

# Paramagnon fractionalization theory of the cuprate pseudogap

Quantum Simulation of Doped Hubbard Systems  
ITAMP, Harvard, Nov 15, 2022

Subir Sachdev



Talk online: [sachdev.physics.harvard.edu](https://sachdev.physics.harvard.edu)

PHYSICS



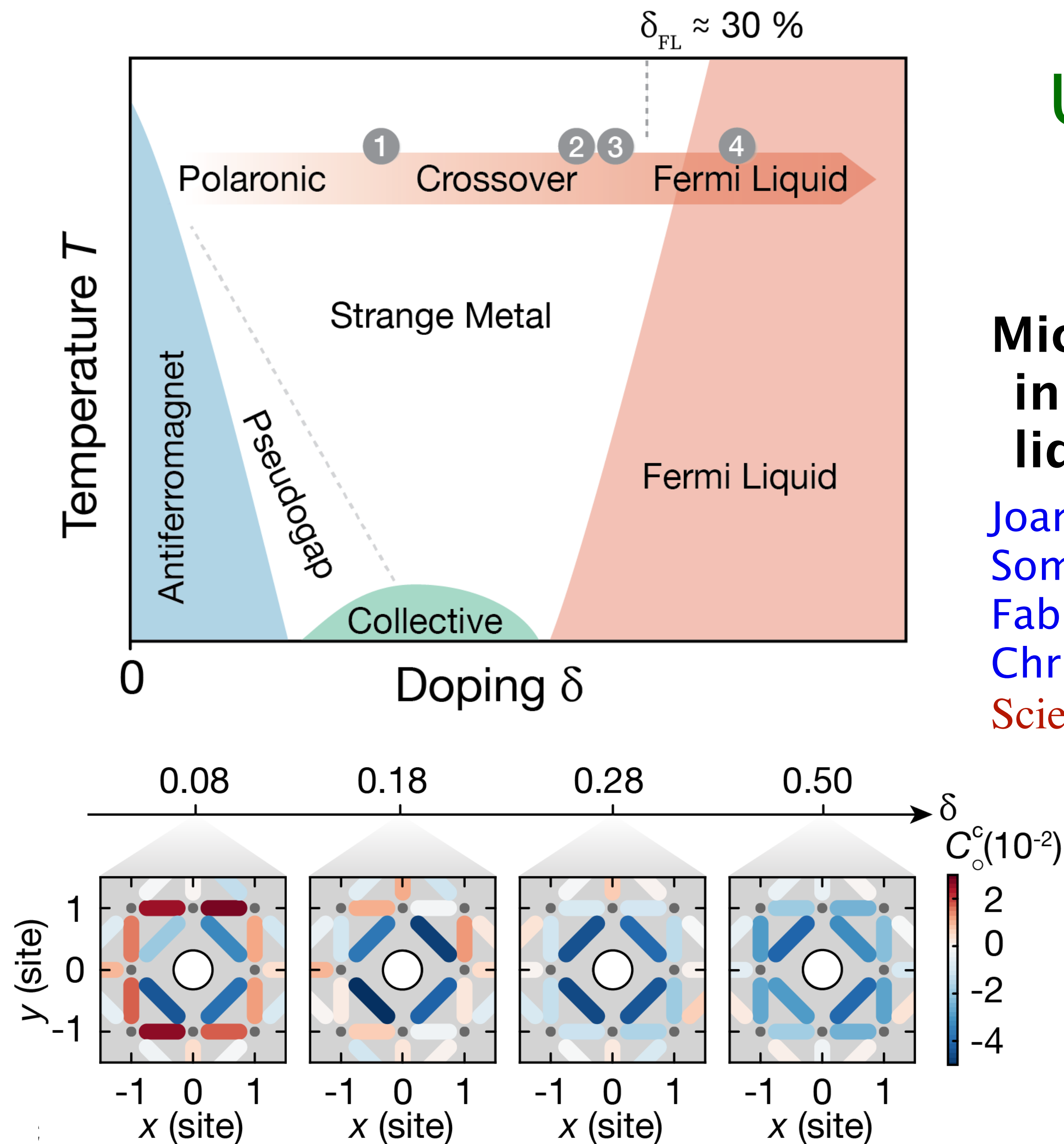
HARVARD

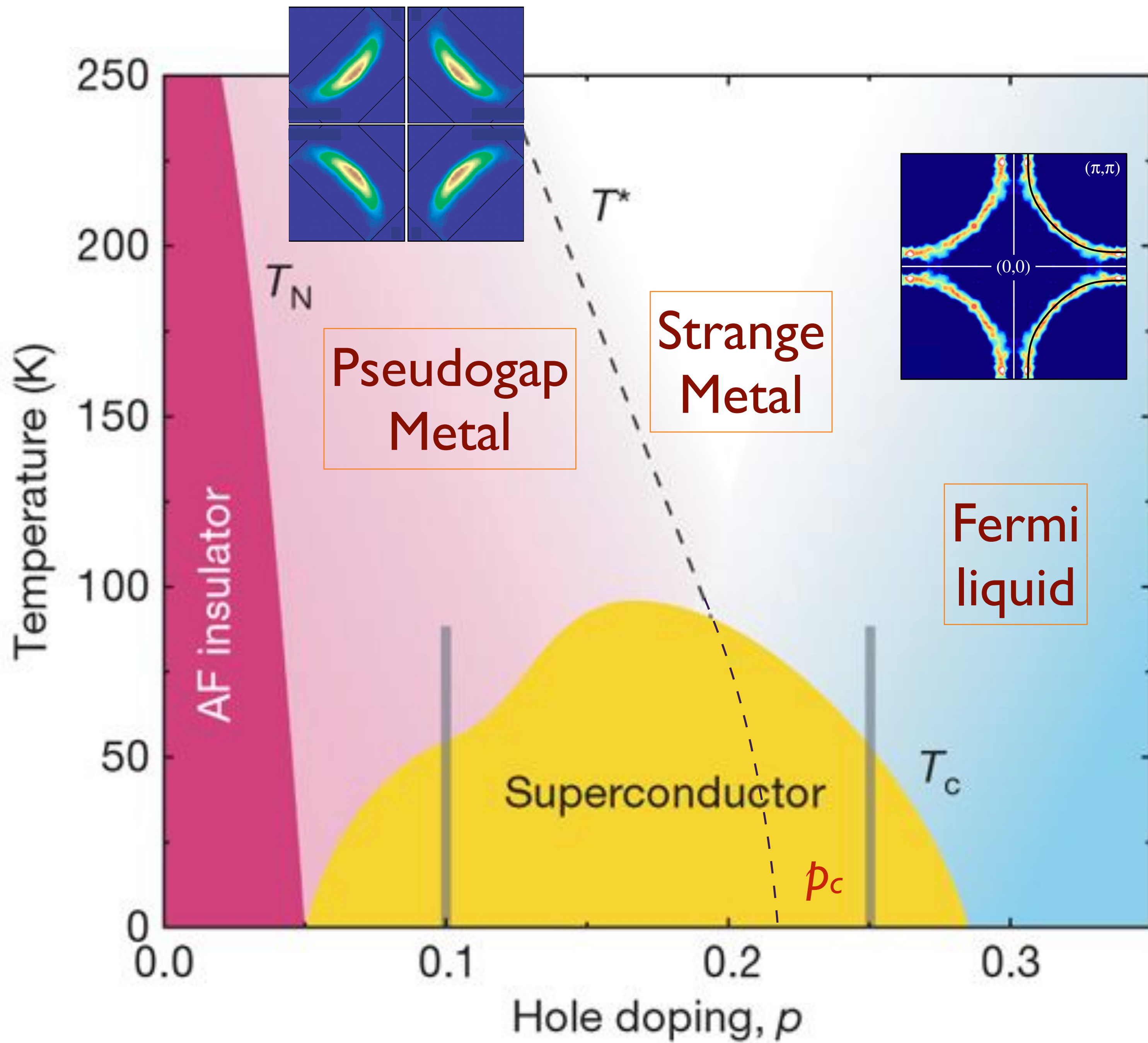
# Ultracold fermionic atoms in optical lattices

## Microscopic evolution of doped Mott insulators from polaronic metal to Fermi liquid

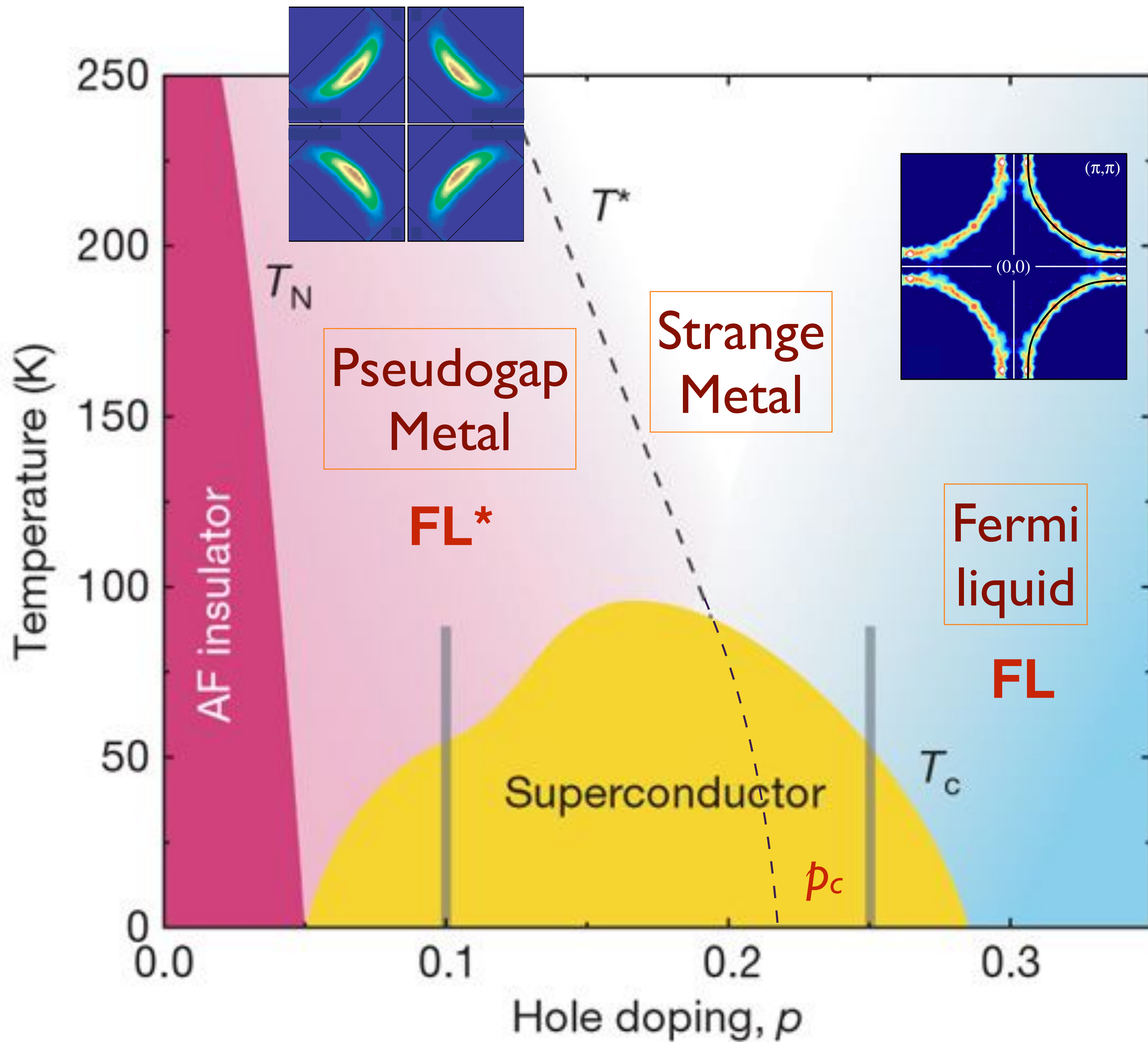
Joannis Koepsell, Dominik Bourgund, Pimonpan Sompet, Sarah Hirthe, Annabelle Bohrdt, Yao Wang, Fabian Grusdt, Eugene Demler, Guillaume Salomon, Christian Gross, Immanuel Bloch

