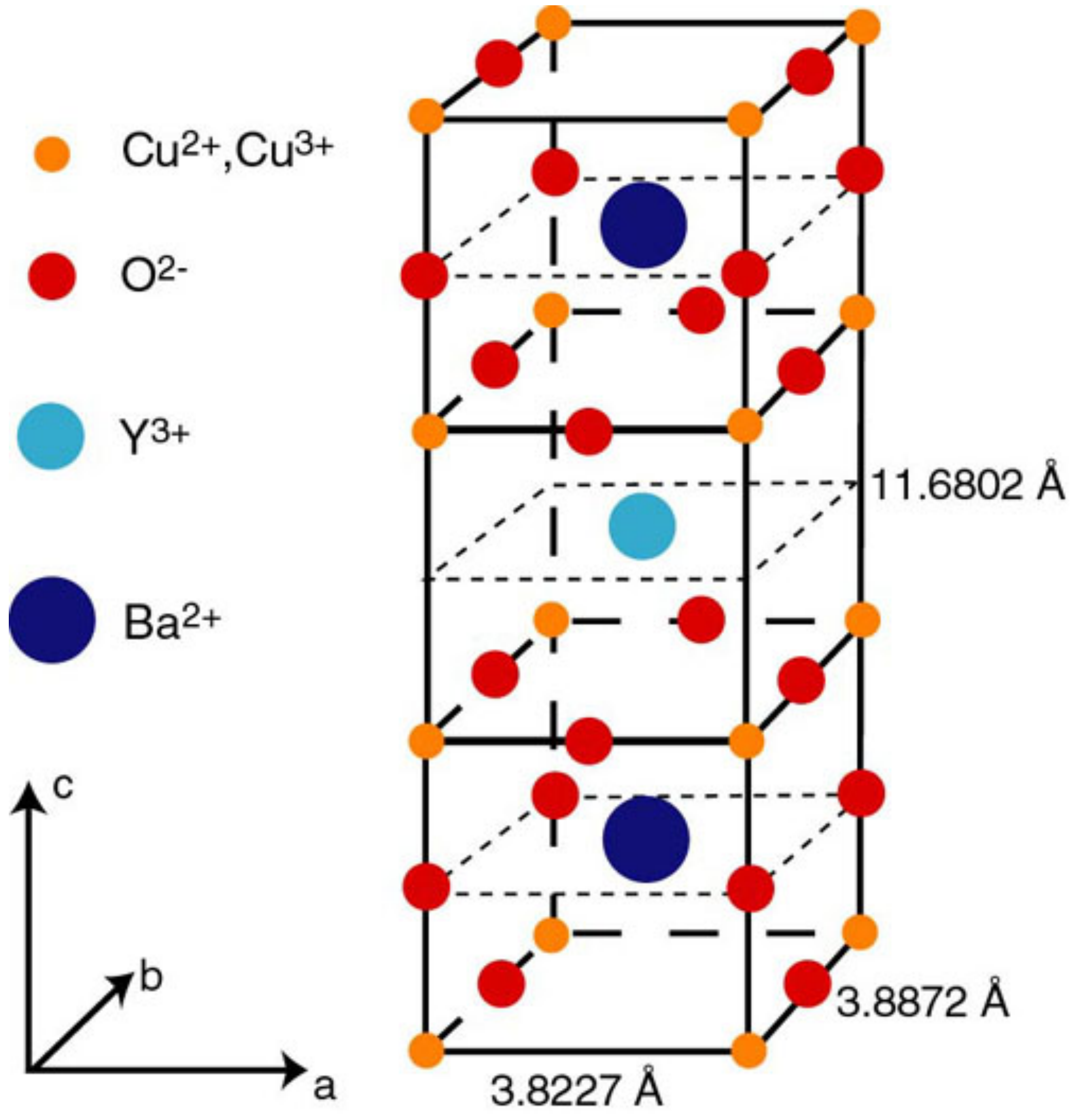
1. Luttinger theorem and U(1) symmetry
2. Anderson lattice model: the large Fermi surface, and the heavy Fermi liquid (HFL)
3. Kondo lattice model: HFL as the Higgs phase of a U(1) gauge theory
4. Kondo lattice model: the FL* phase — fractionalization, emergent gauge fields, and Luttinger violation
5.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

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

High temperature superconductors



CuO_2 plane



$YBa_2Cu_3O_{6+x}$

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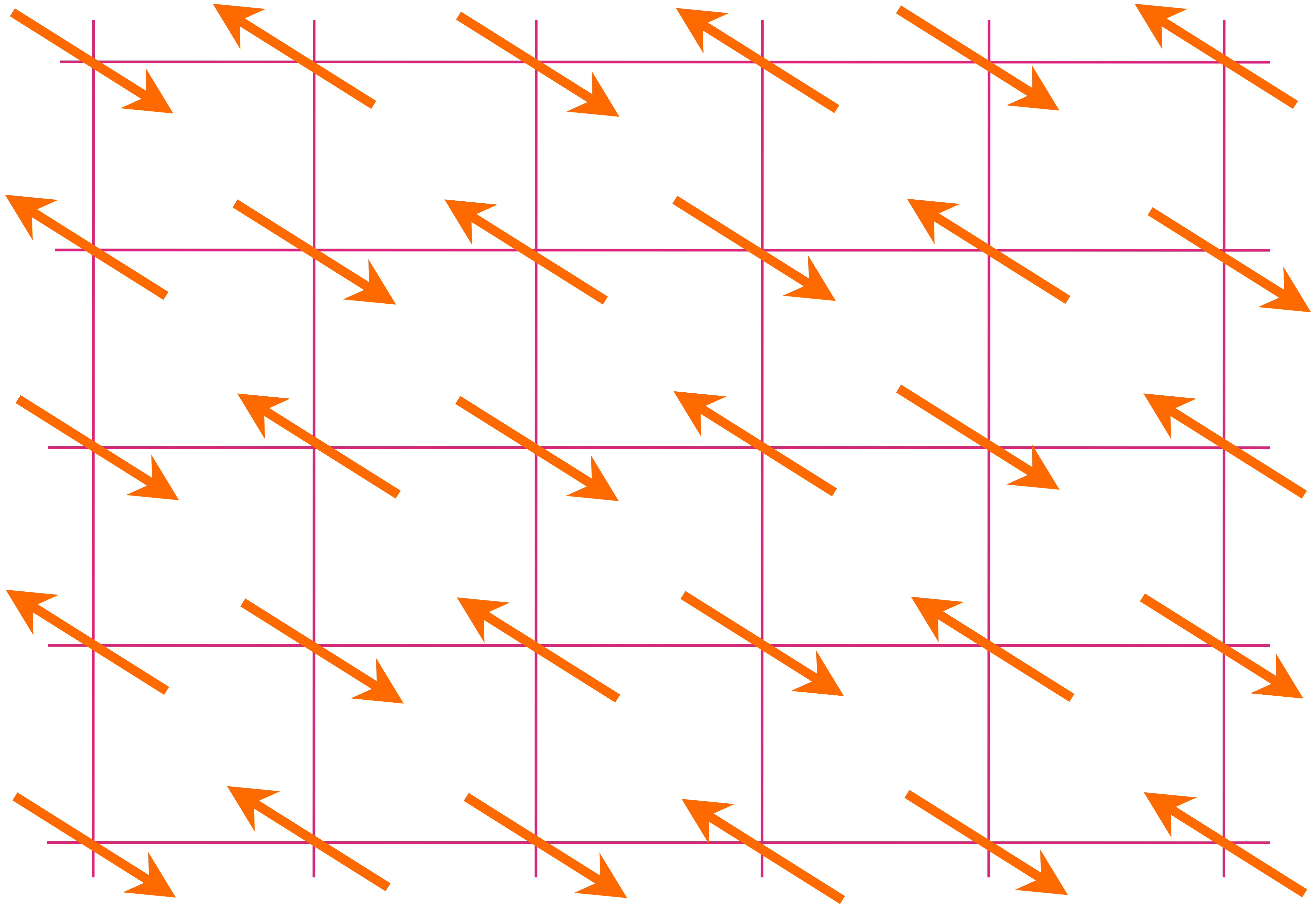

Insulating antiferromagnet

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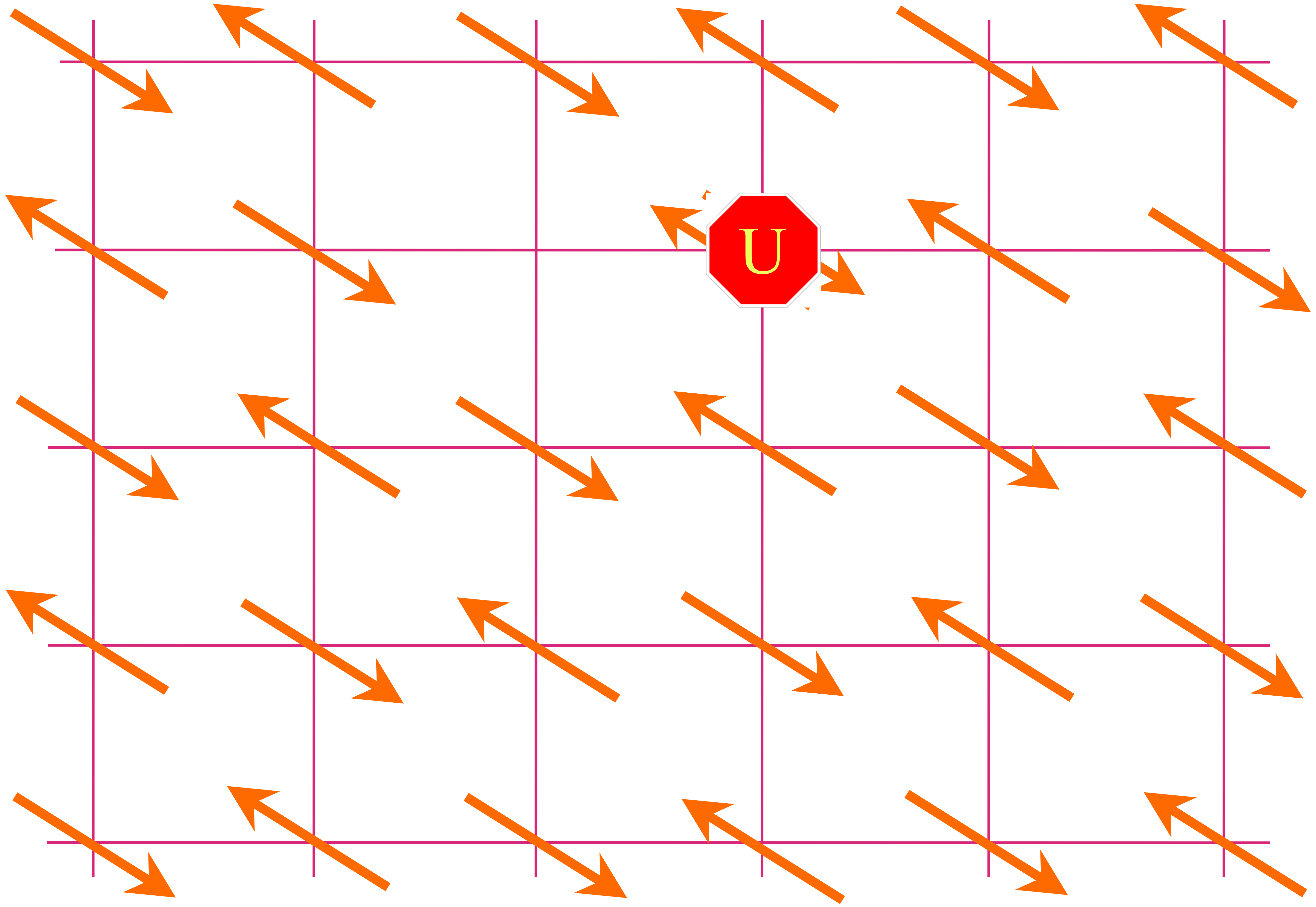

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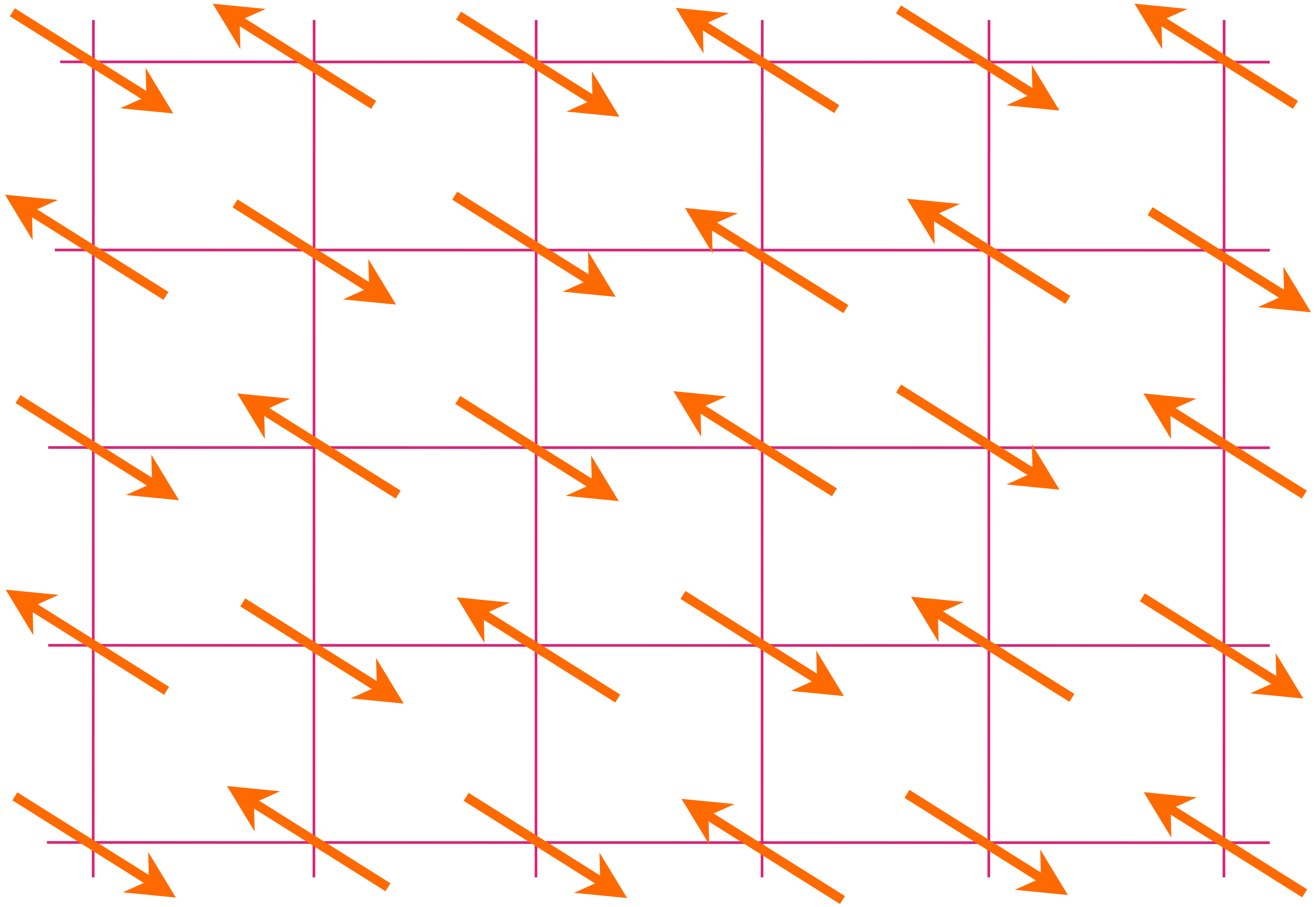