*Science* **374** (2021) 82



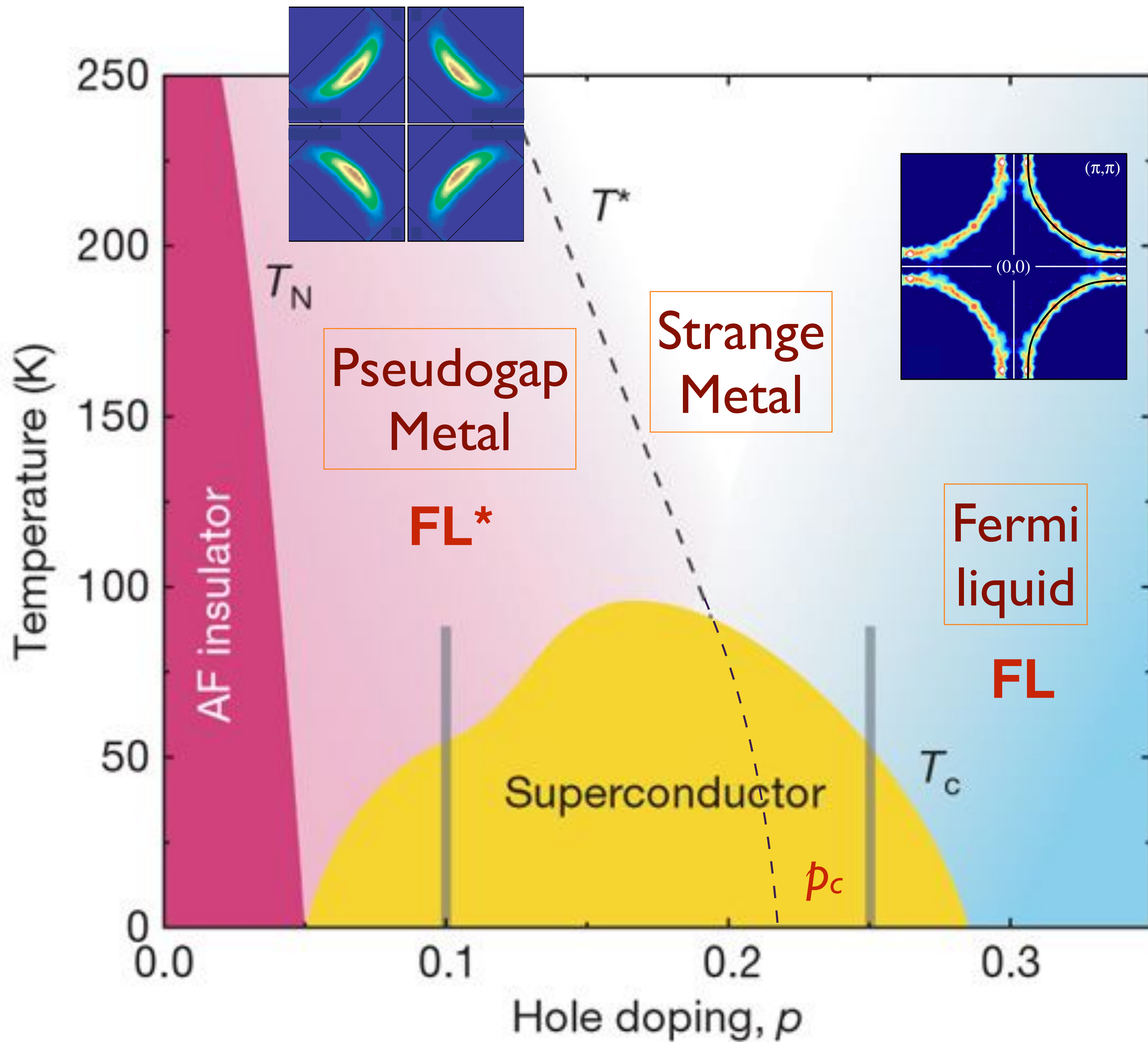






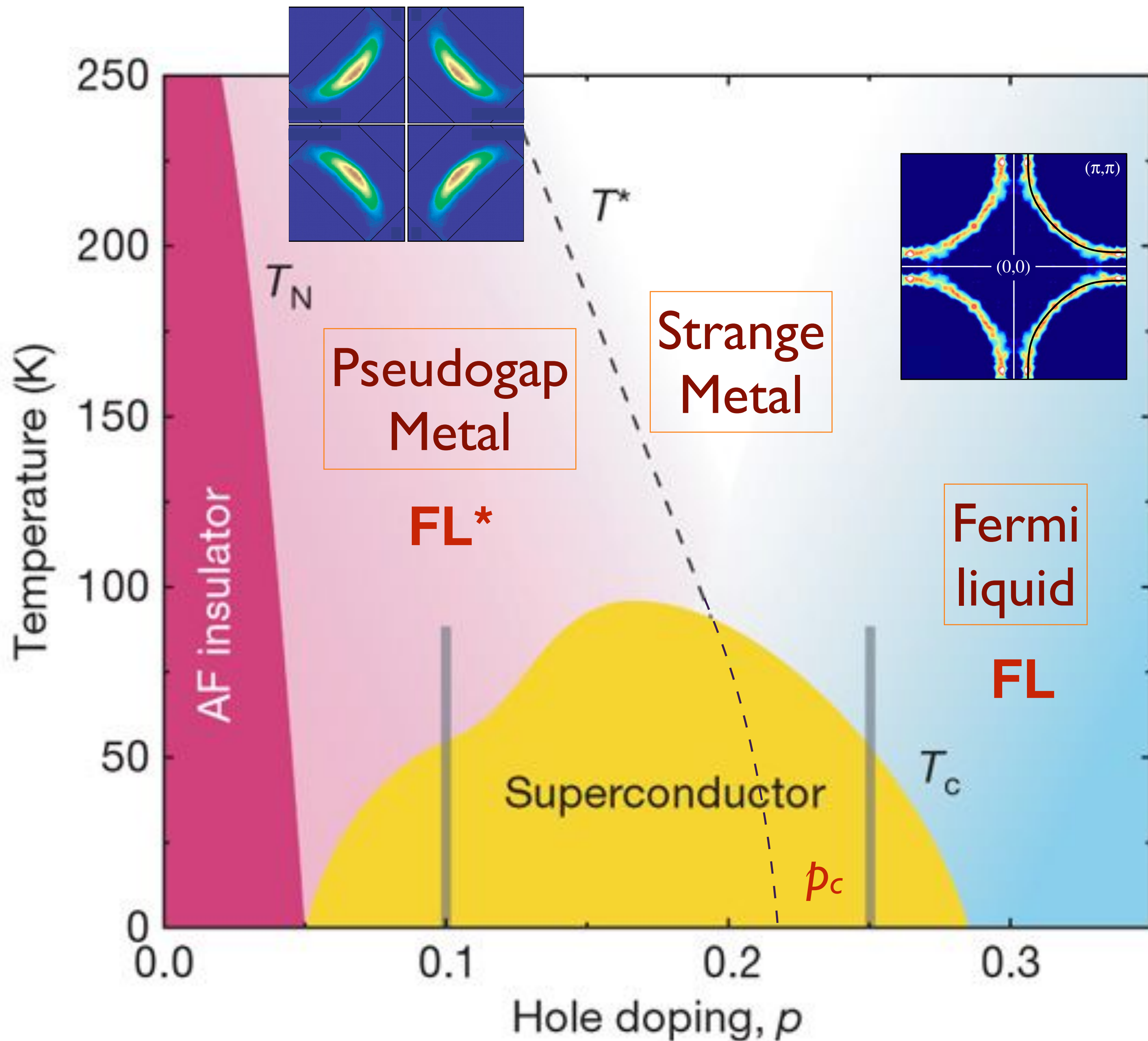
- View the pseudogap metal as quantum state (FL\*), which could be stable at  $T = 0$  under suitable conditions.





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- Start with a mean-field theory of  $FL^*$ , which yields a variational wavefunction.





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- Start with a mean-field theory of  $FL^*$ , which yields a variational wavefunction.
- $FL^*$  will serve as the ‘parent’ for the other regions in the phase diagram.



1. Paramagnon fractionalization theory of the Hubbard model

2. Photoemission in the cuprates

3. Confinement transitions from the pseudogap metal





**Yahui Zhang**

arXiv: 2001.09159

arXiv: 2103.05009



**Alexander  
Nikolaenko**

arXiv: 2006.01140

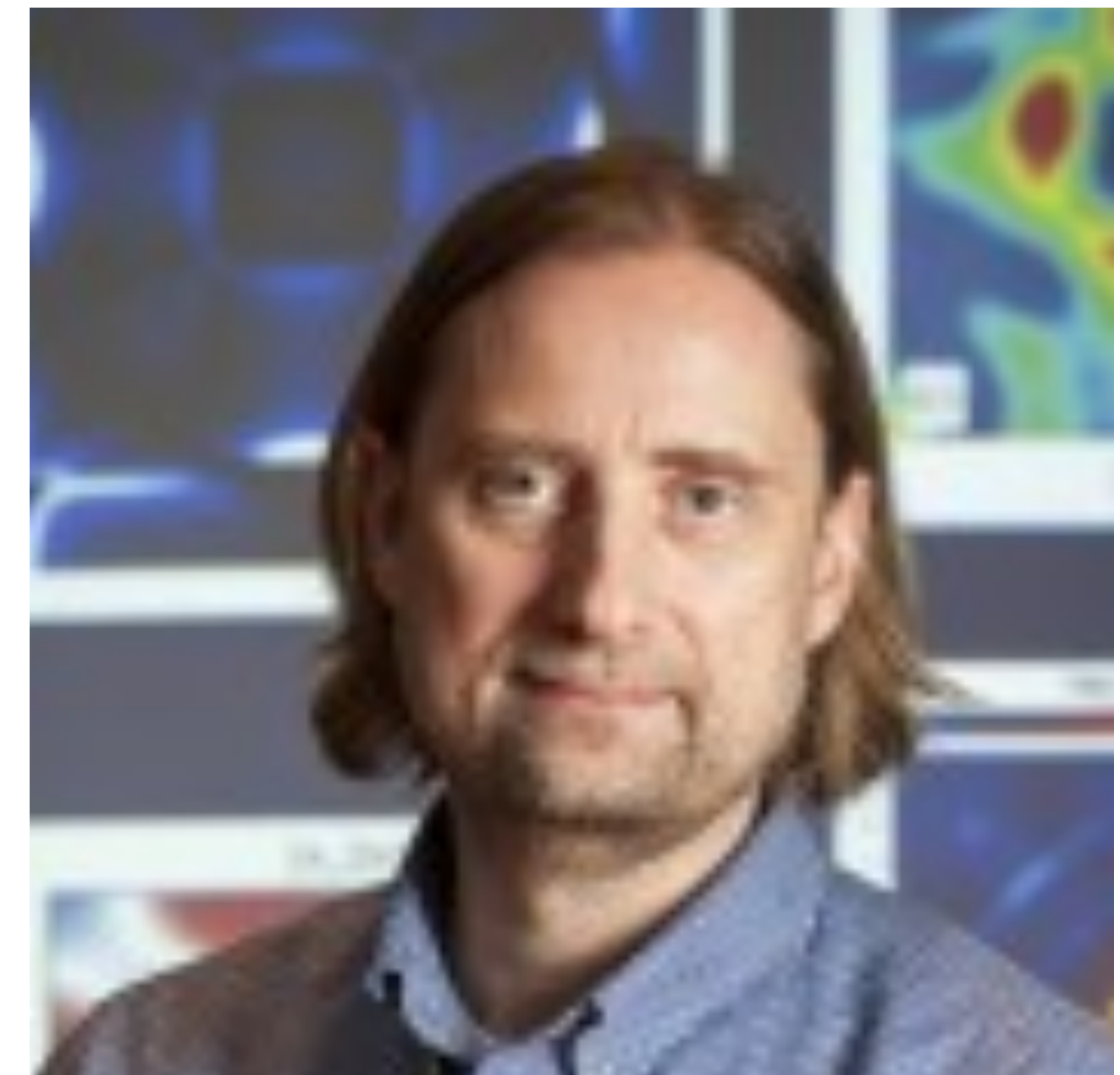
arXiv: 2111.13703



**Maria  
Tikhanovskaya**



**Eric Mascot**



**Dirk Morr**



# 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  $i$ ):

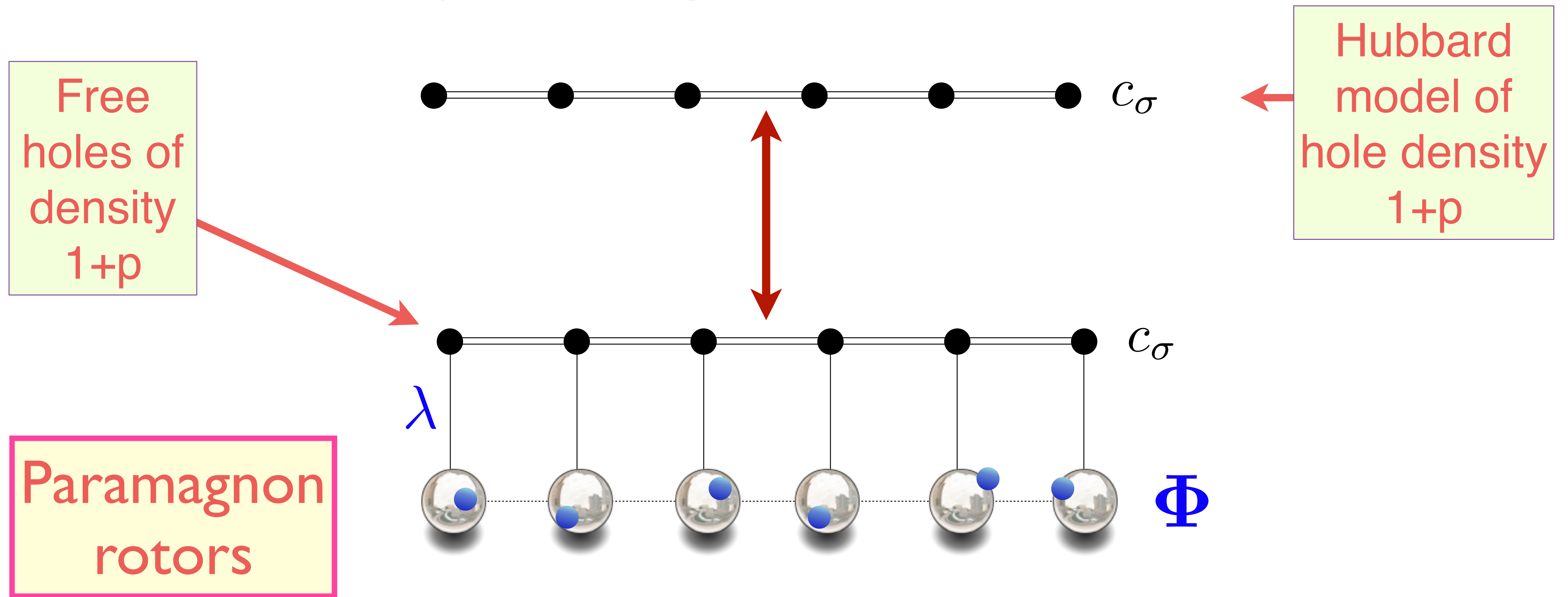
$$U \left( n_\uparrow - \frac{1}{2} \right) \left( n_\downarrow - \frac{1}{2} \right) = -\frac{2U}{3} \mathbf{S}^2 + \frac{U}{4}$$

Then we decouple the interaction via

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

This yields the ‘Scalapino-Pines-Chubukov-Schmalian...’ theory for a ‘paramagnon quantum rotor’  $\Phi_i$  coupled to otherwise free fermions  $c_{i\sigma}$ .

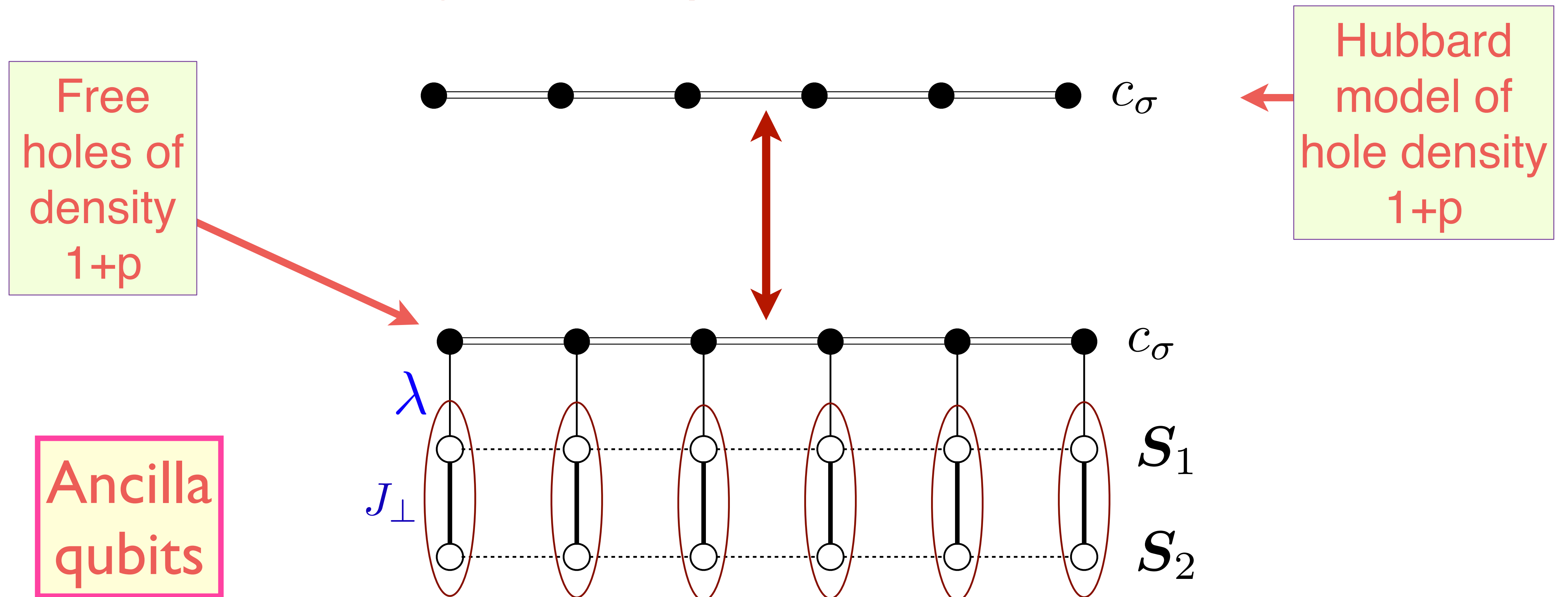
# Paramagnon theory of the Hubbard model



$$\mathcal{H}_{\text{paramagnon}} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} - \lambda \sum_i c_{i\sigma}^\dagger \frac{\tau_{\sigma\sigma'}}{2} c_{i\sigma'} \cdot \Phi_i + \frac{J_\perp}{2} \sum_i P_{\Phi_i}^2 + \sum_i V(\Phi_i) + \dots$$