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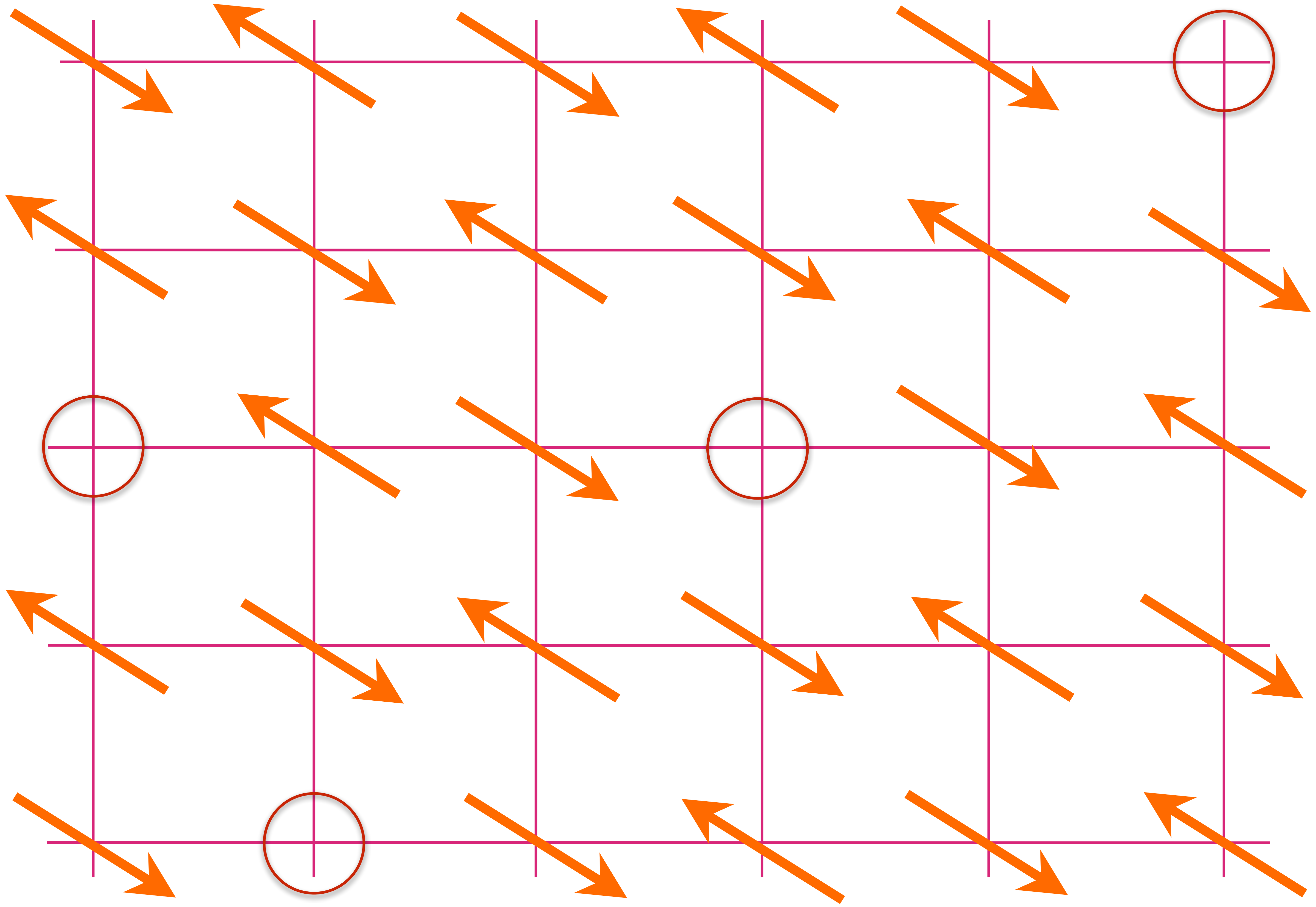

Antiferromagnet doped with hole density p

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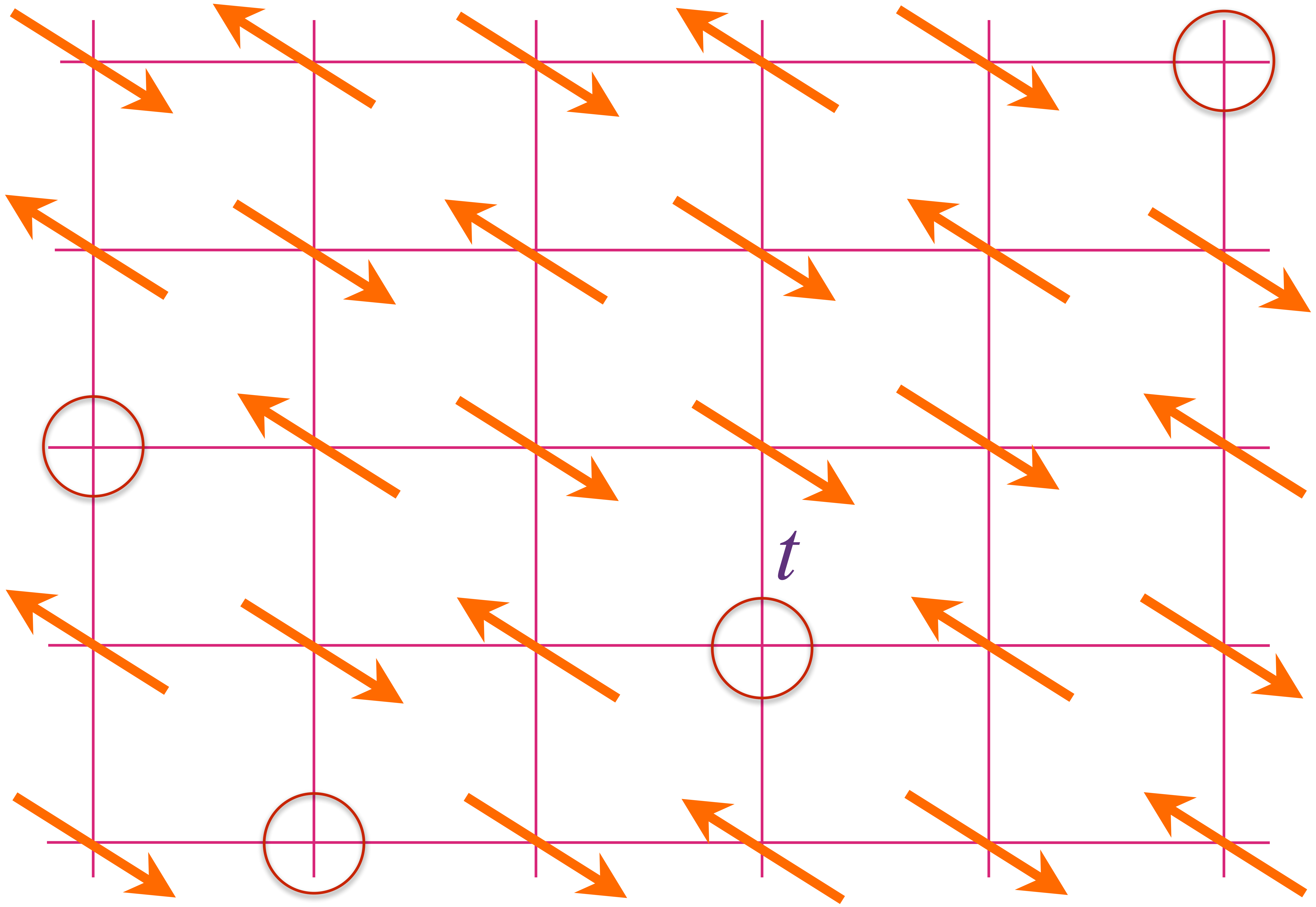

Antiferromagnet doped with hole density p

p mobile holes in a background of fluctuating spins

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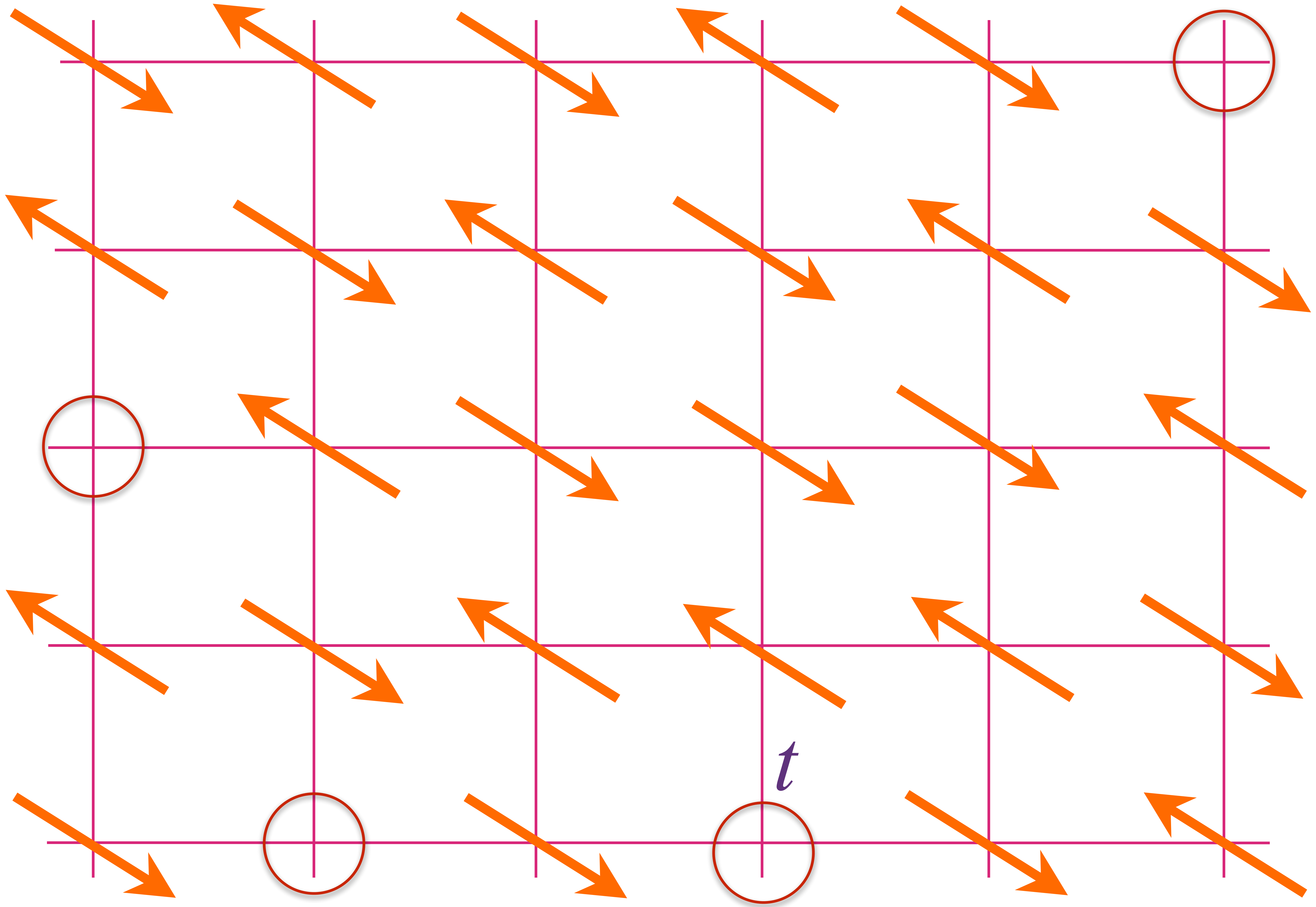