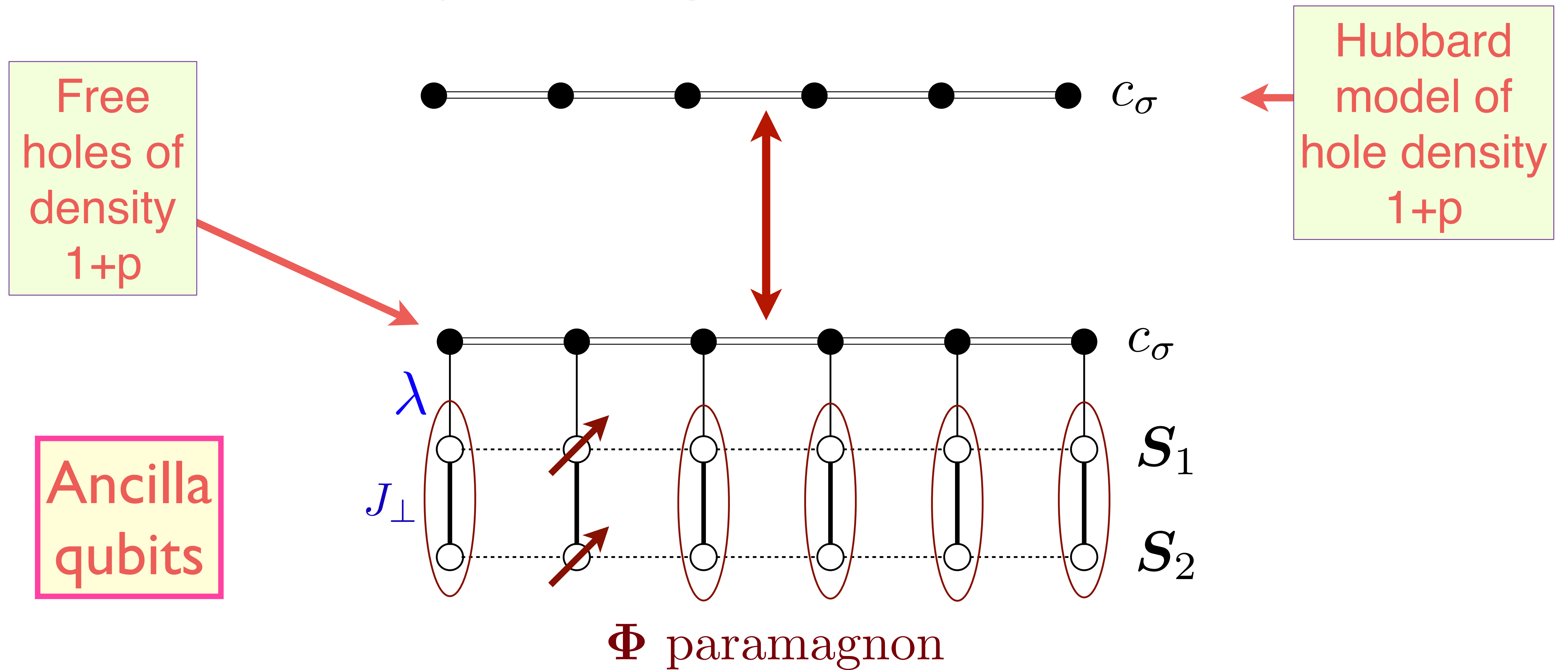


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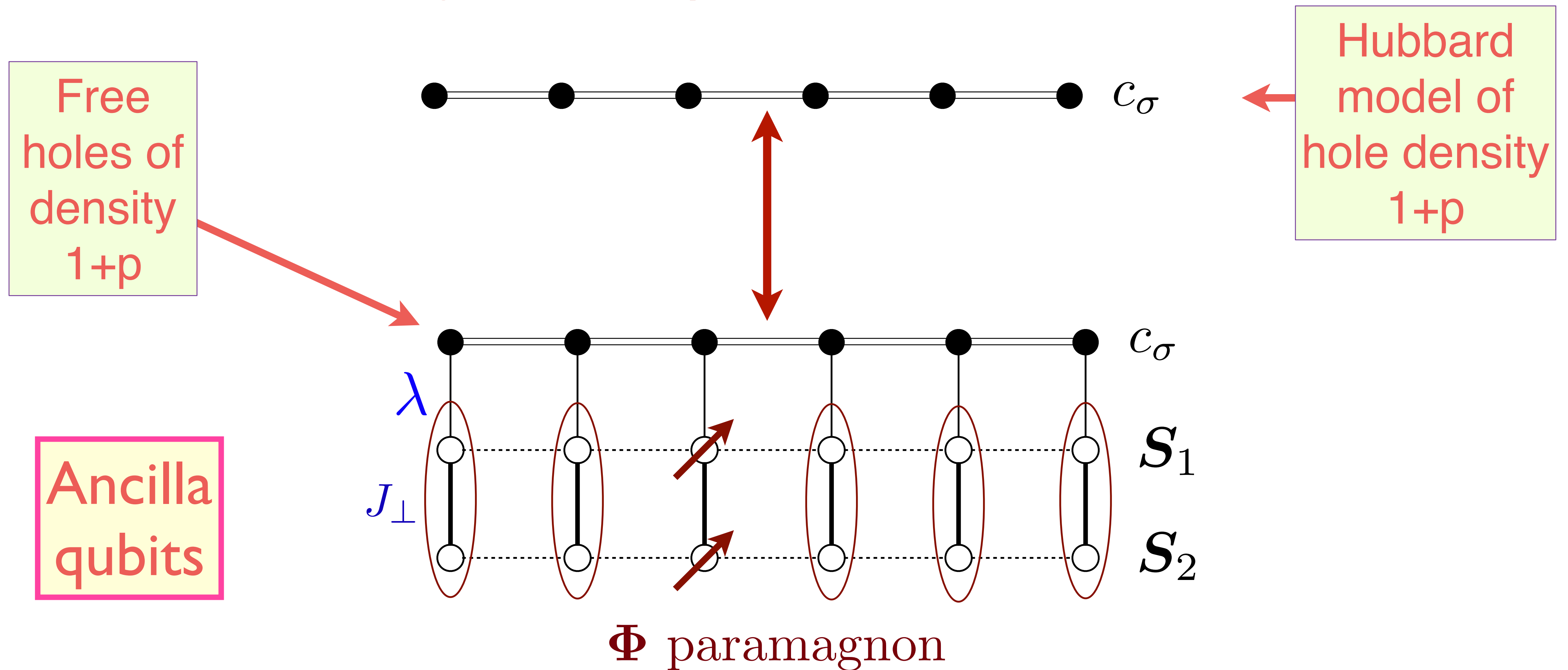
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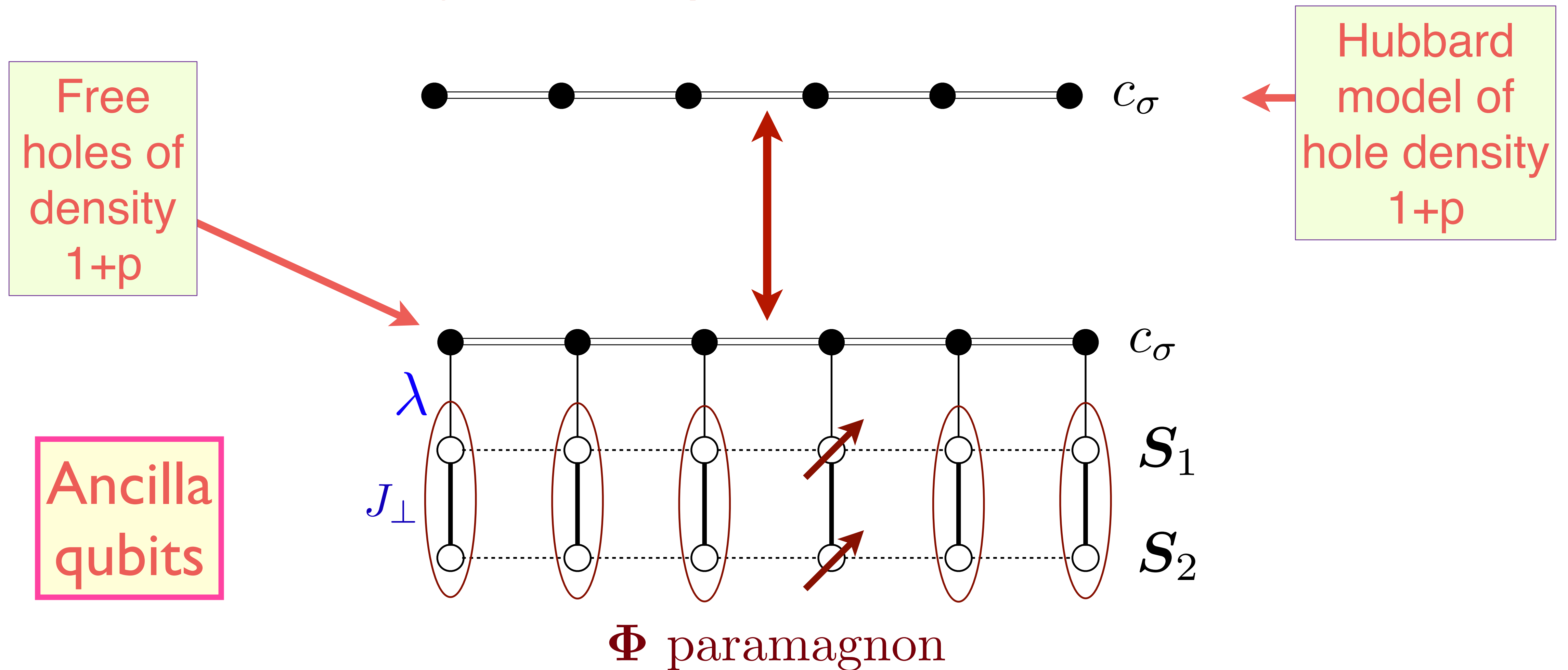


# Paramagnon theory of the Hubbard model



$$\mathcal{H}_{\text{paramagnon}} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c_{\mathbf{p}\sigma}^{\dagger} c_{\mathbf{p}\sigma} - \lambda \sum_i c_{i\sigma}^{\dagger} \frac{\tau_{\sigma\sigma'}}{2} c_{i\sigma'} \cdot \Phi_i + \frac{J_{\perp}}{2} \sum_i P_{\Phi_i}^2 + \sum_i V(\Phi_i) + \dots$$

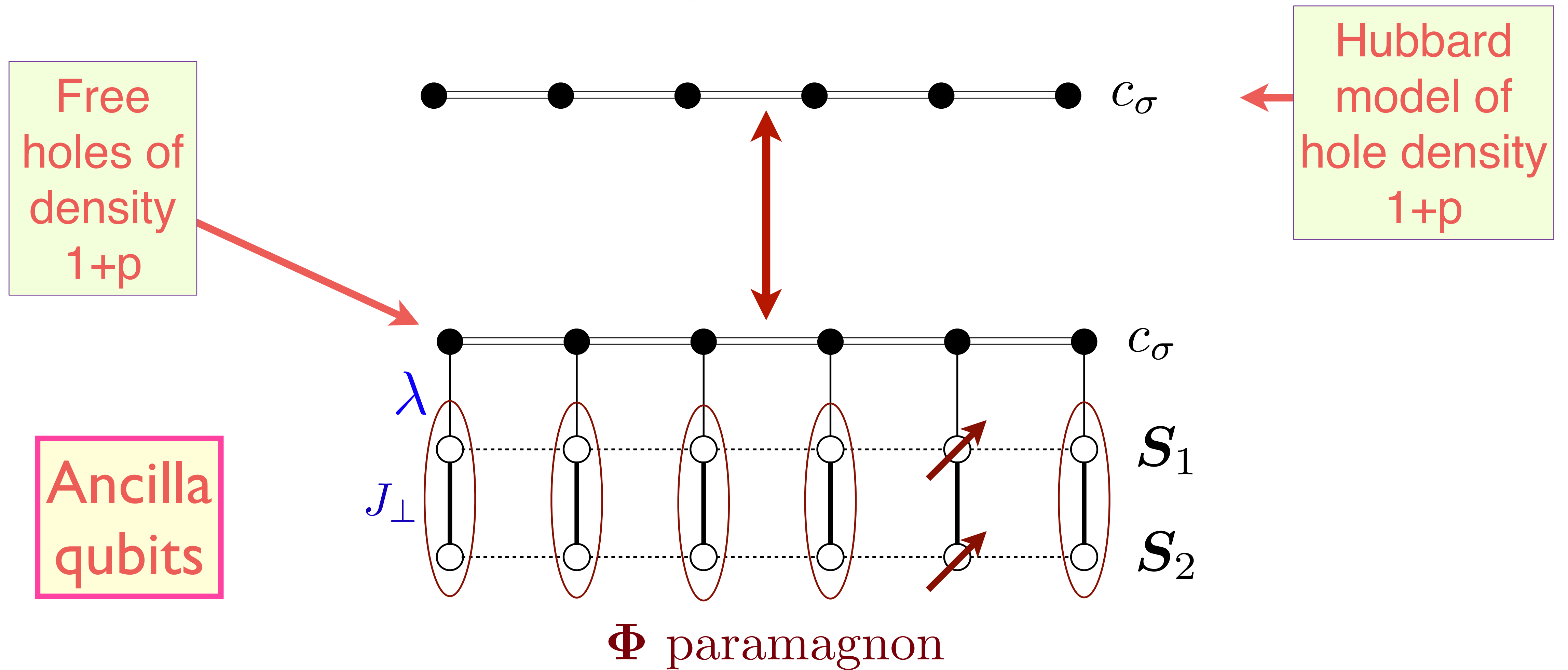
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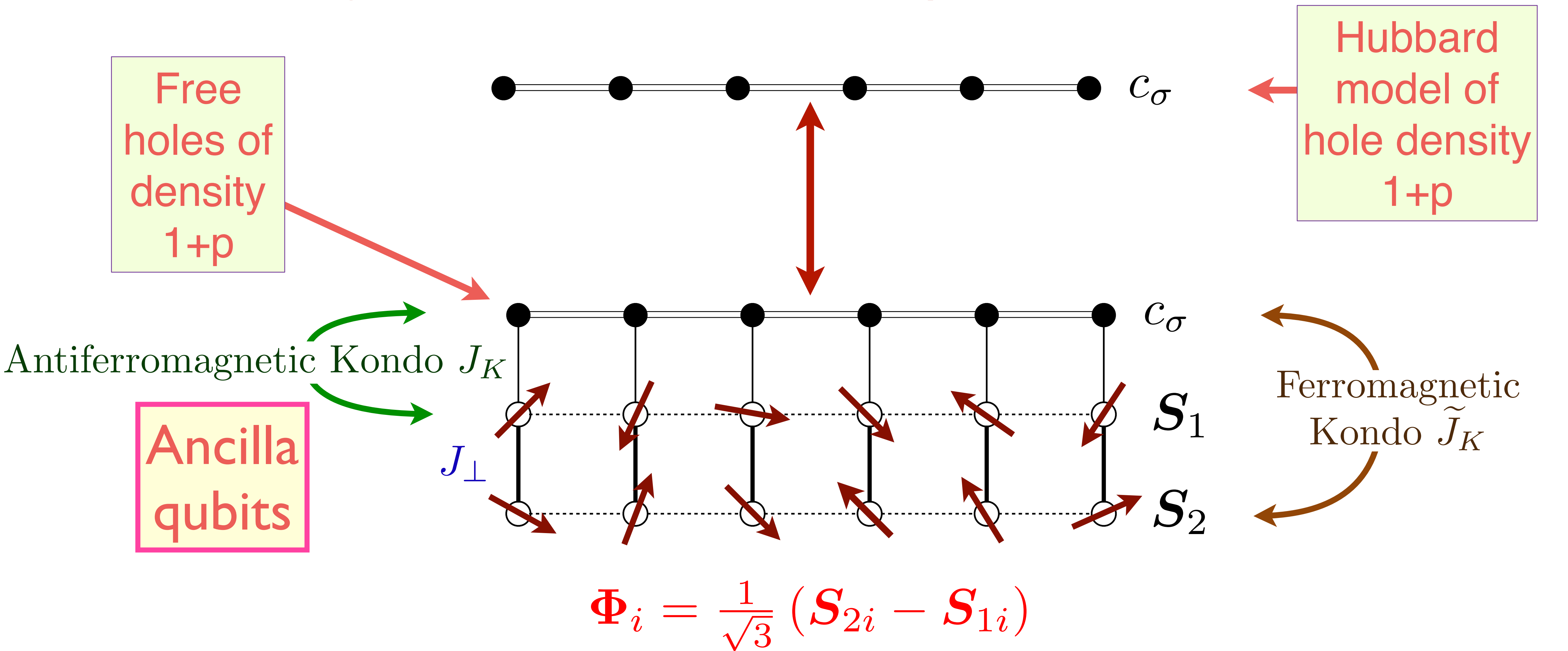