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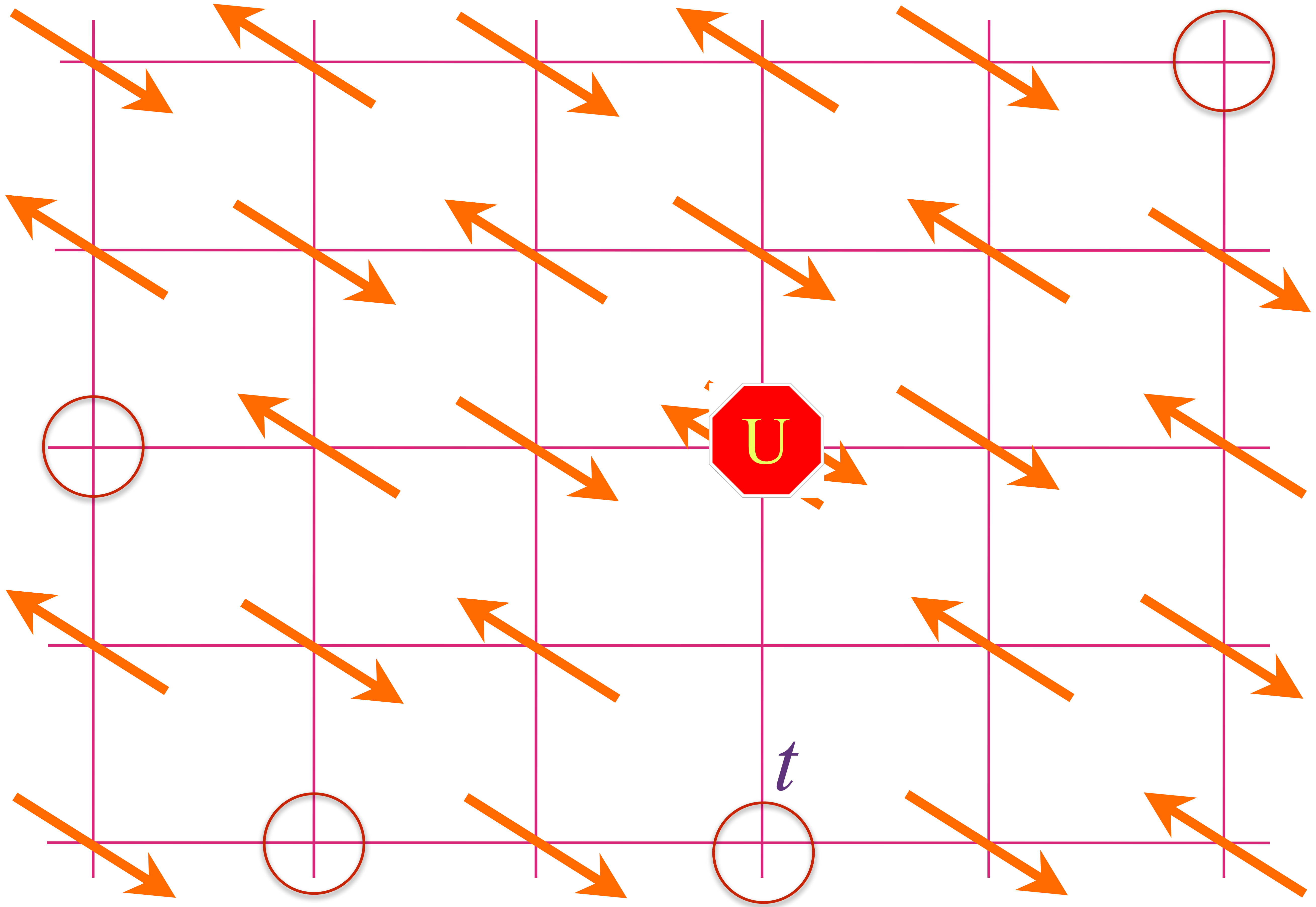

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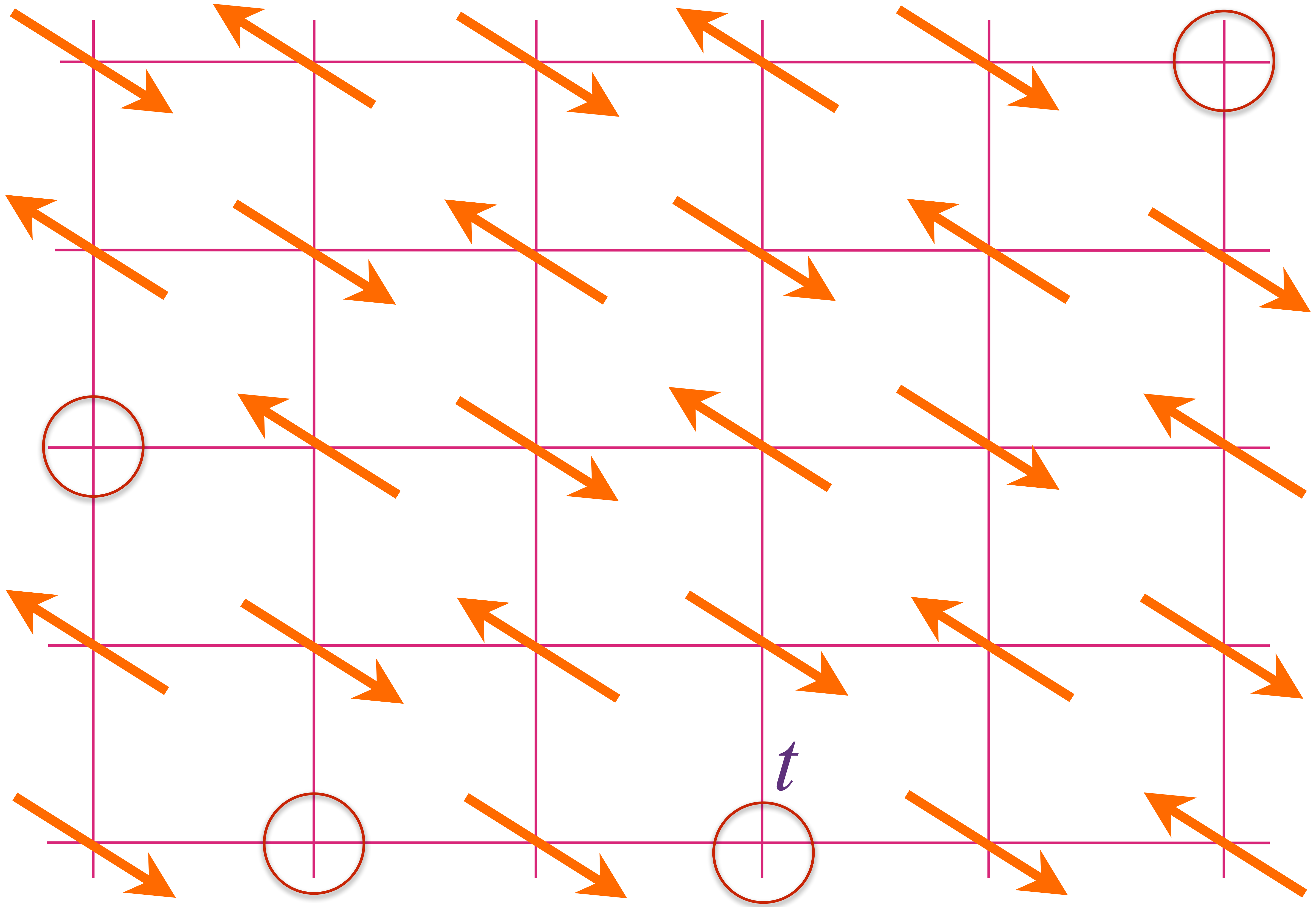

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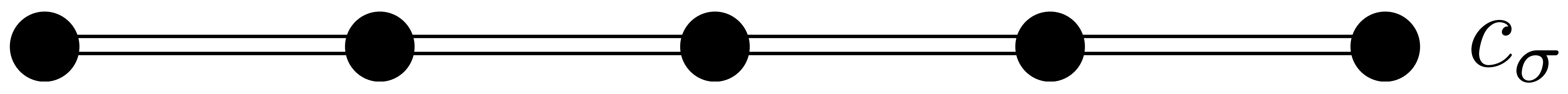
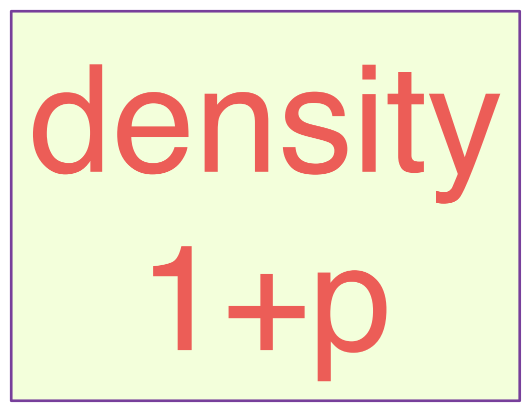
- The Luttinger theorem implies a FL phase with 'large' Fermi surface of size $1 + p$ holes (or $1 - p$ electrons) for all U and all p.





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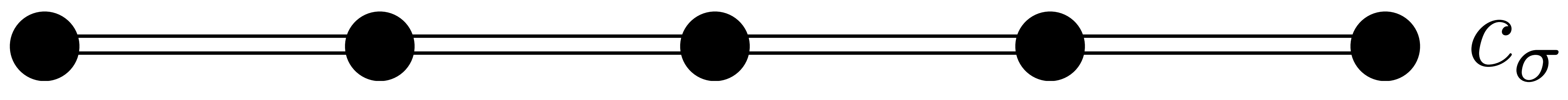
- Vanilla FL theory: Luttinger theorem applies as $p \to 0$ with wavefunction
$|\text{Vanilla}\rangle = [\text{Project out sites with 2 } c\text{'s}] \bowtie |\text{Slater determinant of } c\rangle$



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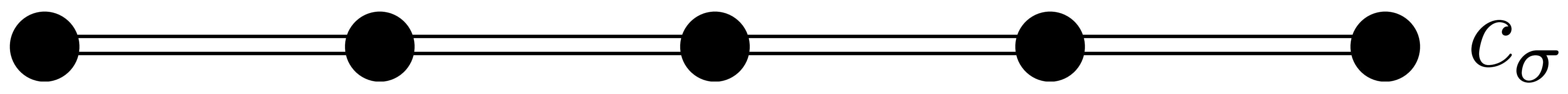
- The main effect of the projection is a 'Brinkman-Rice' enhancement of the quasiparticle mass as $p \to 0$, with $m^*/m \sim 1/p$.



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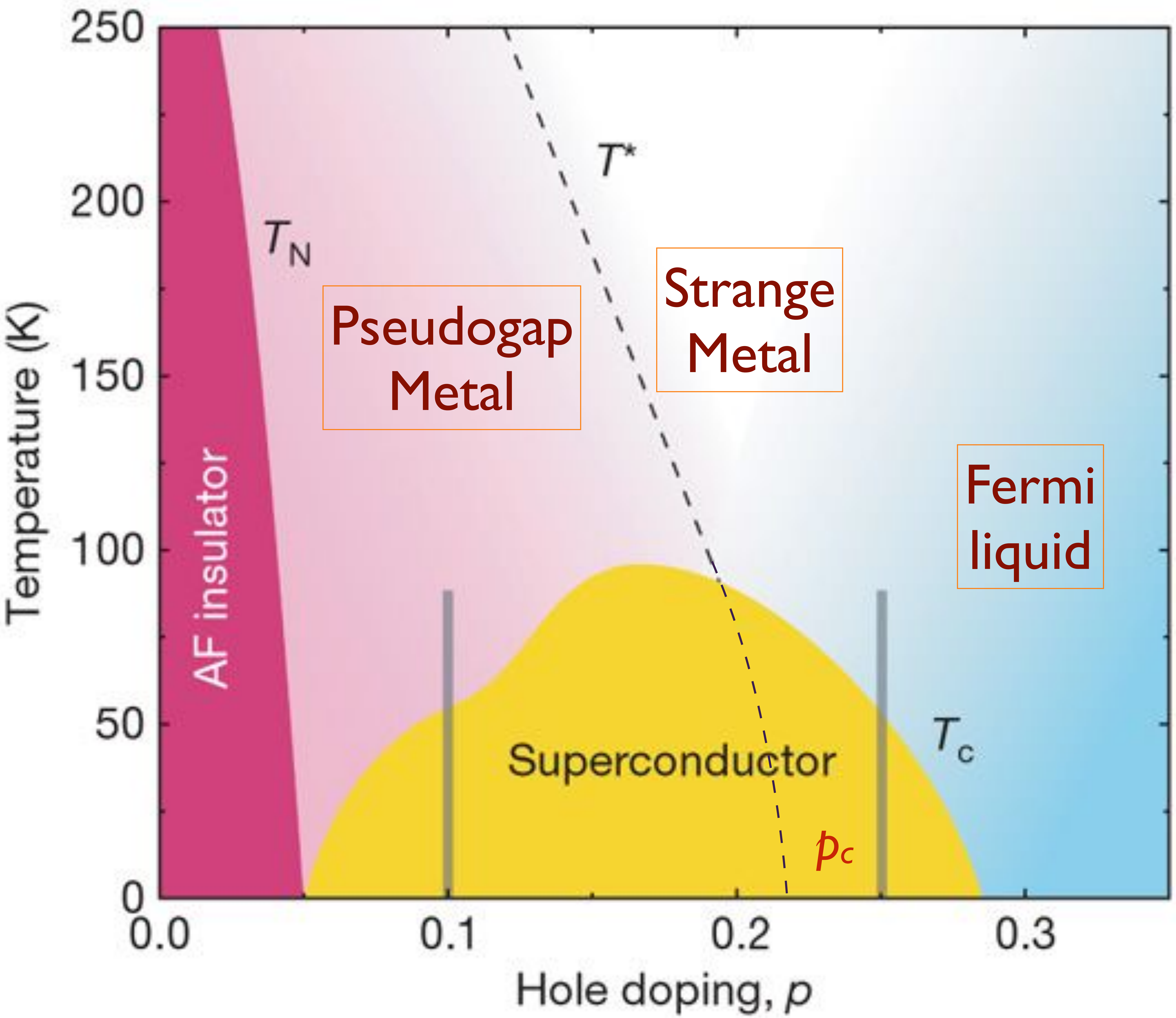
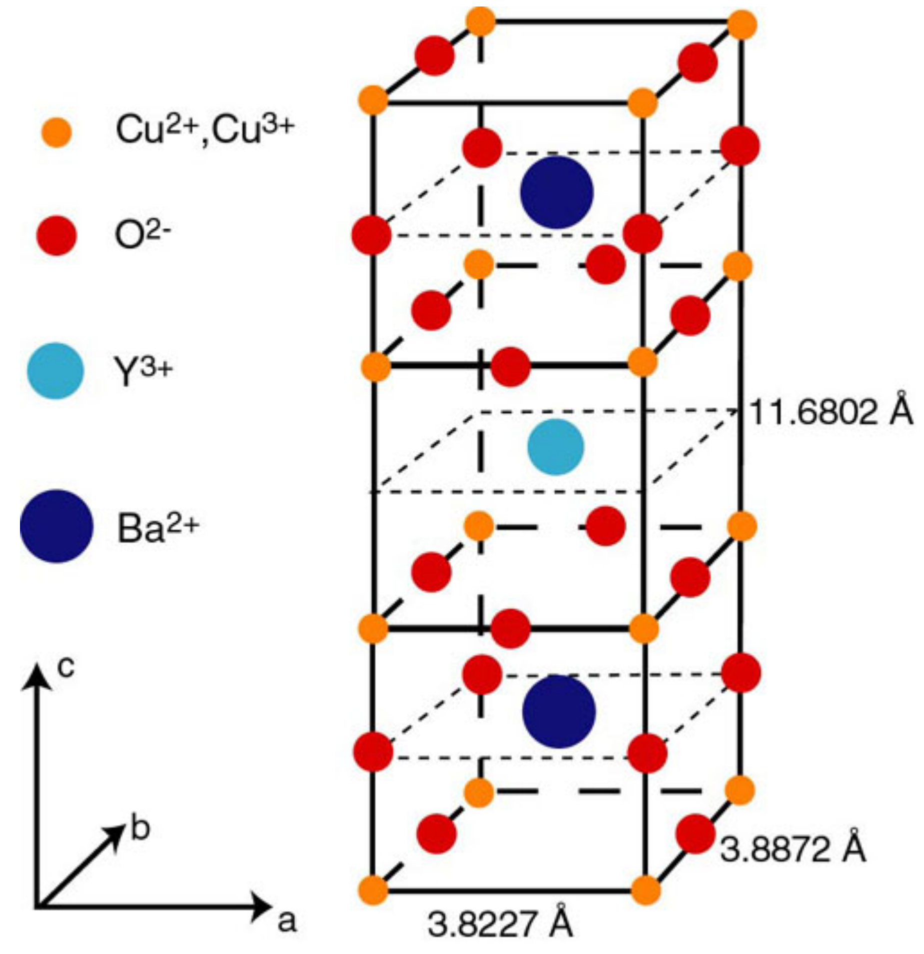
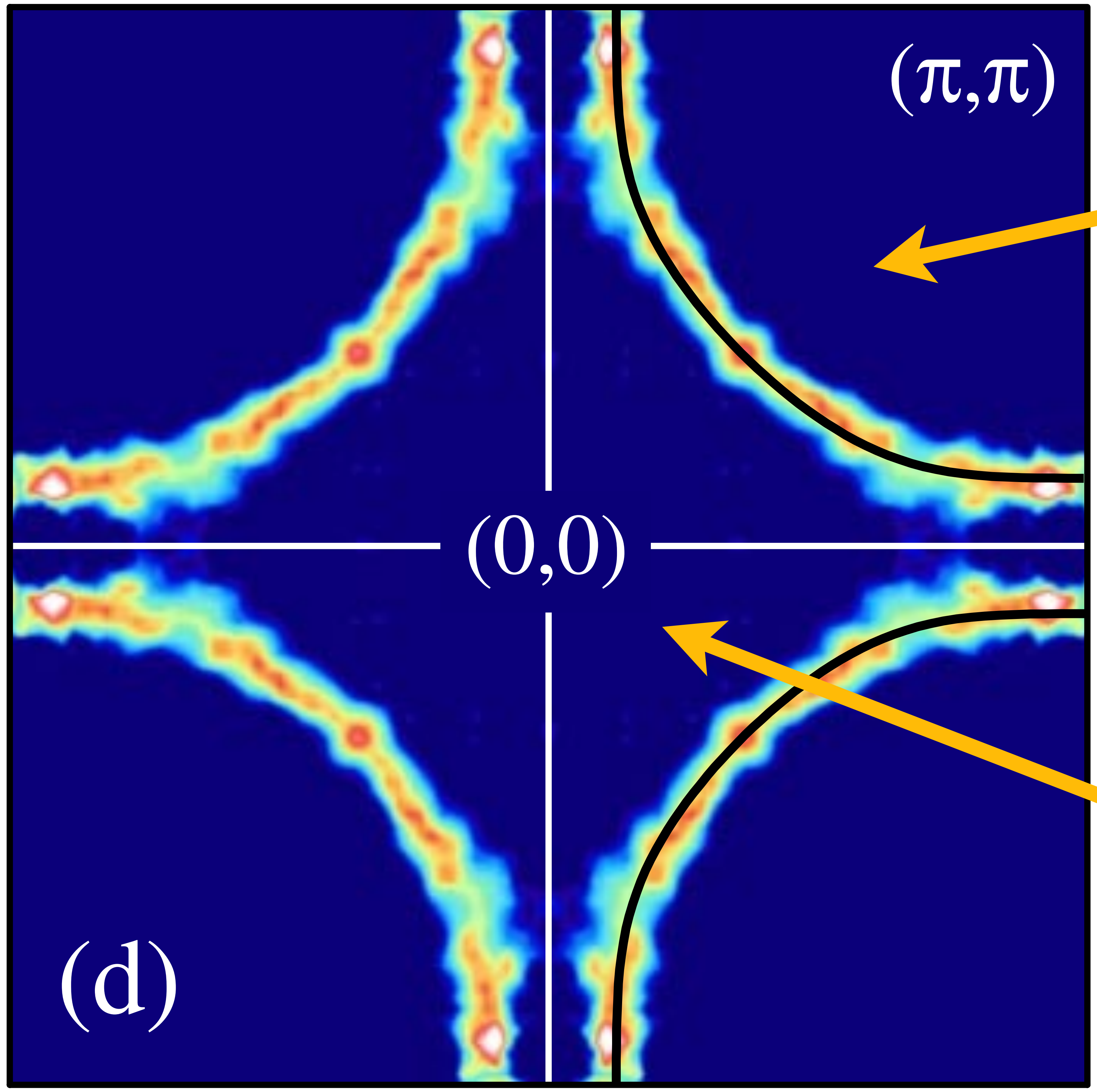