# Paramagnon theory of the Hubbard model



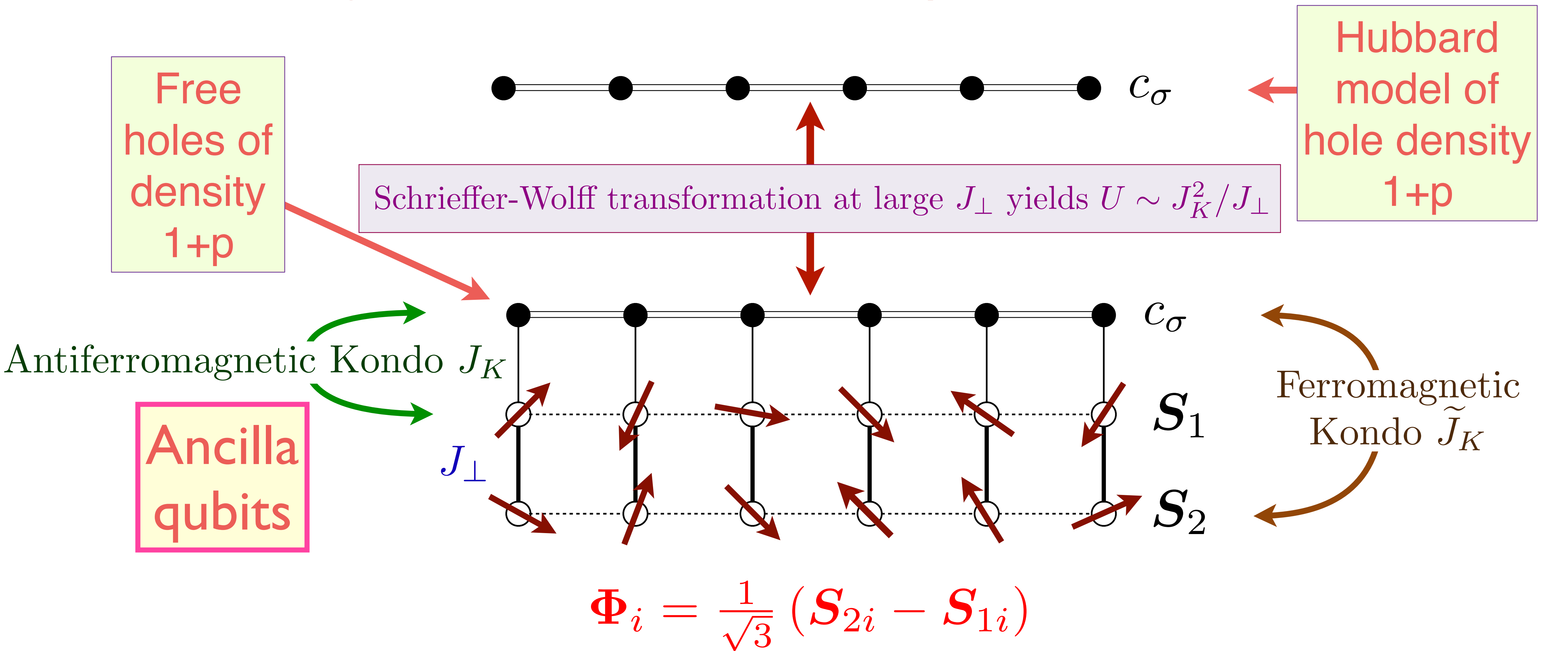
$$\mathcal{H}_{\text{paramagnon}} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} - \lambda \sum_i c_{i\sigma}^\dagger \frac{\tau_{\sigma\sigma'}}{2} c_{i\sigma'} \cdot \Phi_i + \frac{J_\perp}{2} \sum_i P_{\Phi_i}^2 + \sum_i V(\Phi_i) + \dots$$

# Paramagnon fractionalization theory of the Hubbard model



$$\mathcal{H}_{\text{paramagnon}} = \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} c_{\mathbf{p}\sigma}^{\dagger} c_{\mathbf{p}\sigma} + J_K \sum_i c_{i\sigma}^{\dagger} \frac{\tau_{\sigma\sigma'}}{2} c_{i\sigma'} \cdot \mathbf{S}_{1i} - \tilde{J}_K \sum_i c_{i\sigma}^{\dagger} \frac{\tau_{\sigma\sigma'}}{2} c_{i\sigma'} \cdot \mathbf{S}_{2i} + \dots$$

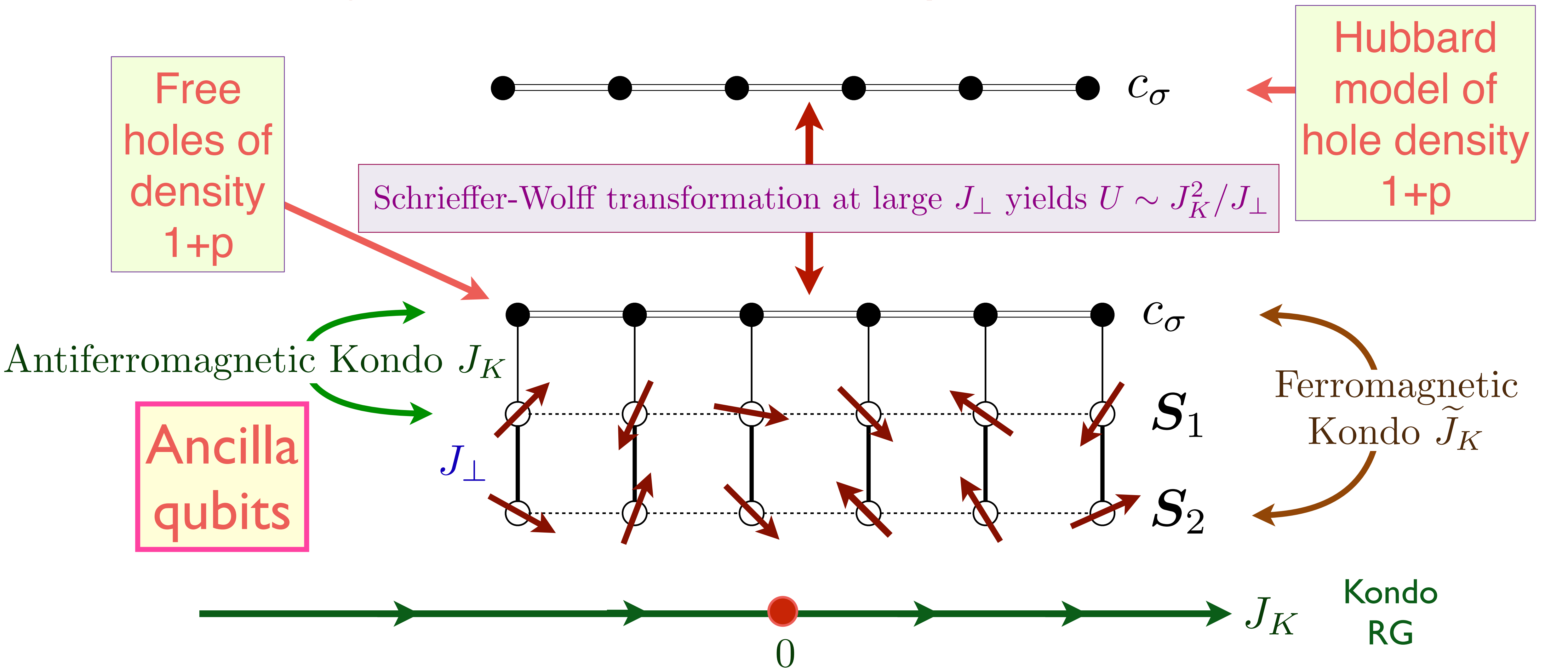
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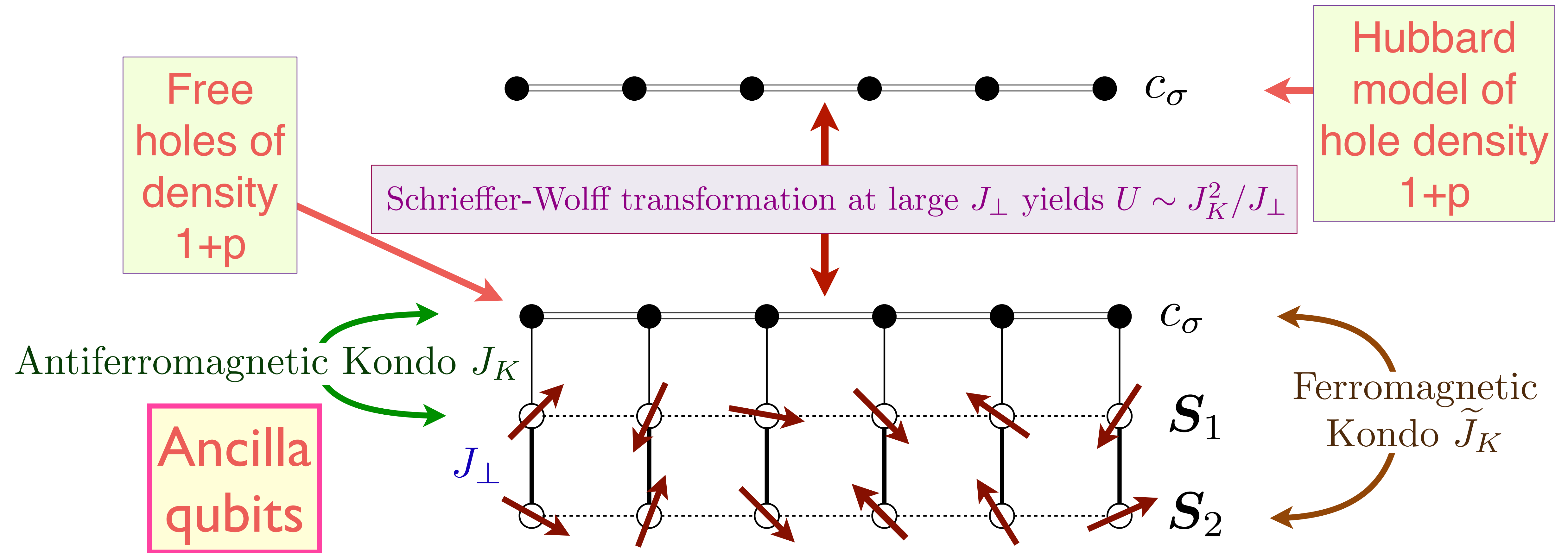


# Paramagnon fractionalization theory of the Hubbard model



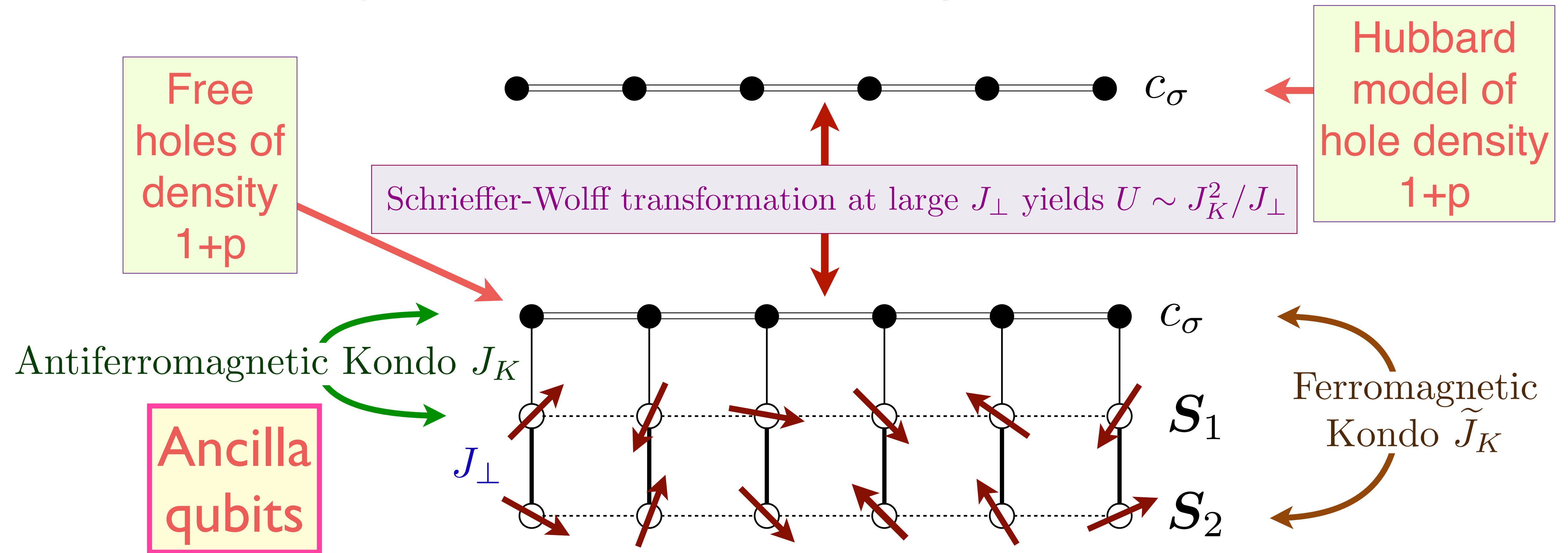
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# Paramagnon fractionalization theory of the Hubbard model