250
200
150
100
50
0
Temperature (K)
0.0
0.1
0.2
0.3
Hole doping, p
AF insulator
T_N
T*
Pseudogap Metal
Strange Metal
Fermi liquid
Superconductor
T_c
p_c


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

Photoemission at large p



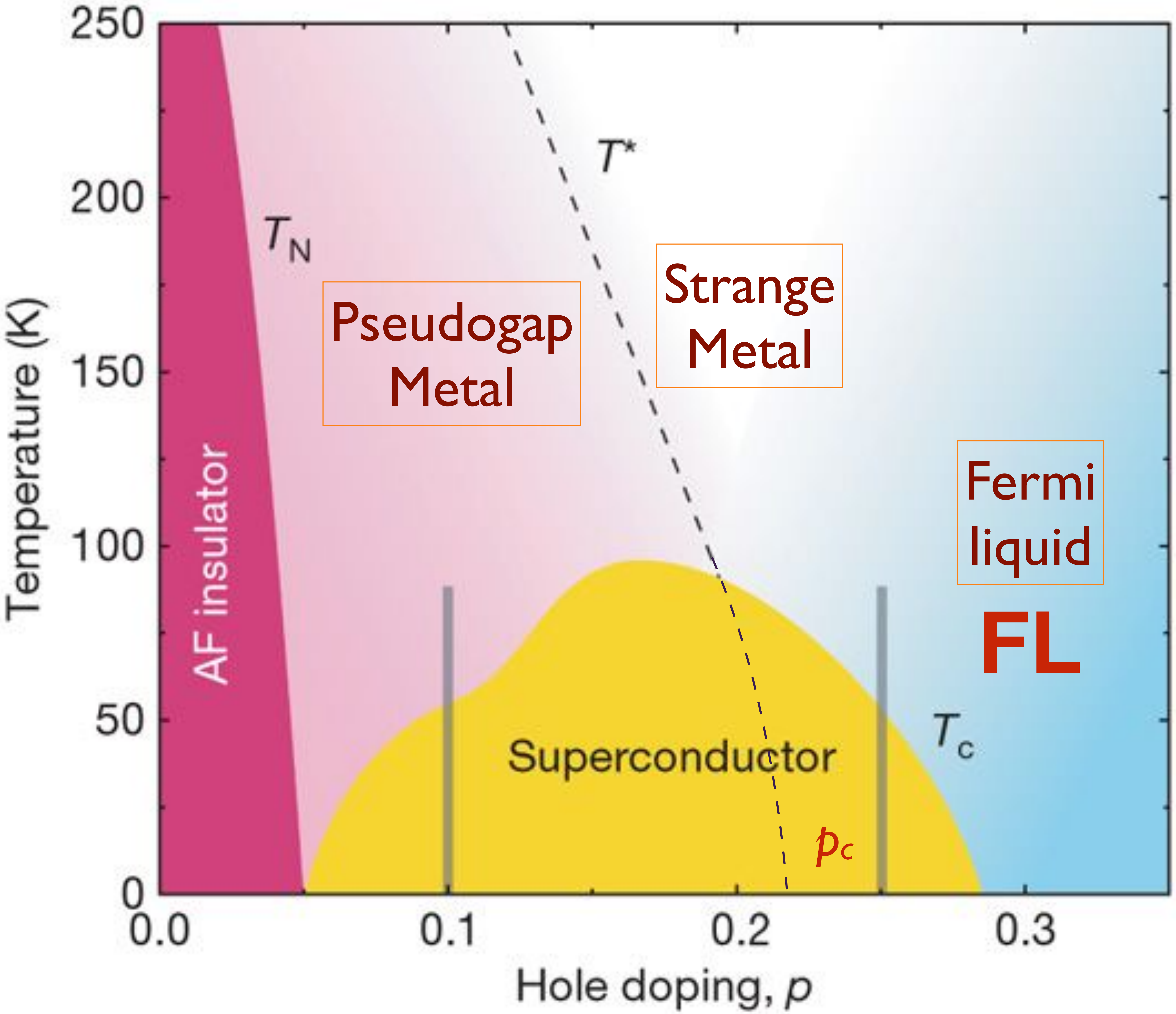
$1+p$ holes

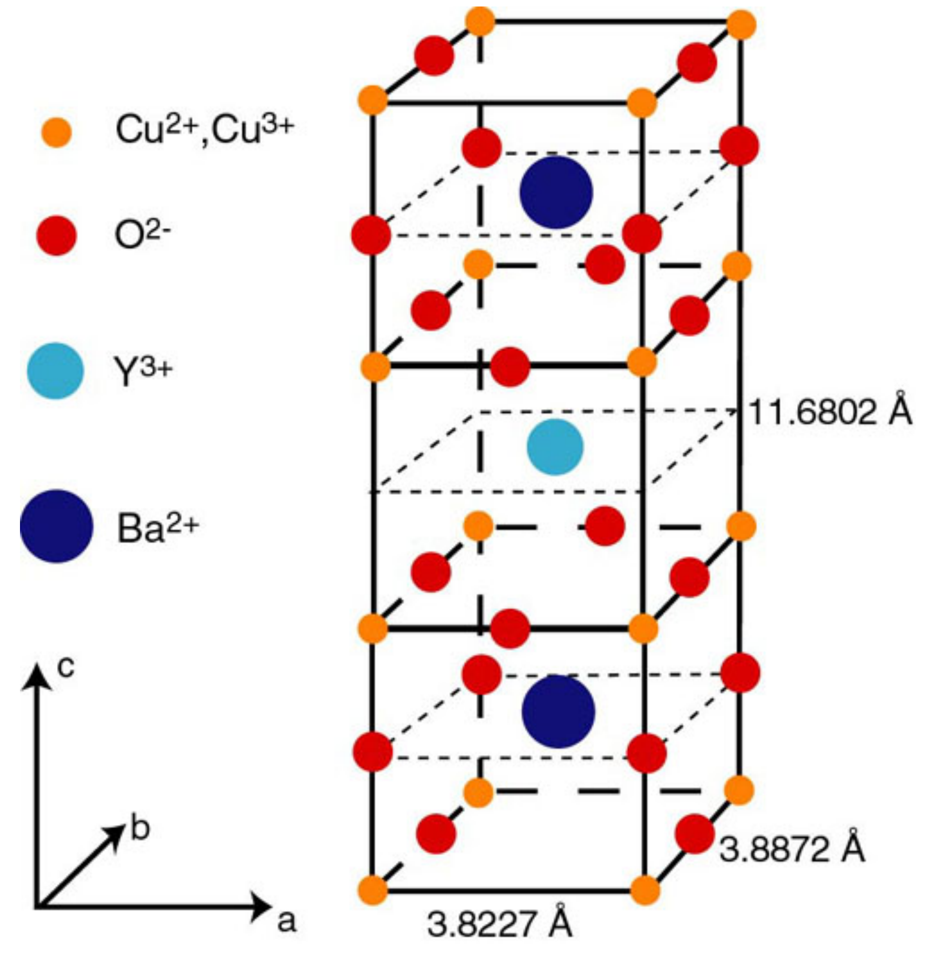
1-p electrons

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

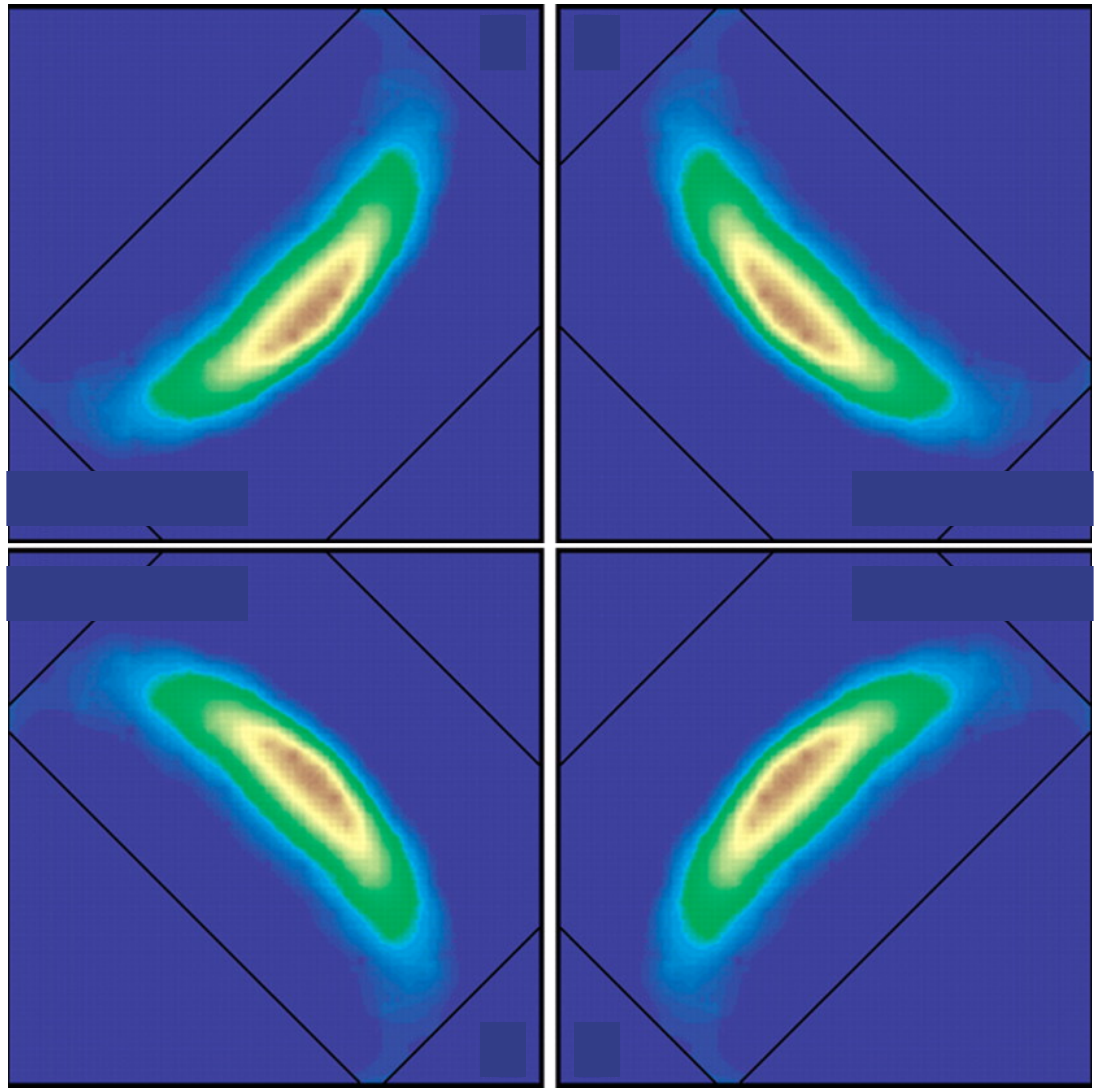
$1+p$ mobile holes in a filled band

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)


250
200
150
100
50
0
Temperature (K)
0.0
0.1
0.2
0.3
Hole doping, p
AF insulator
T_N
Pseudogap Metal
T^*
Strange Metal
Fermi liquid
FL
Superconductor
T_c
p_c


Cu^{2+},Cu^{3+}
O^{2-}
Y^{3+}
Ba^{2+}
c
b
a
11.6802 Å
3.8872 Å
3.8227 Å

Photoemission at small p



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

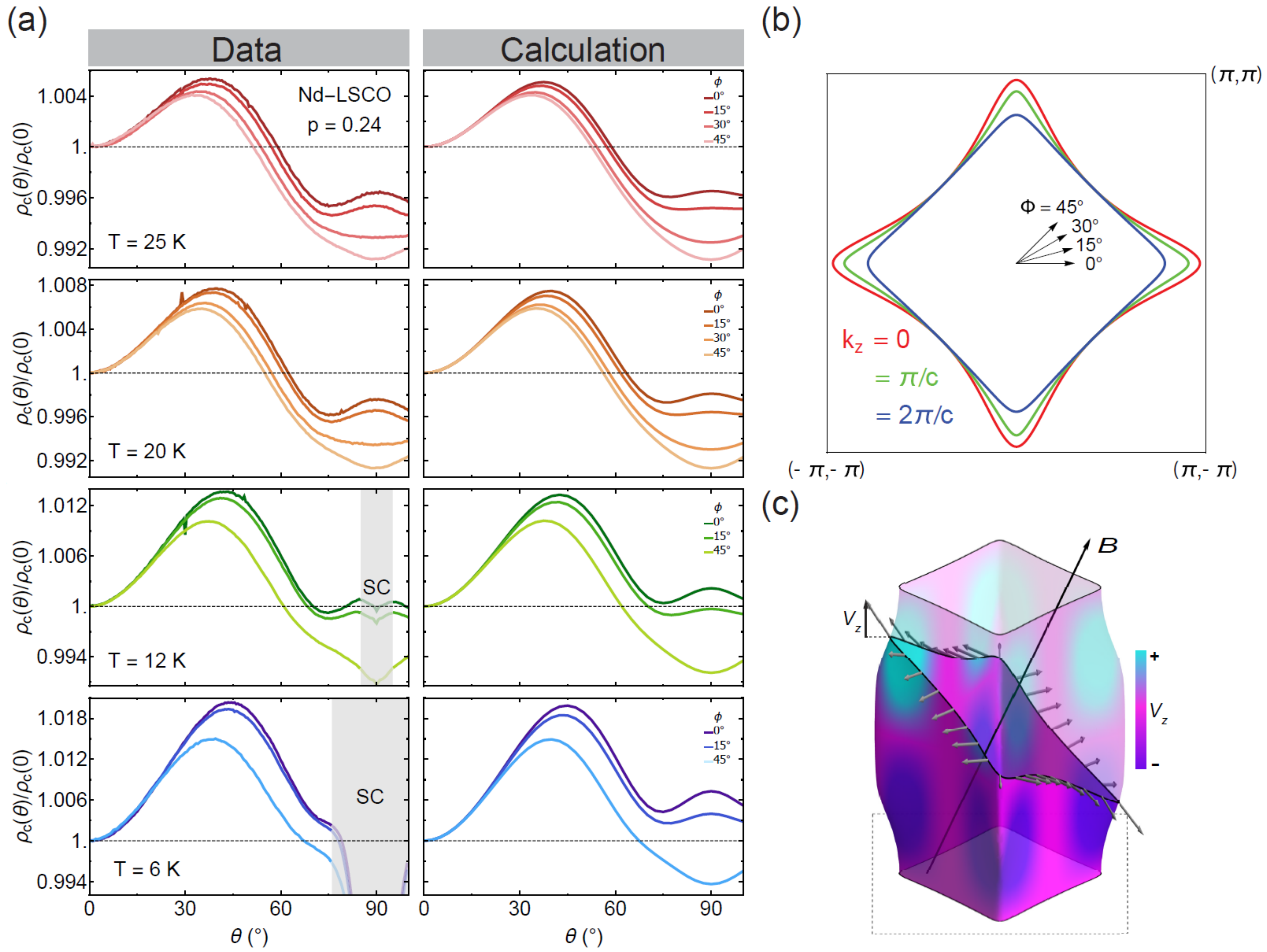
“Fermi arcs”

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)

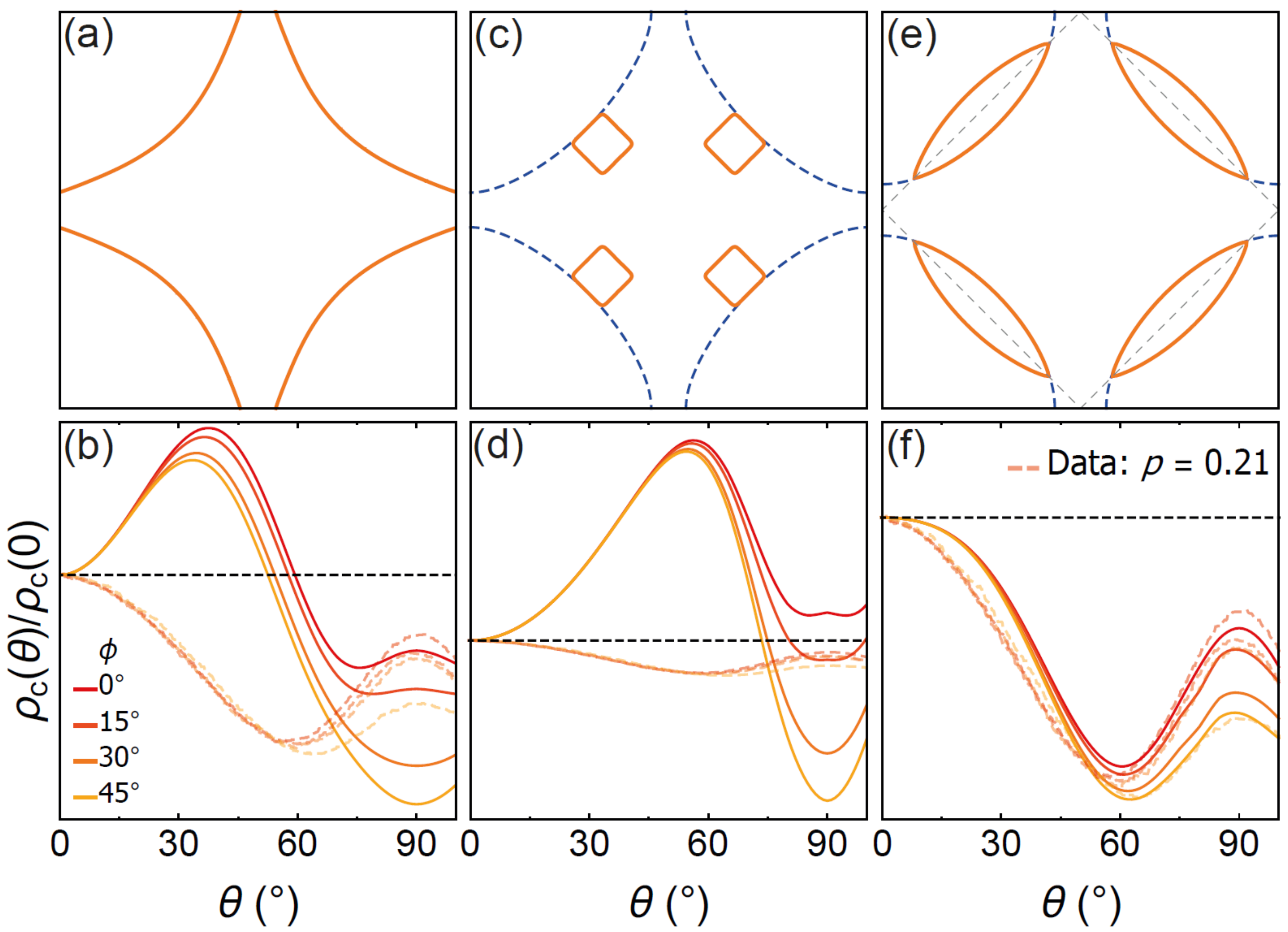
Fermi surface transformation at the pseudogap critical point of a cuprate superconductor

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

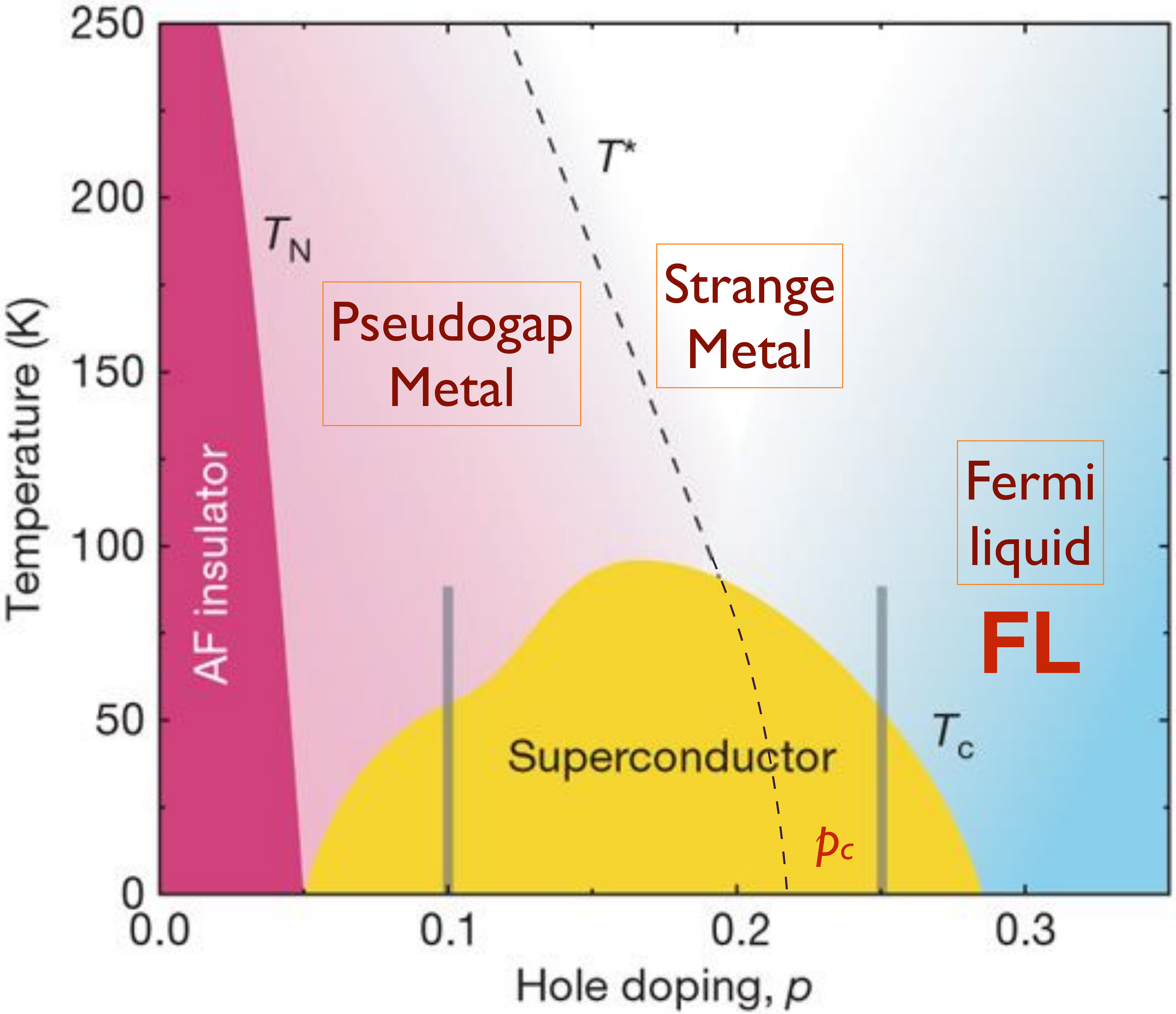
We use angle-dependent magnetoresistance (ADMR) to measure the Fermi surface of the cuprate $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$. Above the critical doping p* — outside of the pseudogap phase — we find a Fermi surface that is in quantitative agreement with angle-resolved photoemission. Below p*, however, the 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
200
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50
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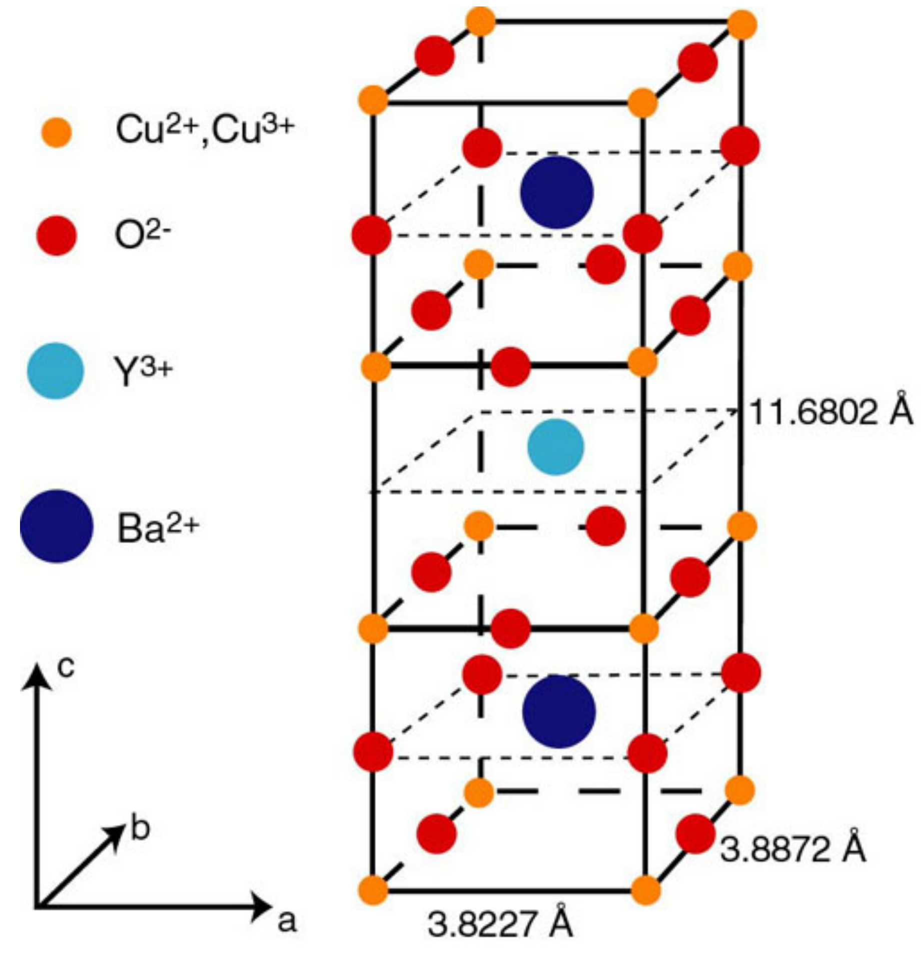
0.1
0.2
0.3
Temperature (K)
Hole doping, p
AF insulator
T_N
Pseudogap Metal
T^*
Strange Metal
Fermi liquid
FL
Superconductor
T_c
p_c