A FL\* state is realized when the antiferromagnetic Kondo coupling dominates over  $J_\perp$ , and the  $c_\sigma$  and  $S_1$  form a heavy Fermi liquid state (as found in the heavy fermion compounds) of hole density  $(1+p) + 1 = 2+p = p \text{ mod } 2!$

# Paramagnon fractionalization theory of the Hubbard model

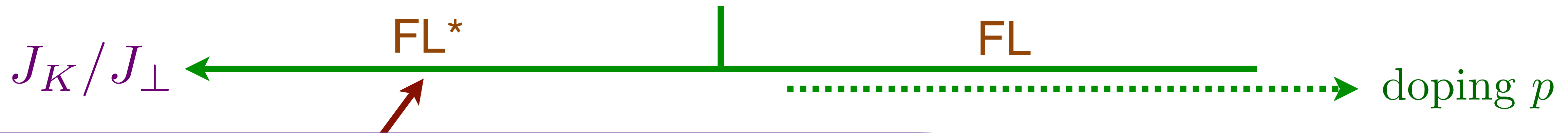
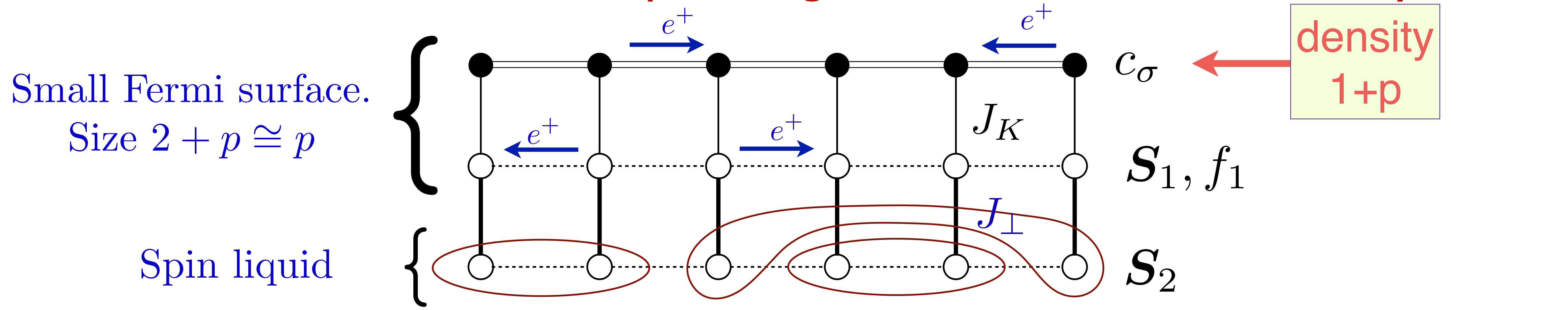


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The  $S_2$  must form an 'odd' spin liquid which does not break translational symmetry, to obtain a metal with a non-Luttinger volume Fermi surface.



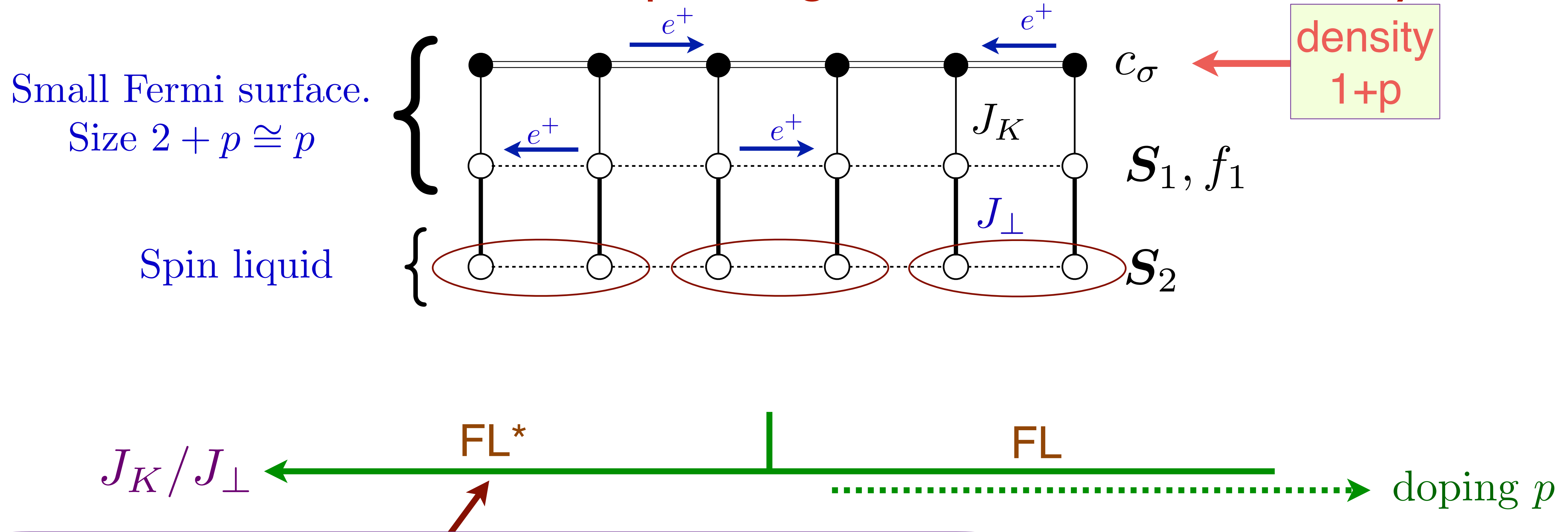
# Trial wavefunctions in the paramagnon fractionalization theory



Small Fermi surface of size  $p$

$$\begin{aligned}
 |\text{FL}^*\rangle = & [\text{Projection onto rung singlets of } S_1, S_2] \\
 & \bowtie |\text{Slater determinant of } (c, f_1)\rangle \\
 & \otimes |\text{Spin liquid of } S_2\rangle
 \end{aligned}$$

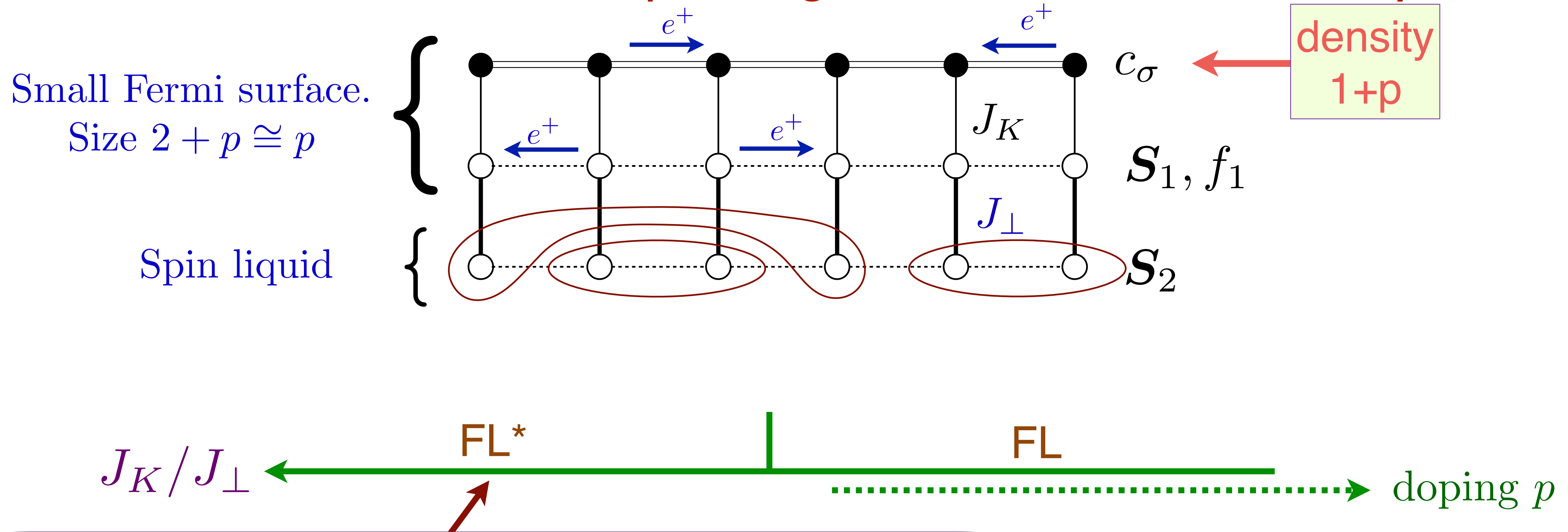
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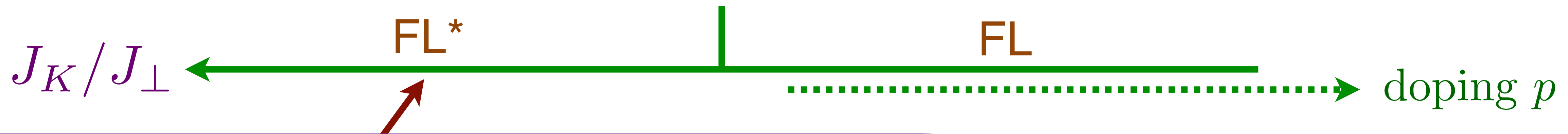
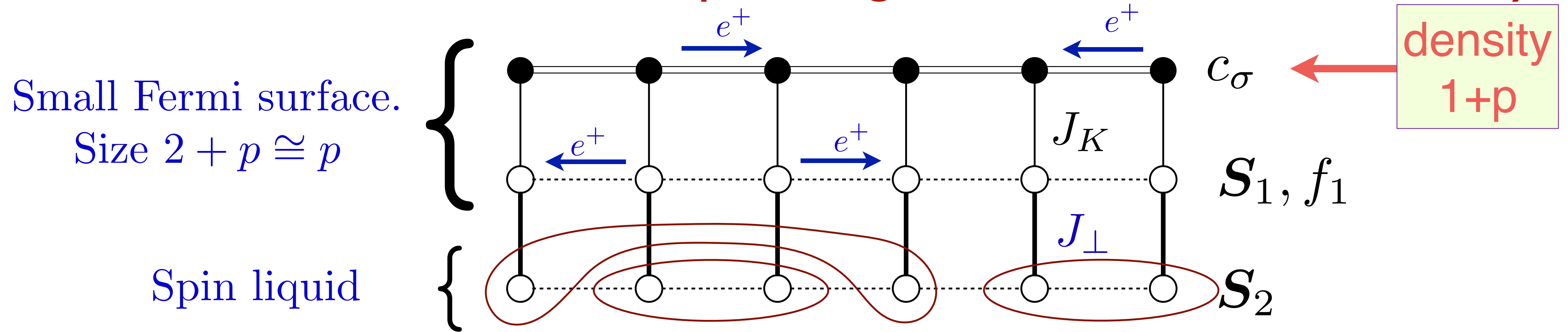


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# Trial wavefunctions in the paramagnon fractionalization theory

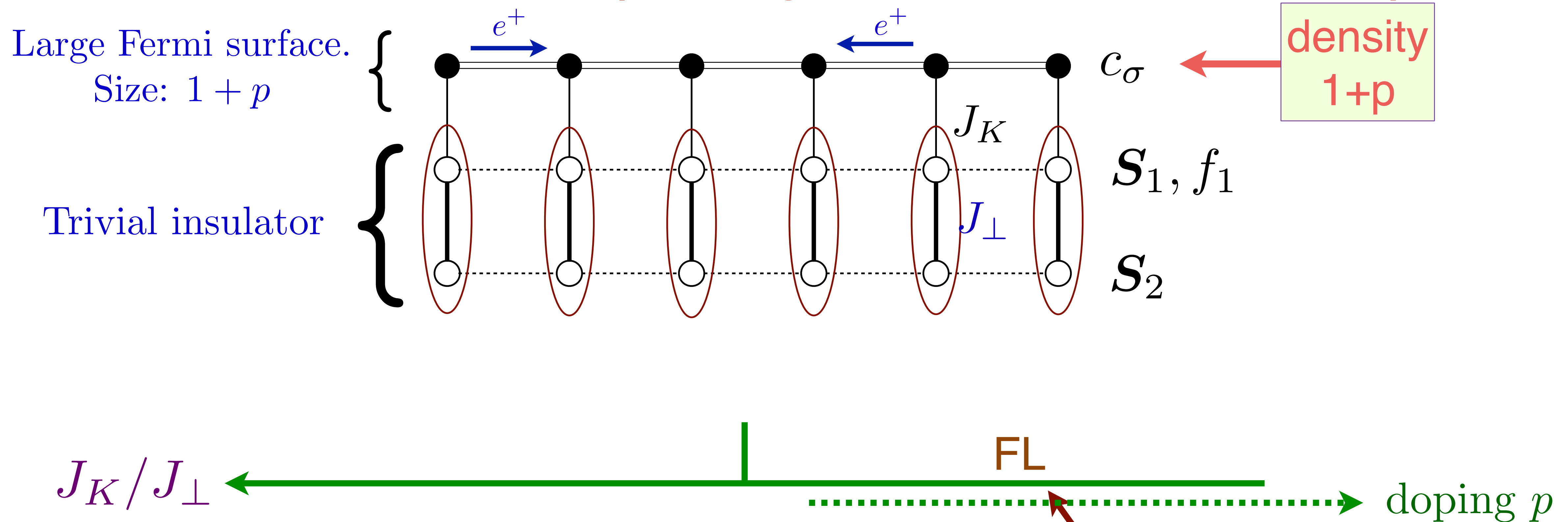


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 \end{aligned}$$

Pseudogap metal =  
Kondo Lattice Heavy  
Fermi Liquid  
 $\oplus$   
Spin Liquid