Cu^{2+},Cu^{3+}
O^{2-}
Y^{3+}
Ba^{2+}
c
b
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11.6802 Å
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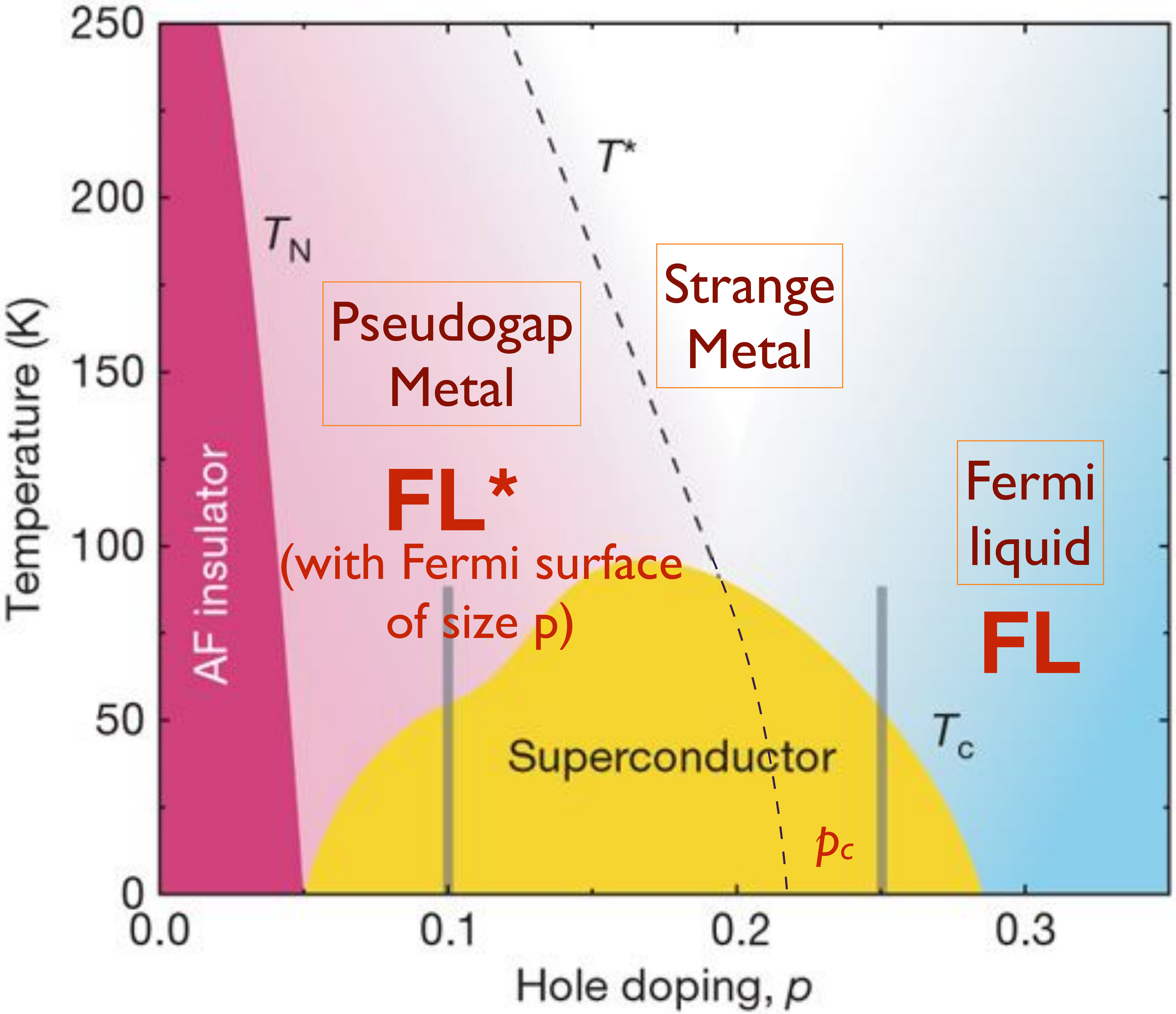
250
200
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0.1
0.2
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Temperature (K)
Hole doping, p
AF insulator
T_N
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Pseudogap Metal
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(with Fermi surface of size p)
Fermi liquid
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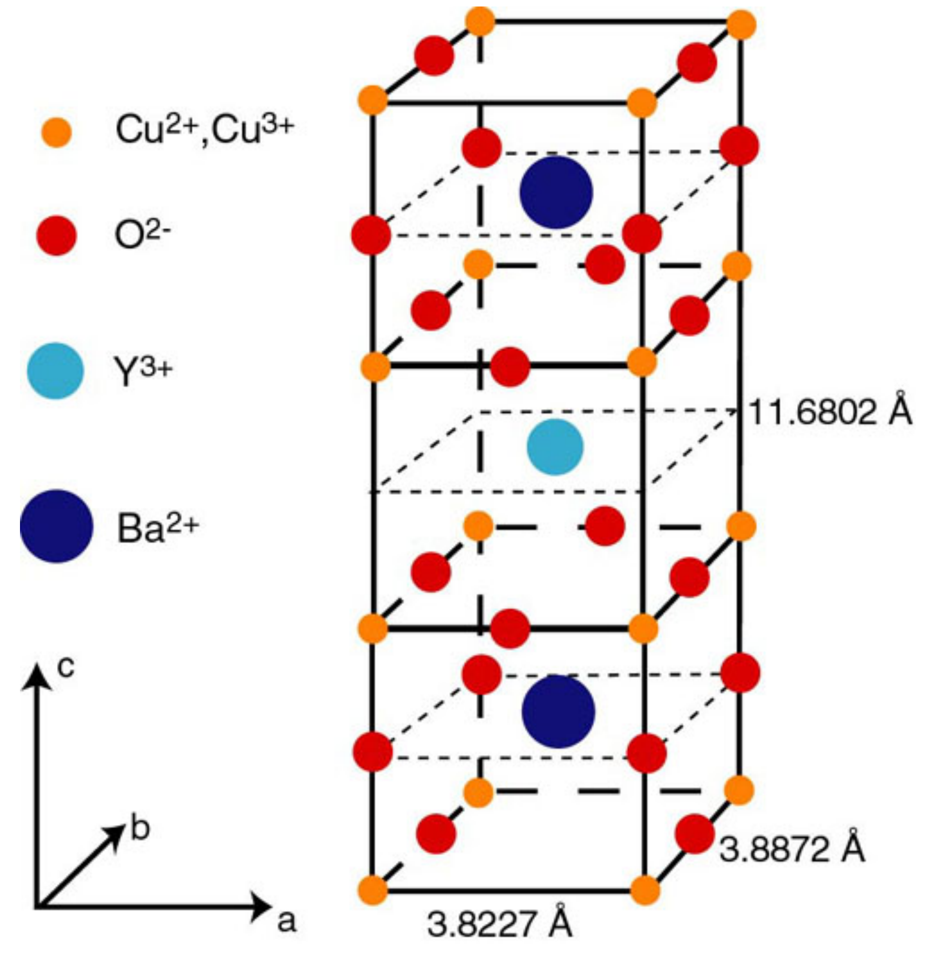
T_c
p_c


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

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

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].

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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].

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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].

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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].

Yahui Zhang

arXiv: 2001.09159
arXiv: 2006.01140
arXiv: 2103.05009

Maria Tikhanovskaya

Alexander Nikolaenko

Paramagnon theory of the Hubbard model

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

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

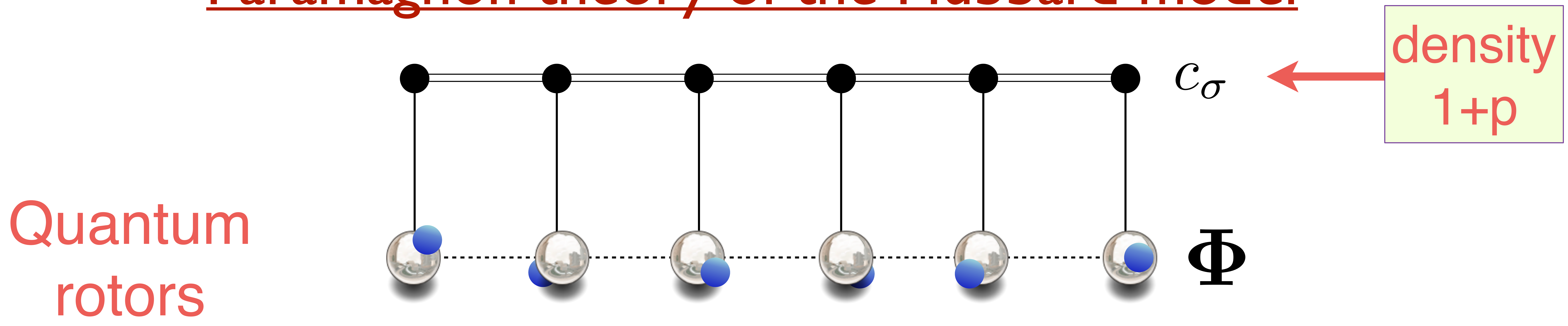
$$U\left(n_{\uparrow} - \frac{1}{2}\right)\left(n_{\downarrow} - \frac{1}{2}\right) = -\frac{2U}{3}\boldsymbol{S}^2 + \frac{U}{4}$$

Then we decouple the interaction via

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

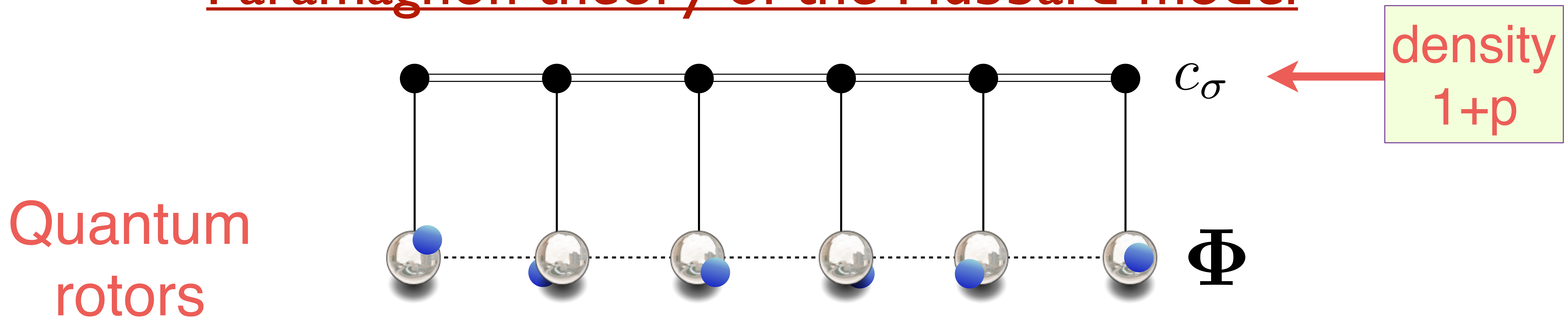
This yields the 'Hertz-Millis' theory for a 'paramagnon quantum rotor' $\boldsymbol{\Phi}_i$ coupled to otherwise free fermions $c_{i\sigma}$.

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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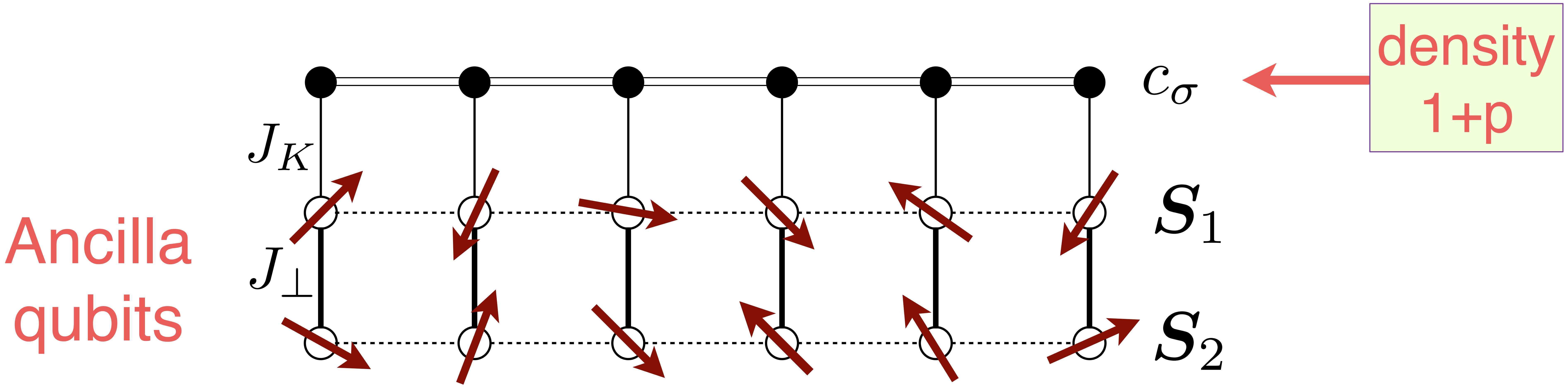
Key idea:

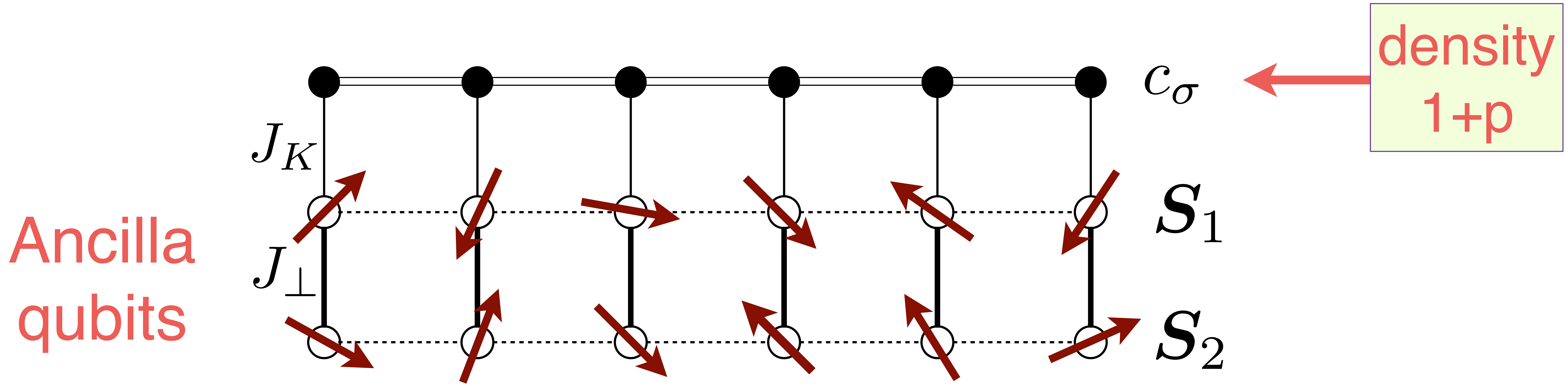
Fractionalize the ‘paramagnon rotor’ $\boldsymbol{\Phi}_i$
into 2 “ancilla qubits”,
$S = 1/2$ spins $\boldsymbol{S}_{1i}$ and $\boldsymbol{S}_{2i}$ on each site,
and don’t fractionalize the mobile electron $c_{i\sigma}$.

Ancilla theory of the Hubbard model



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

Ancilla theory of the Hubbard model



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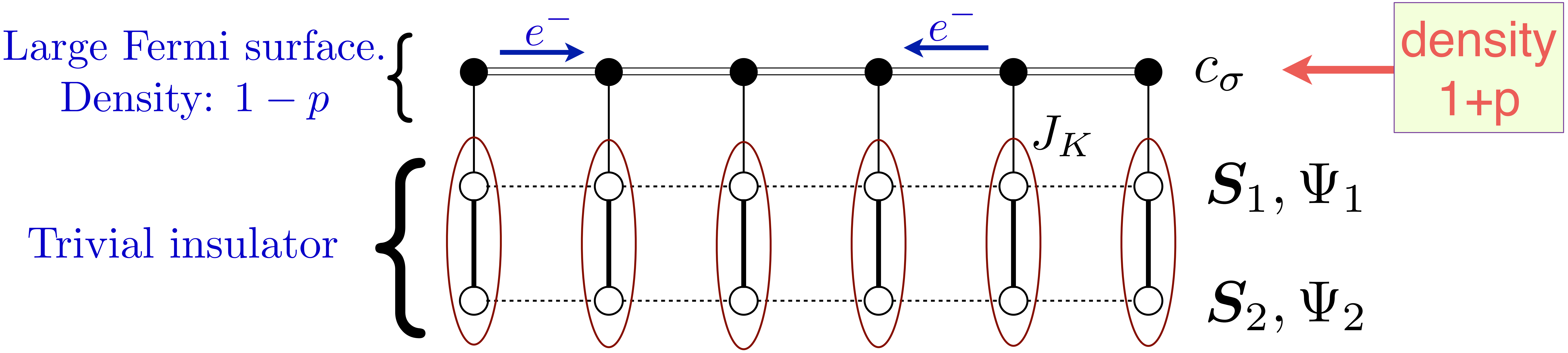
Performing a Schrieffer-Wolff transformation in powers of $1/J_\perp$, we obtain

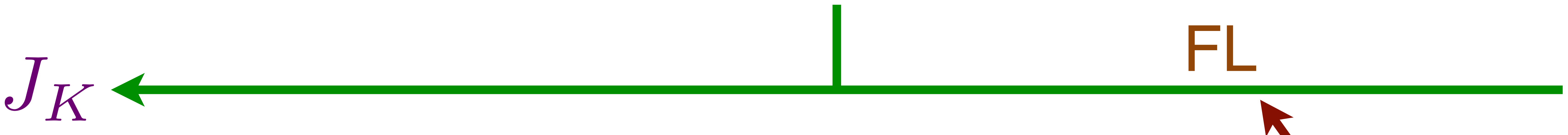
$$\mathcal{H} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} + U \sum_i \left[c_{i\uparrow}^\dagger c_{i\uparrow} \right] \left[c_{i\downarrow}^\dagger c_{i\downarrow} \right] + J \sum_{\langle ij \rangle} \left[c_{i\sigma}^\dagger \frac{\boldsymbol{\tau}_{\sigma\sigma'}}{2} c_{i\sigma'} \right] \cdot \left[c_{j\rho}^\dagger \frac{\boldsymbol{\tau}_{\rho\rho'}}{2} c_{j\rho'} \right]$$

i.e. we recover a Hubbard-Heisenberg model with *no ancillas* and

$$U = \frac{3J_K^2}{8J_\perp} + \frac{3J_K^3}{16J_\perp^2} + \ldots \quad , \quad J = \frac{J_K^2 (J_1 + J_2)}{4J_\perp^2}$$

Ancilla theory of the Hubbard model

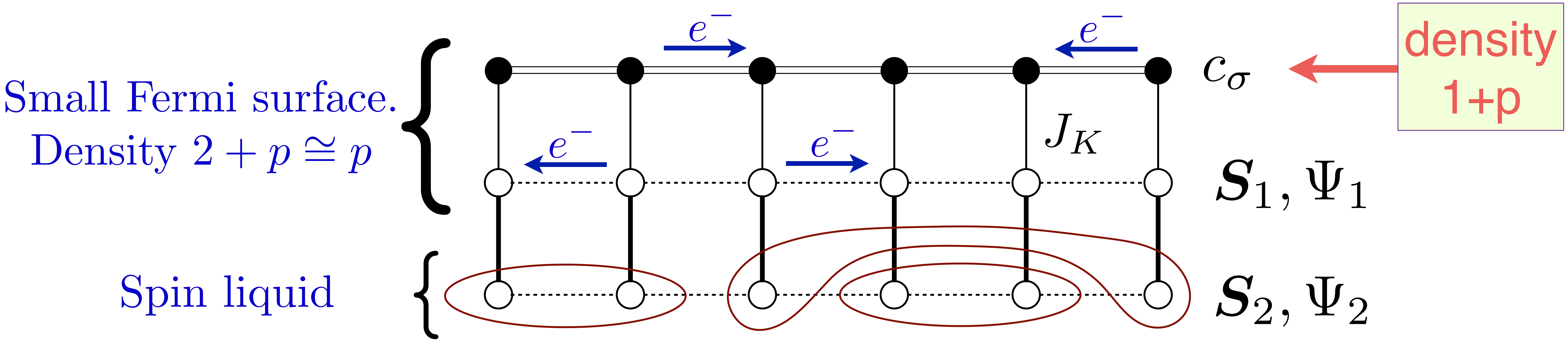


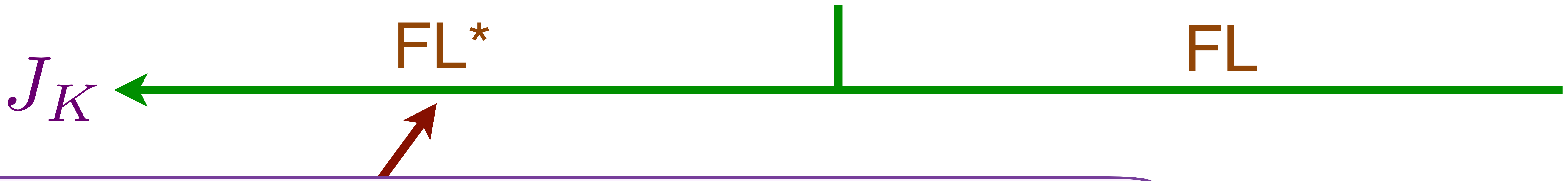


Large Fermi surface of size $1+p$

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

Ancilla theory of the Hubbard model

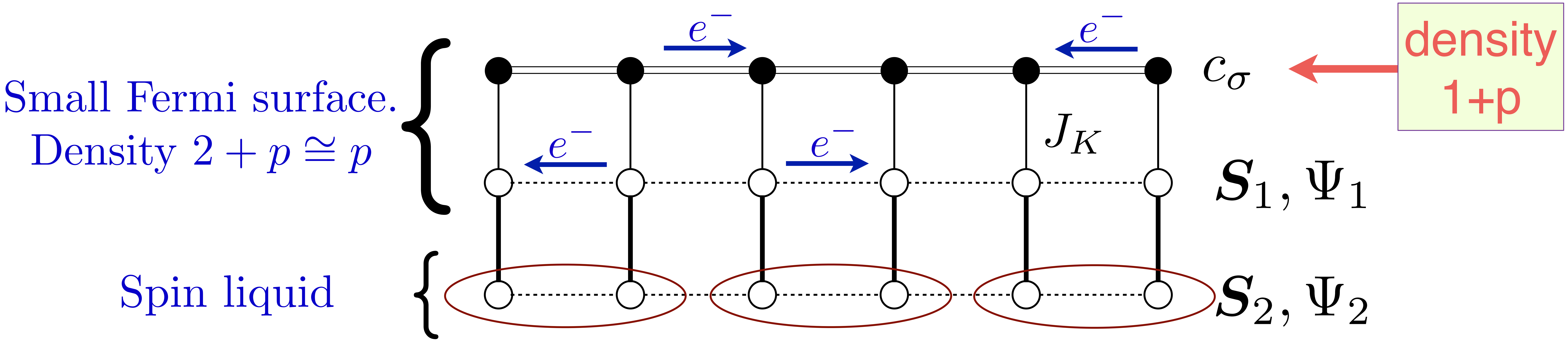


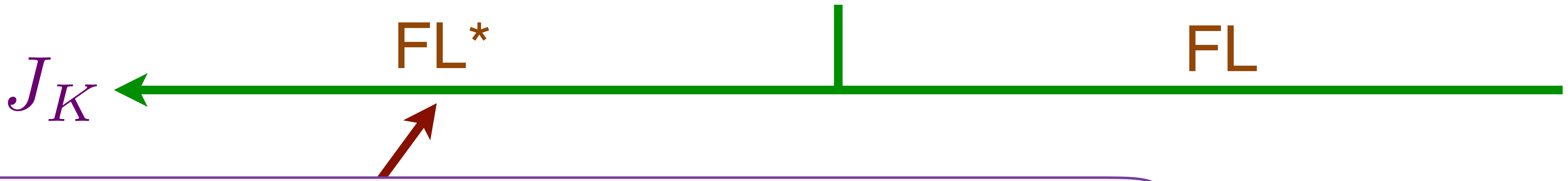


Small Fermi surface of size p

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

Ancilla theory of the Hubbard model





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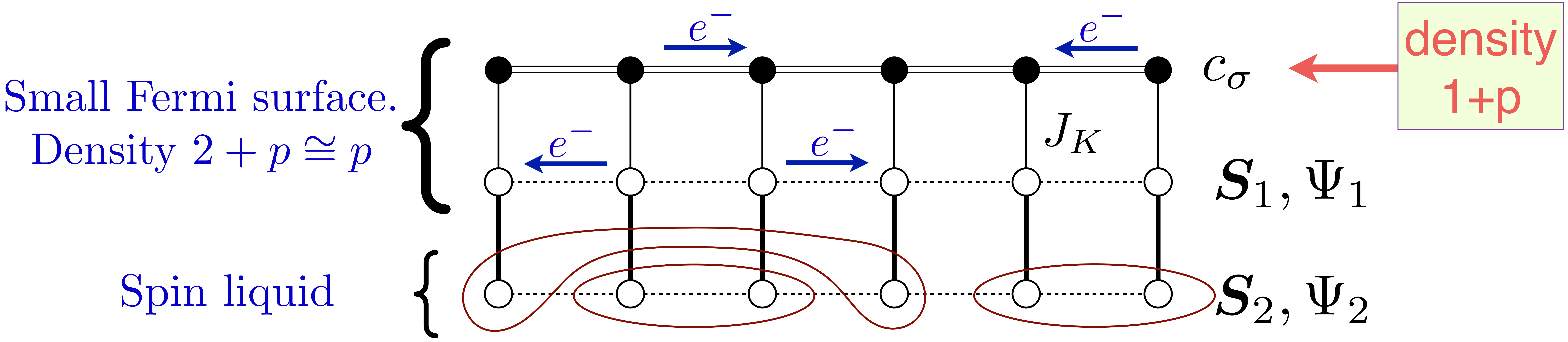