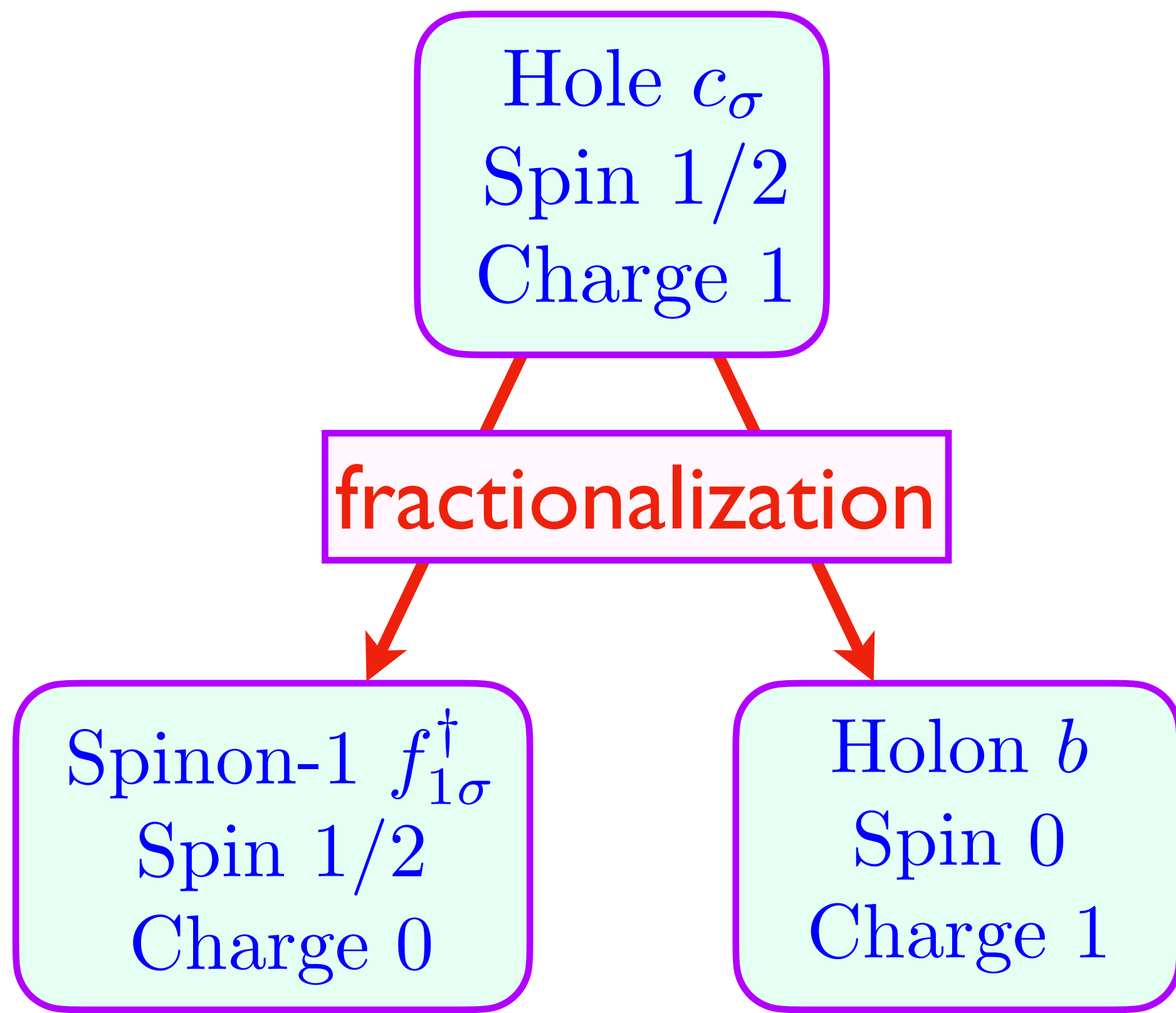
# Trial wavefunctions in the paramagnon fractionalization theory



Large Fermi surface of size  $1 + p$

$|\text{FL}\rangle = |\text{Rung singlets of } \mathcal{S}_1, \mathcal{S}_2\rangle$

$\otimes |\text{Slater determinant of } c\rangle$



## Electron fractionalization



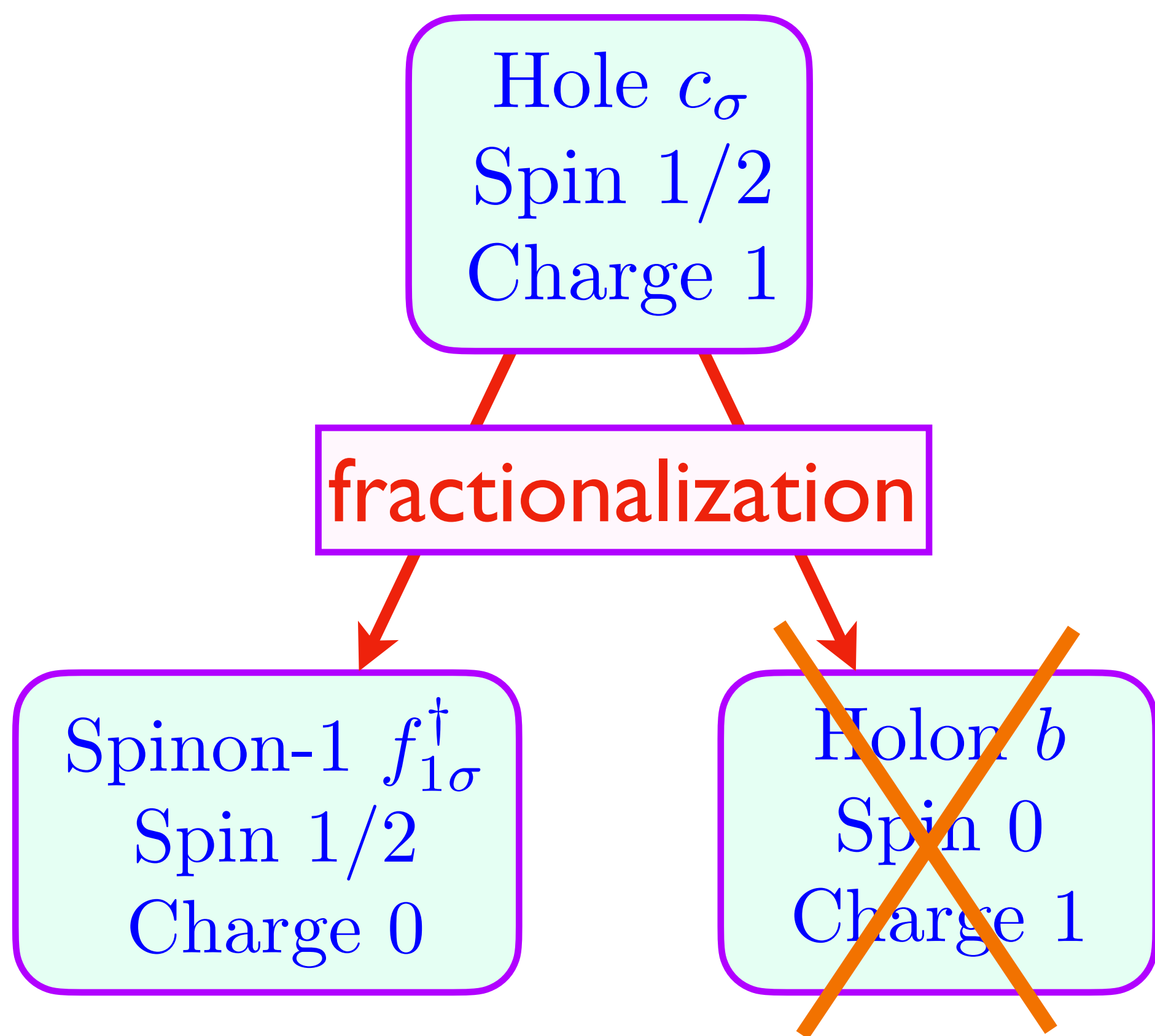
Hole  $c_\sigma$   
Spin  $1/2$   
Charge 1

**fractionalization**

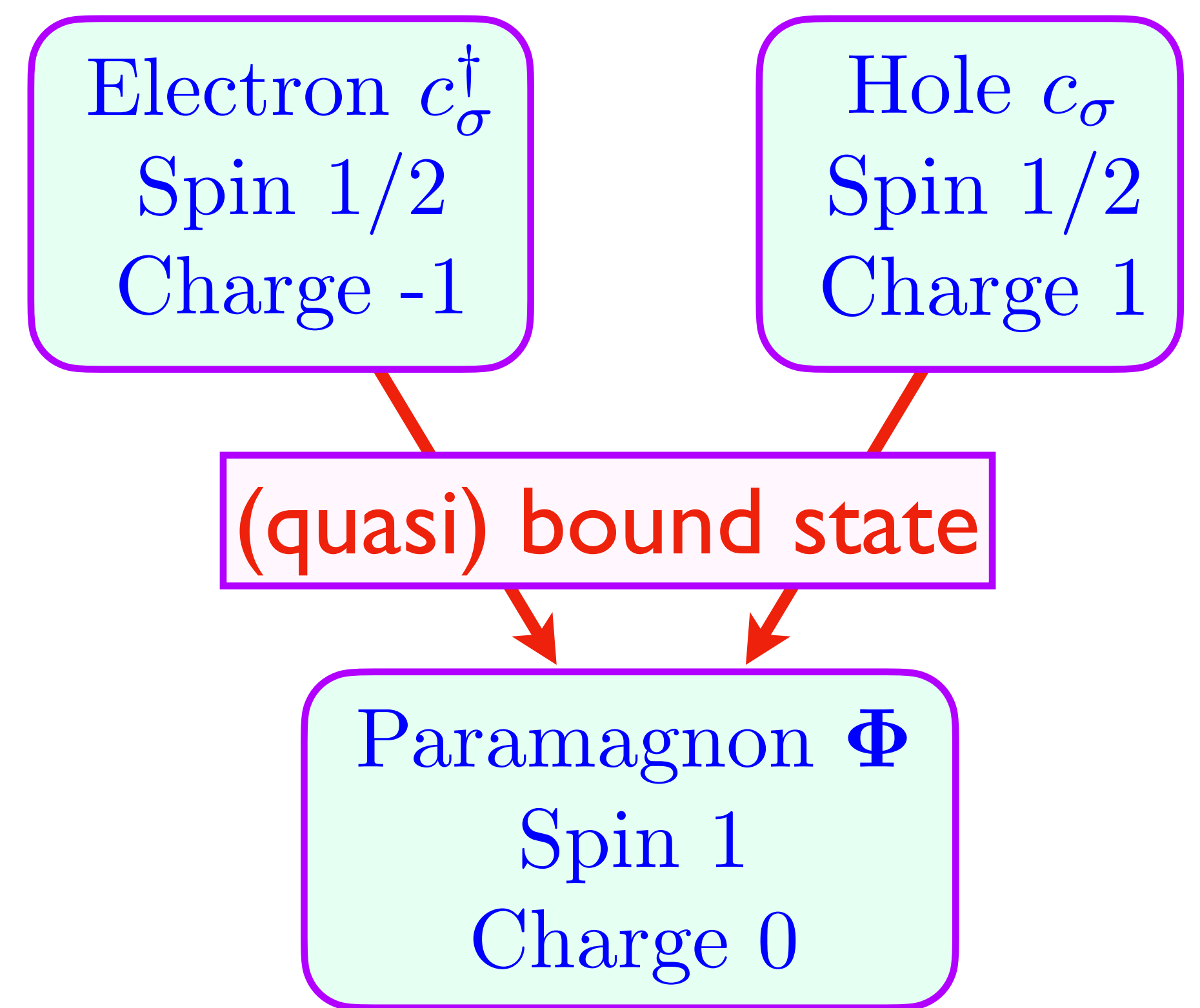
Spinon-1  $f_{1\sigma}^\dagger$   
Spin  $1/2$   
Charge 0