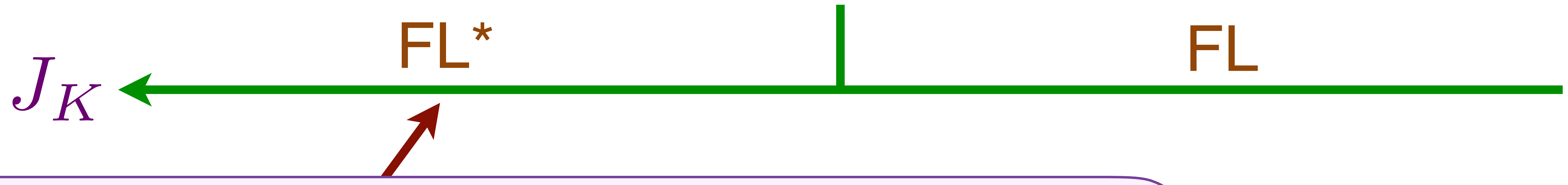

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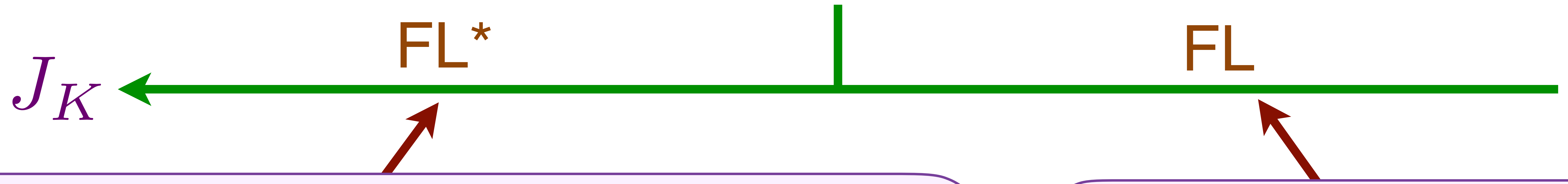
Ancilla theory of the Hubbard model



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Large Fermi surface of size $1 + p$

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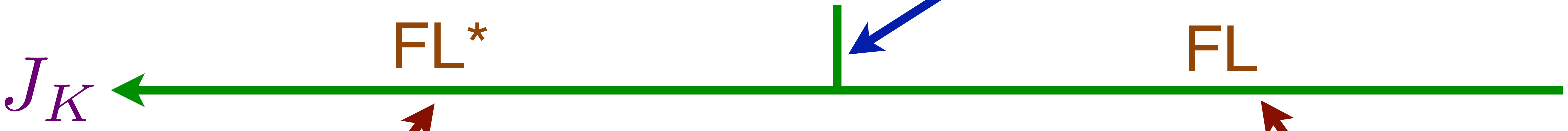
Ancilla theory of the Hubbard model

- Deconfined criticality of a $(\mathrm{SU}(2)_S \times \mathrm{U}(1)_1)/Z_2$ gauge theory.



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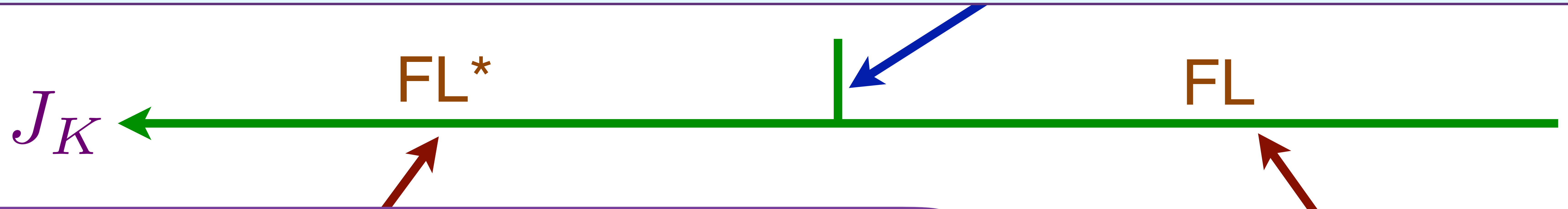

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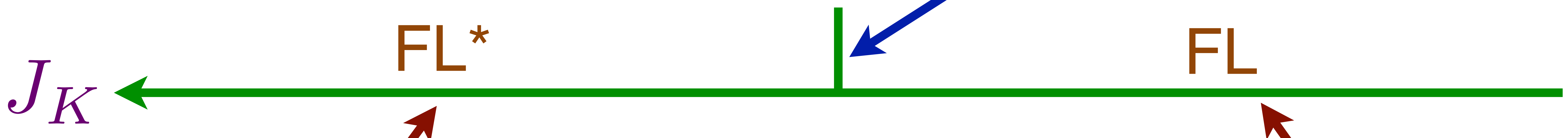

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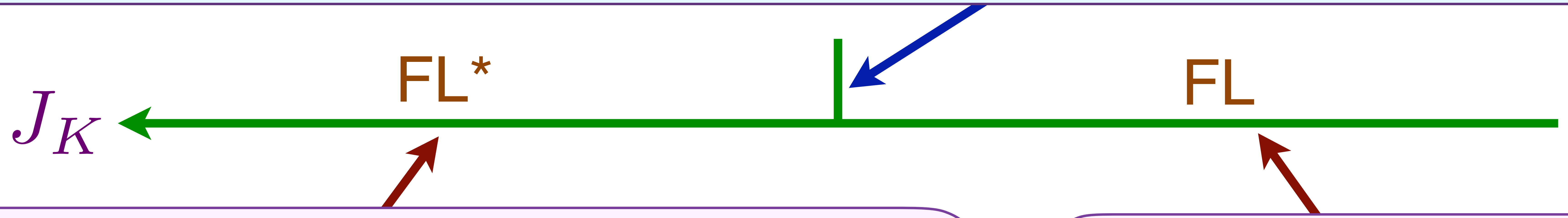

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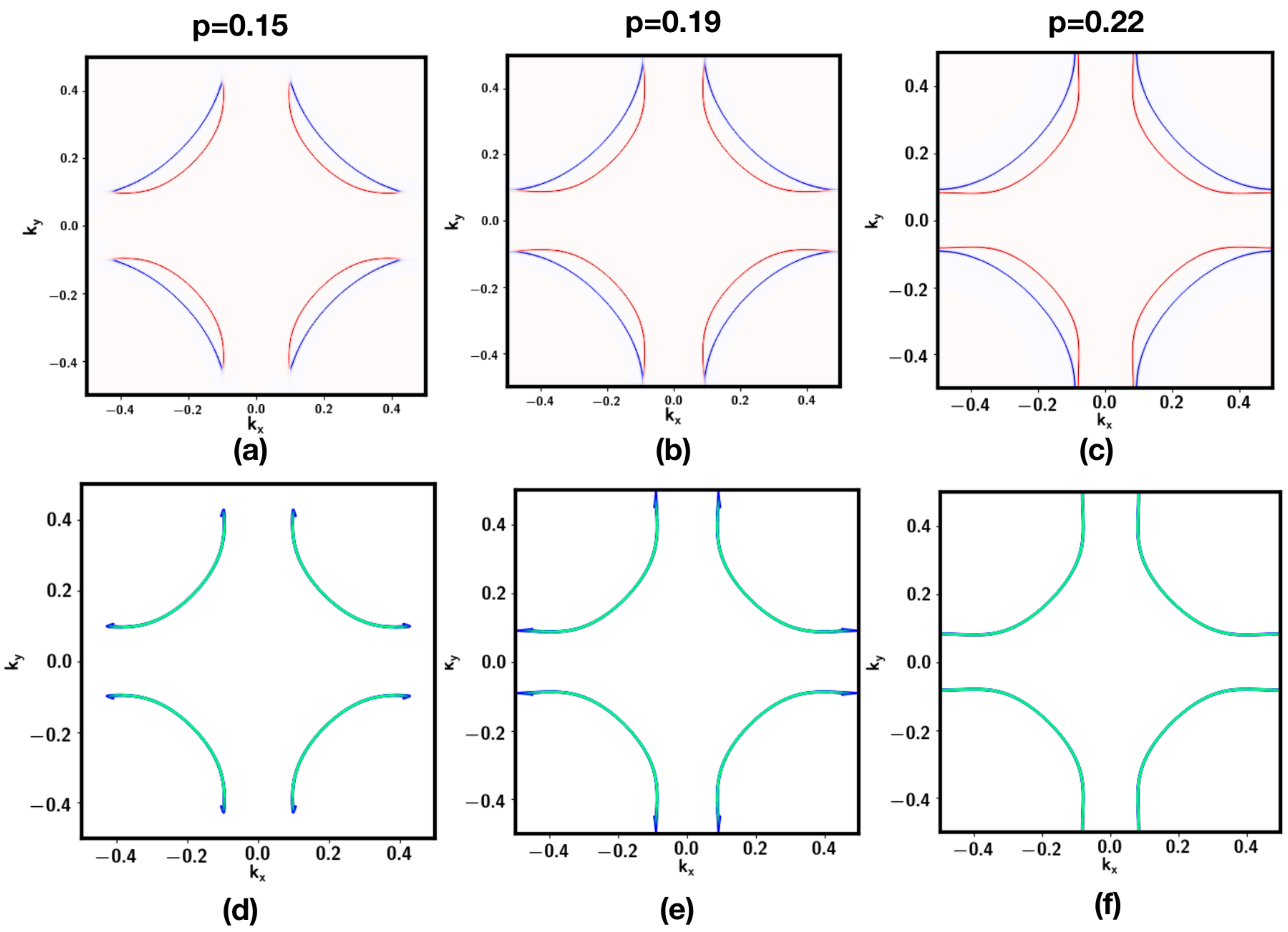
FL* in a ***one-band*** model



Zero frequency spectral density of electrons (red) and ghosts (blue)

“Fermi arc” spectral functions in the FL* phase

Ya-Hui Zhang

Ya-Hui Zhang, S. Sachdev, PRR **2**, 023172; PRB **102**, 155124 (2020)

FL*

- Theory of FL-FL* transition on a Kondo lattice: Emergent U(1) gauge field coupled to a hybridization boson and a gauge-neutral *small* Fermi surface of electrons.

FL*

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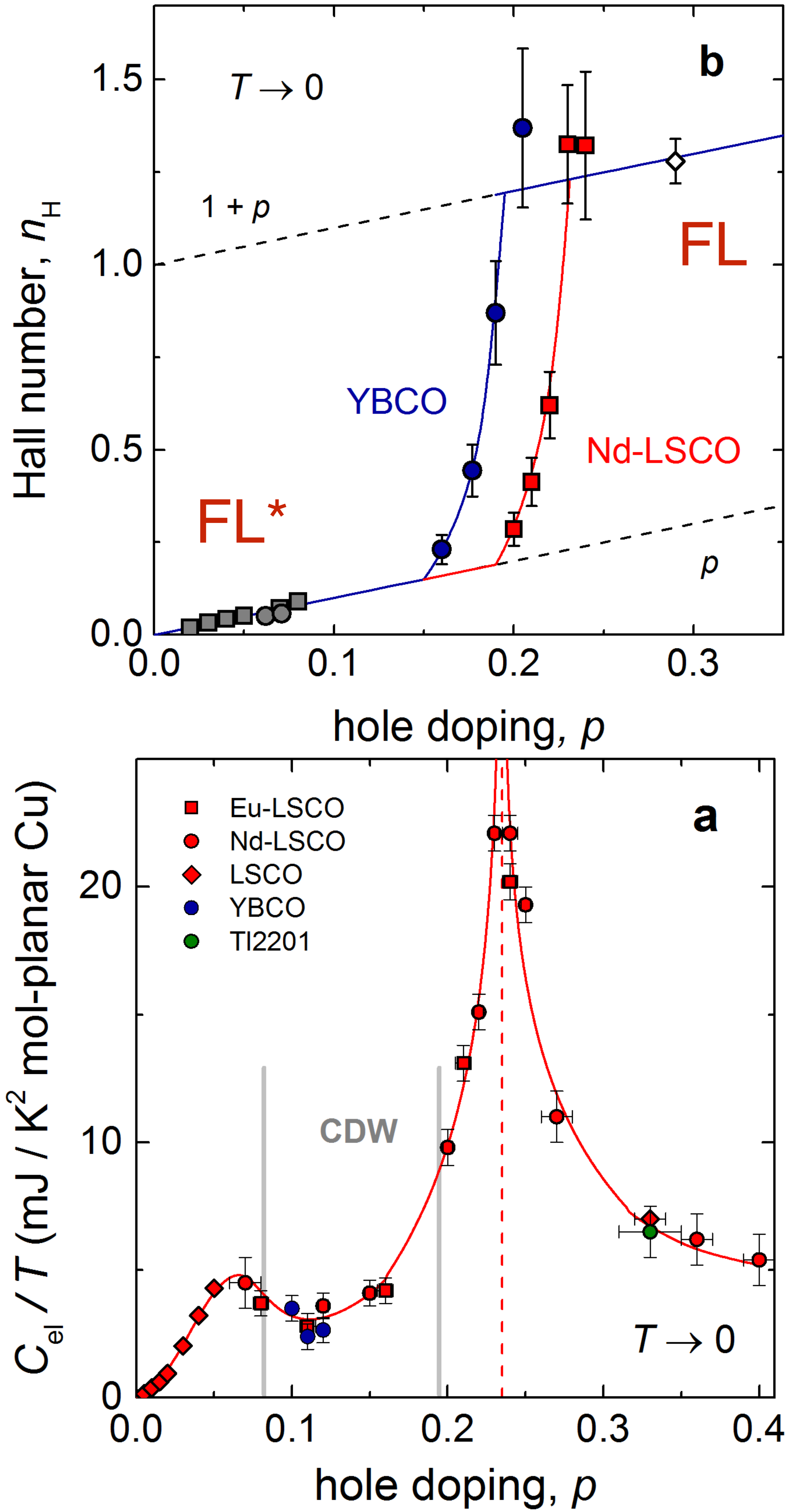
- Theory of FL-FL* transition on a single band Hubbard model: Emergent SU(2)×U(1) gauge theory coupled to hybridization boson, a gauge-neutral *large* Fermi surface of electrons, and a 'ghost' Fermi surface.
  Prediction: critical 'ghost' Fermi surfaces near the transition.

Cuprates



Evidence for
ghost Fermi surfaces
in the
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$CeCoIn_5$