~~Holon  $b$   
Spin 0  
Charge 1~~

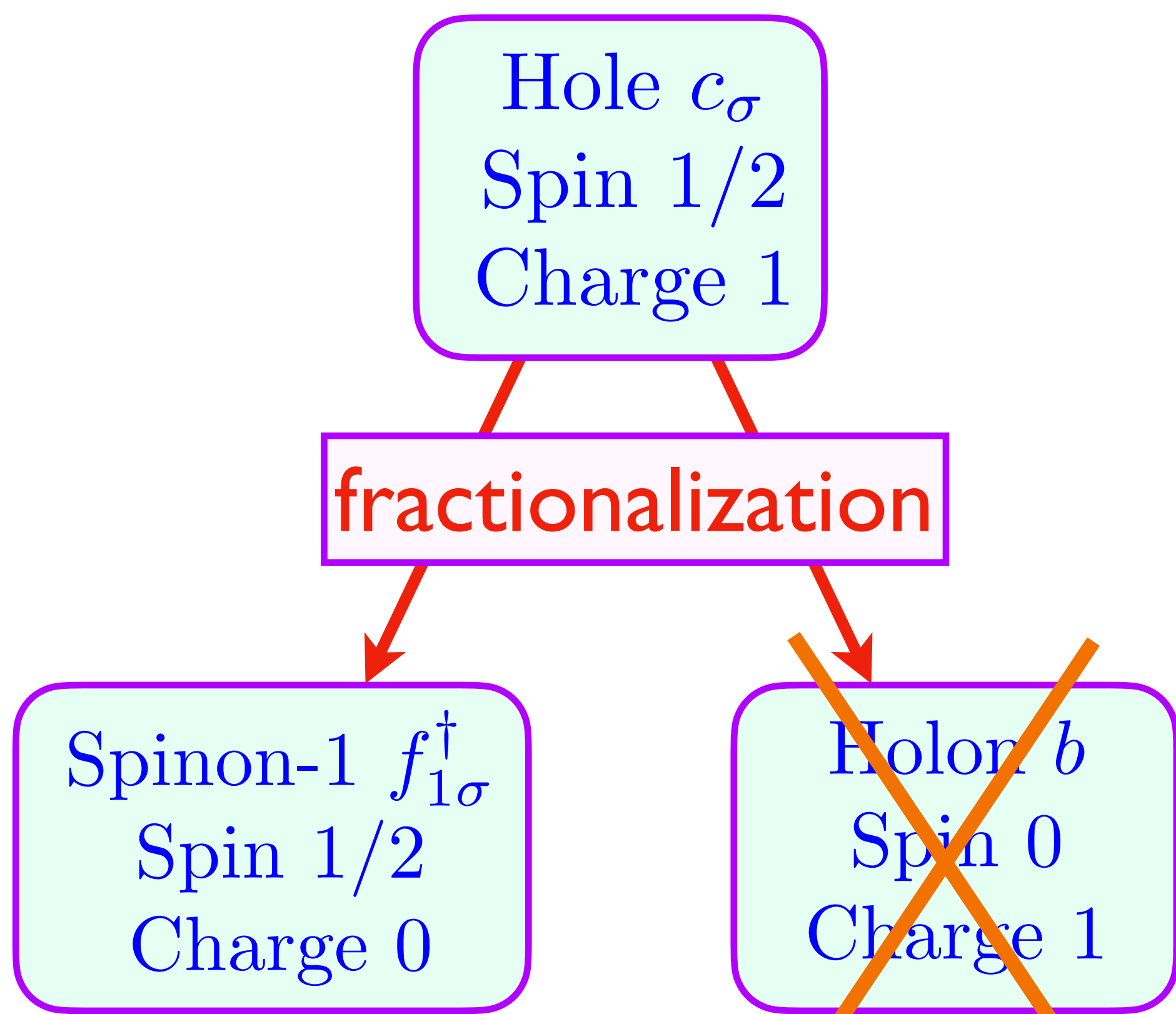
**Electron fractionalization**



Electron fractionalization

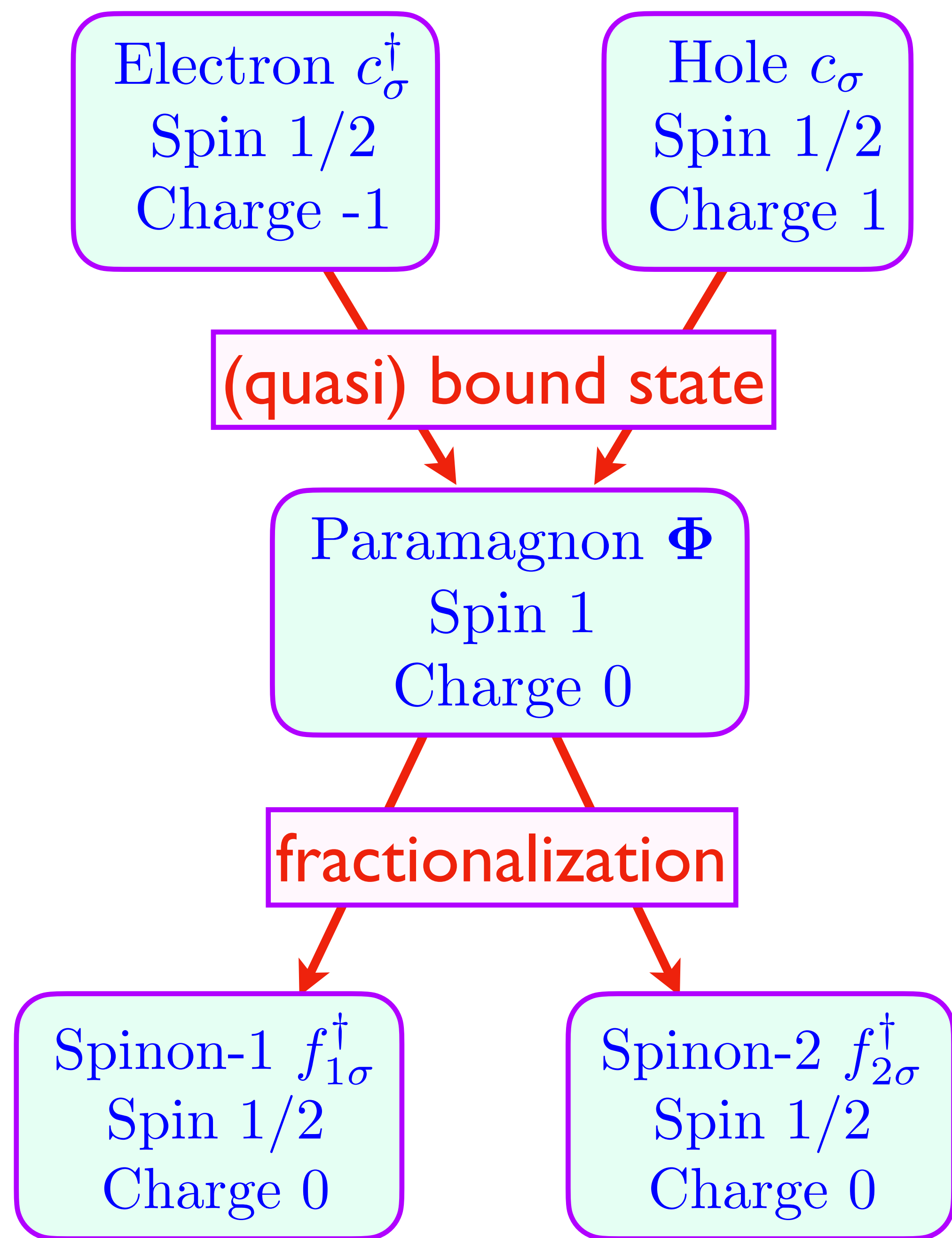


Don't fractionalize the electron;  
fractionalize the paramagnon!



Electron fractionalization

Don't fractionalize the electron;  
fractionalize the paramagnon!



Paramagnon fractionalization

1. Paramagnon fractionalization theory of the Hubbard model

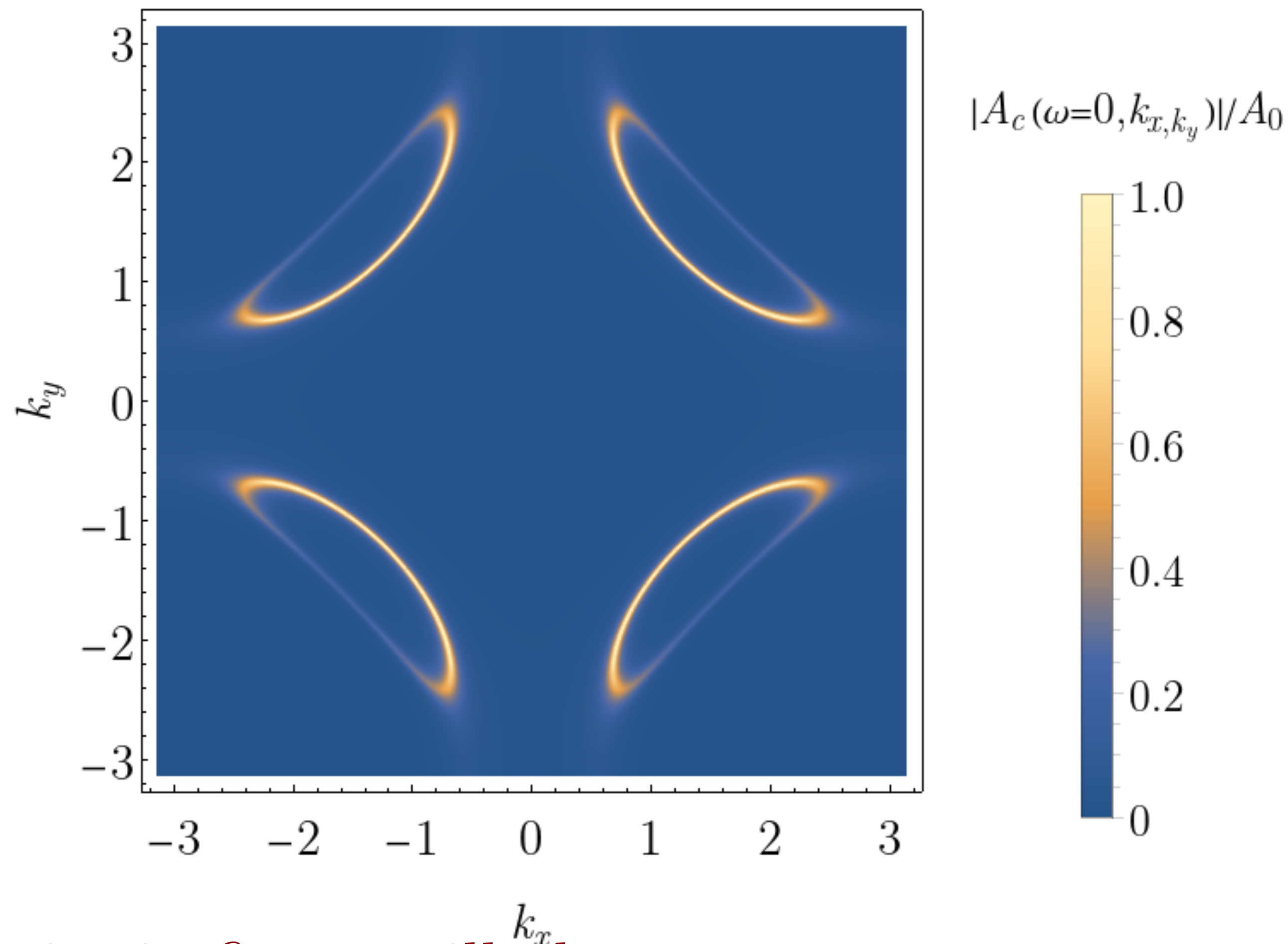
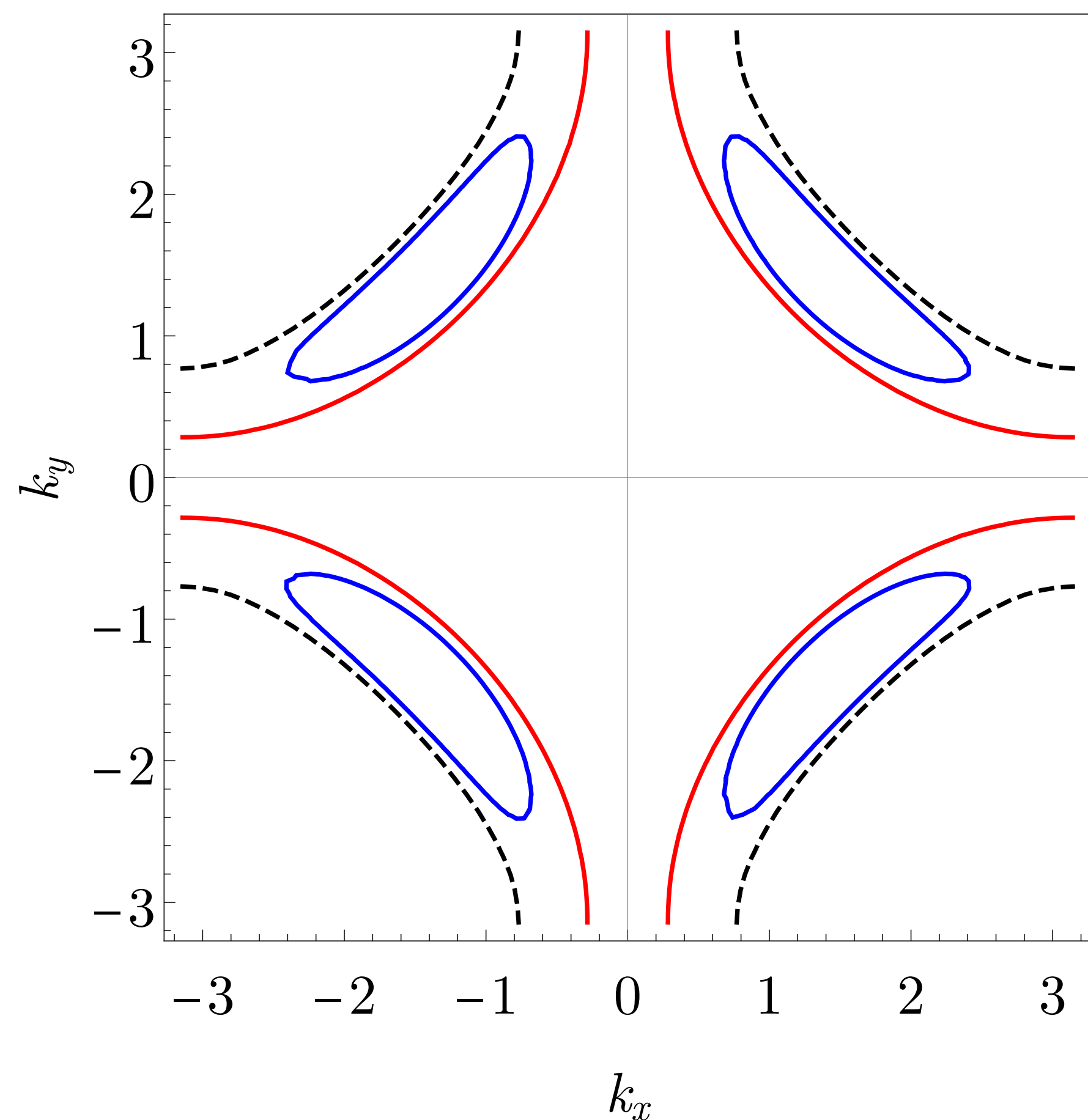
2. Photoemission in the cuprates

3. Confinement transitions from the pseudogap metal



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

# “Fermi arc” spectral functions

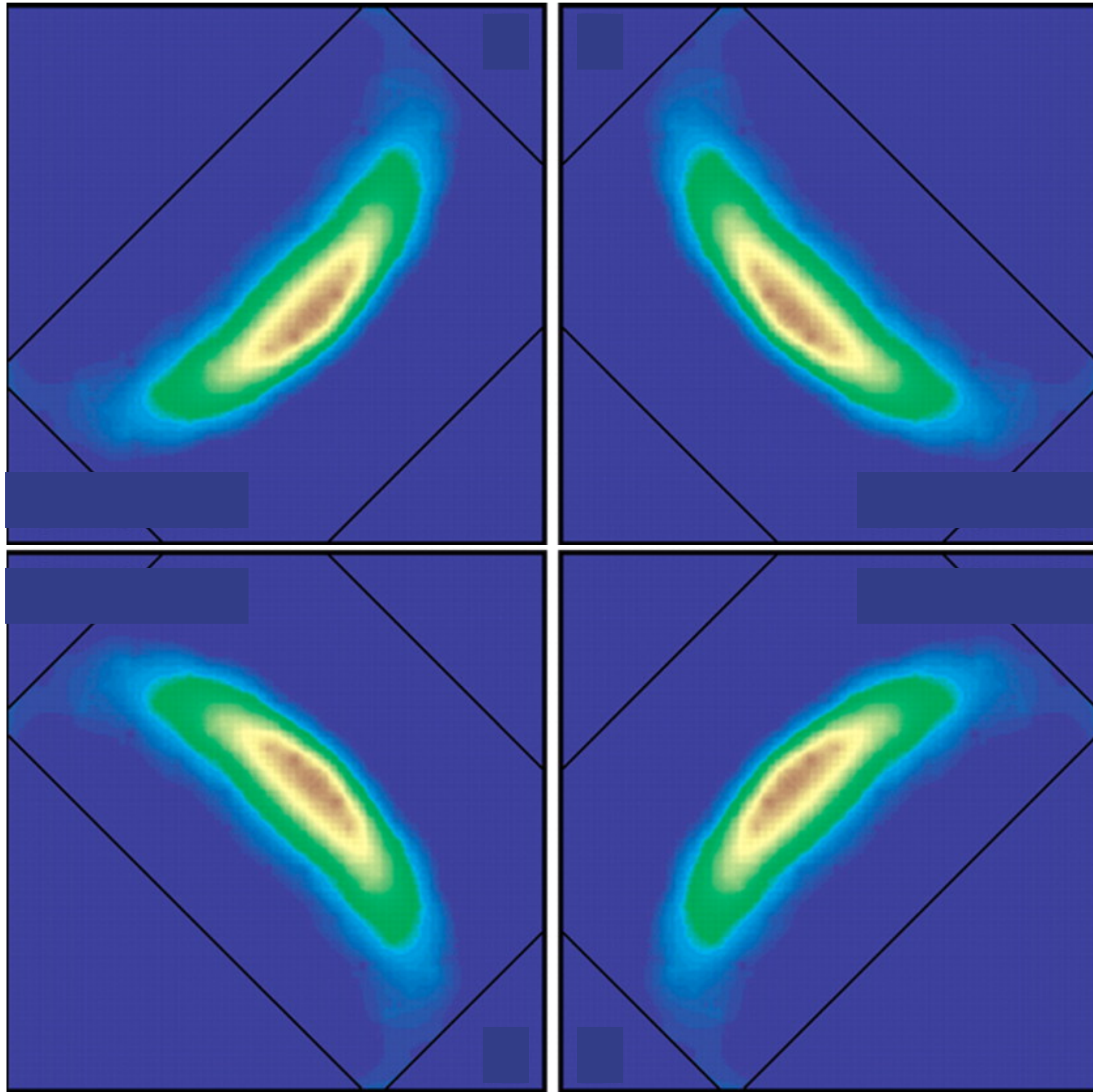


**FL\***: Condensate  $B$  breaks gauge symmetries in first ancilla layer.

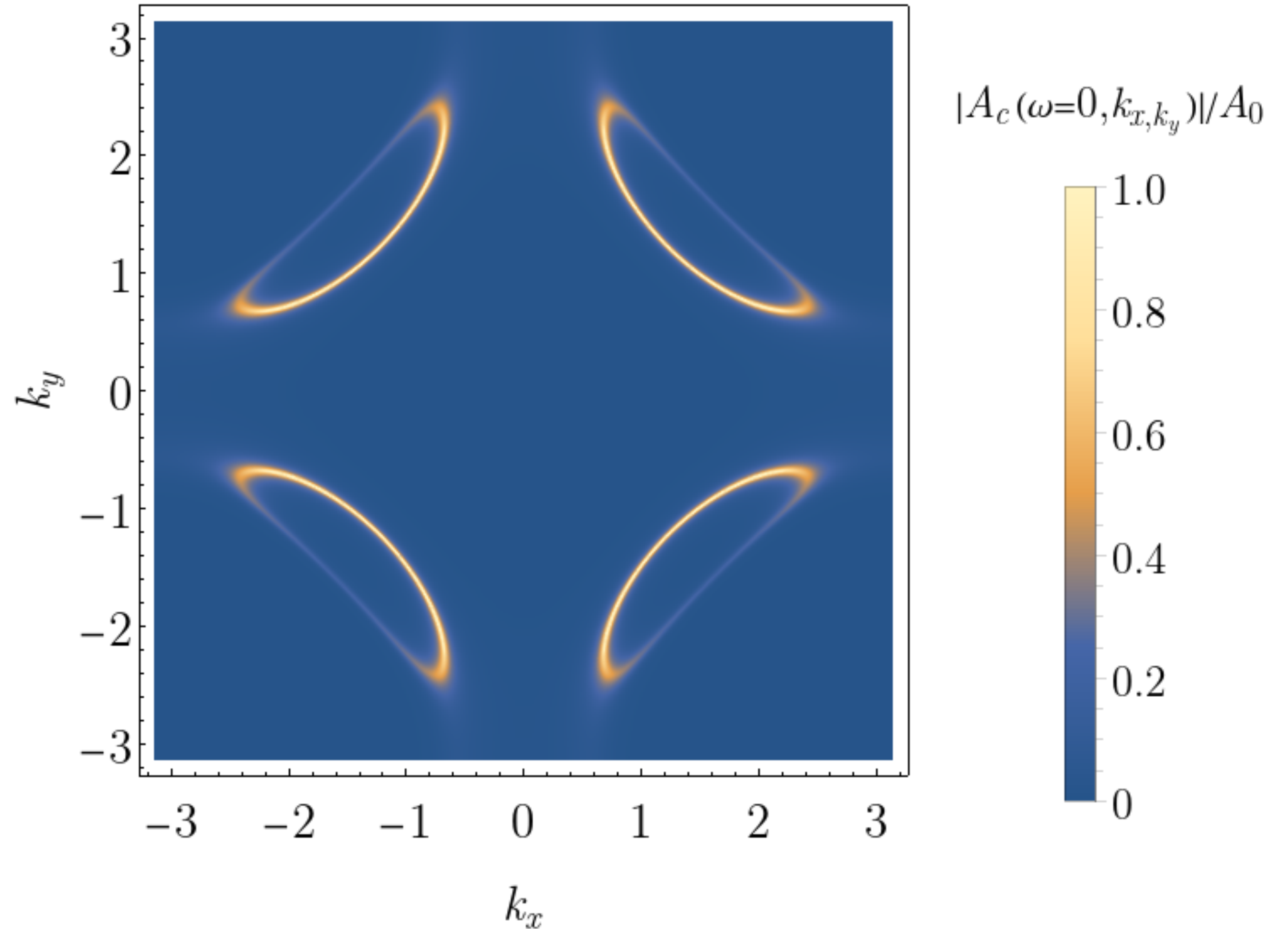
$$H = - \sum_{i,j} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,j} t_{1,ij} f_{1i\sigma}^\dagger f_{1j\sigma} + \sum_i B (c_{i\sigma}^\dagger f_{1i\sigma} + f_{1i\sigma}^\dagger c_{i\sigma})$$

Precursors:  
 Kai-Yu Yang, T. M. Rice, Fu-Chun Zhang,  
 PRB **73**, 174501 (2006)  
 Yang Qi, SS, PRB **81**, 115129 (2010)  
 Eun-Gook Moon, SS,  
 PRB **83**, 224508 (2011)

# Photoemission at small $p$



$\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$   
at  $x = 0.10$

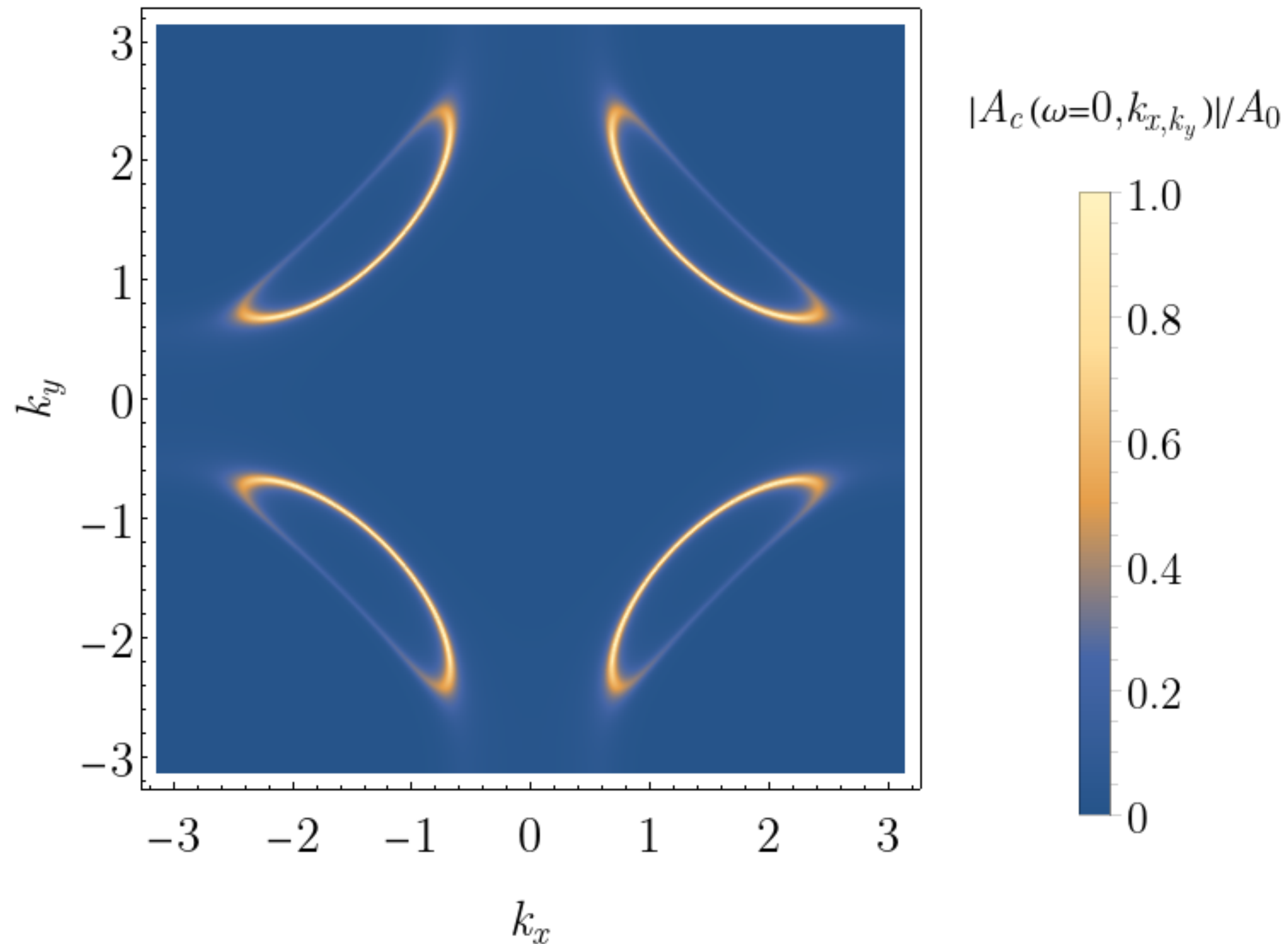
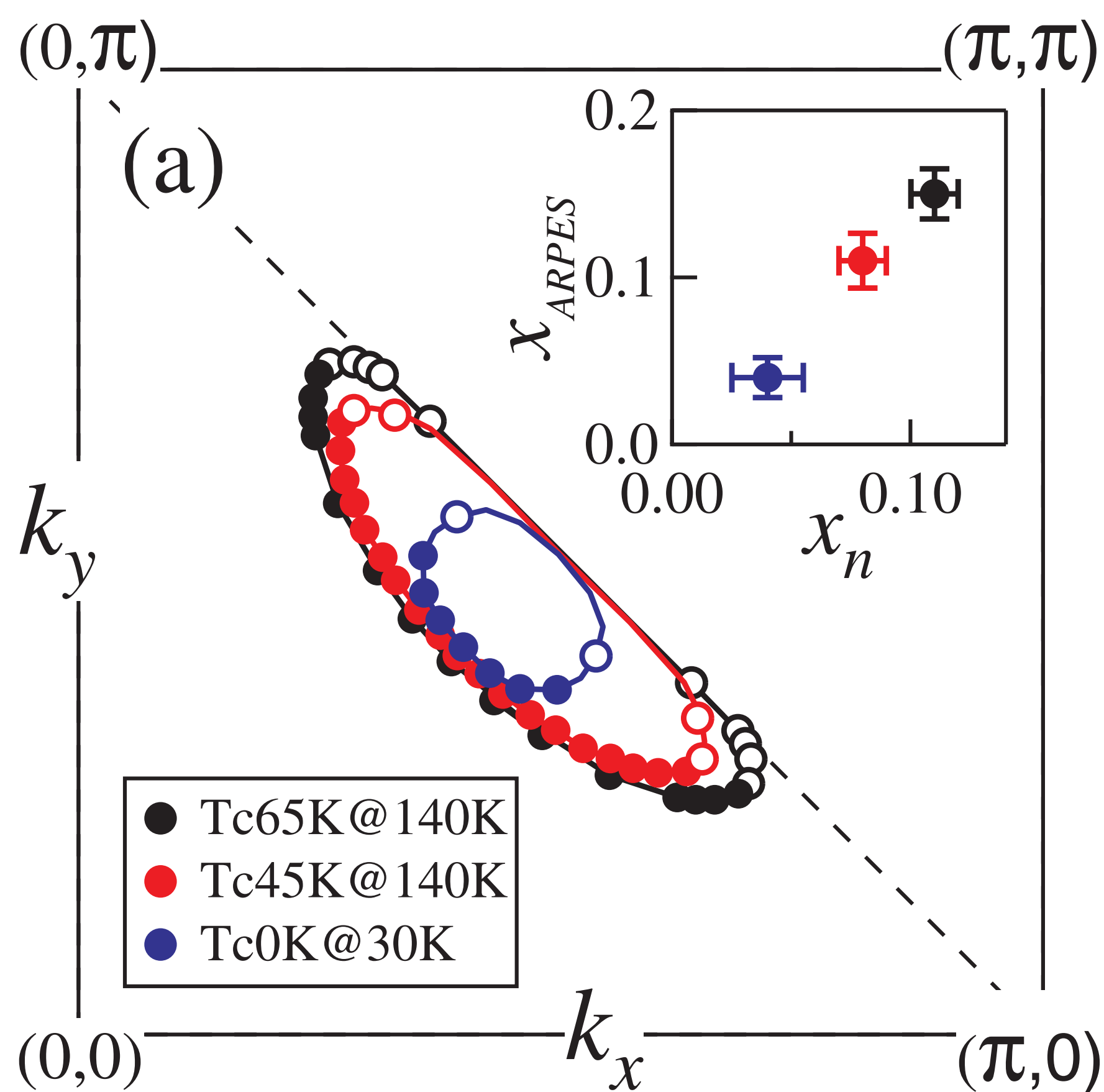


“*Fermi arcs*”

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)

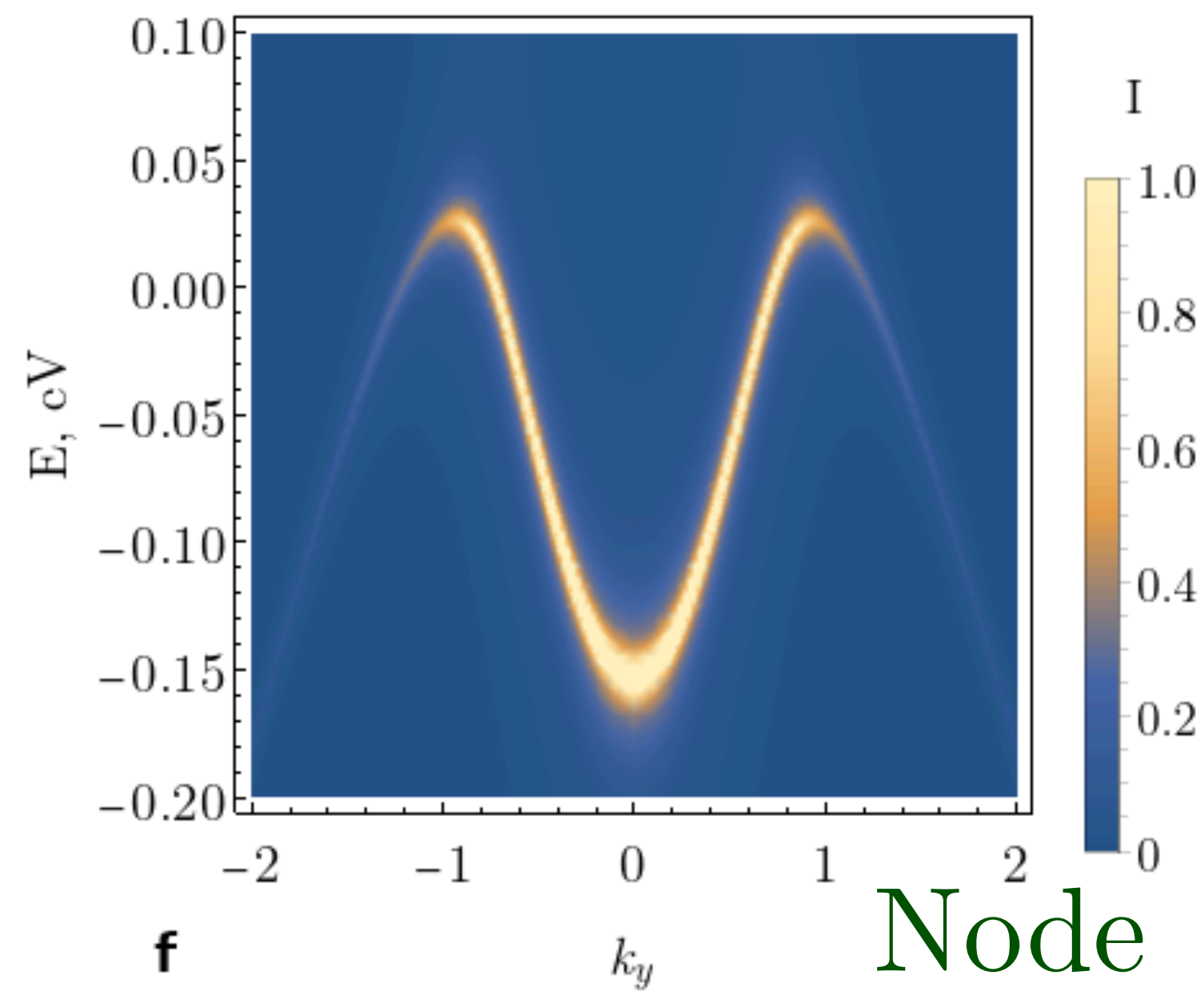
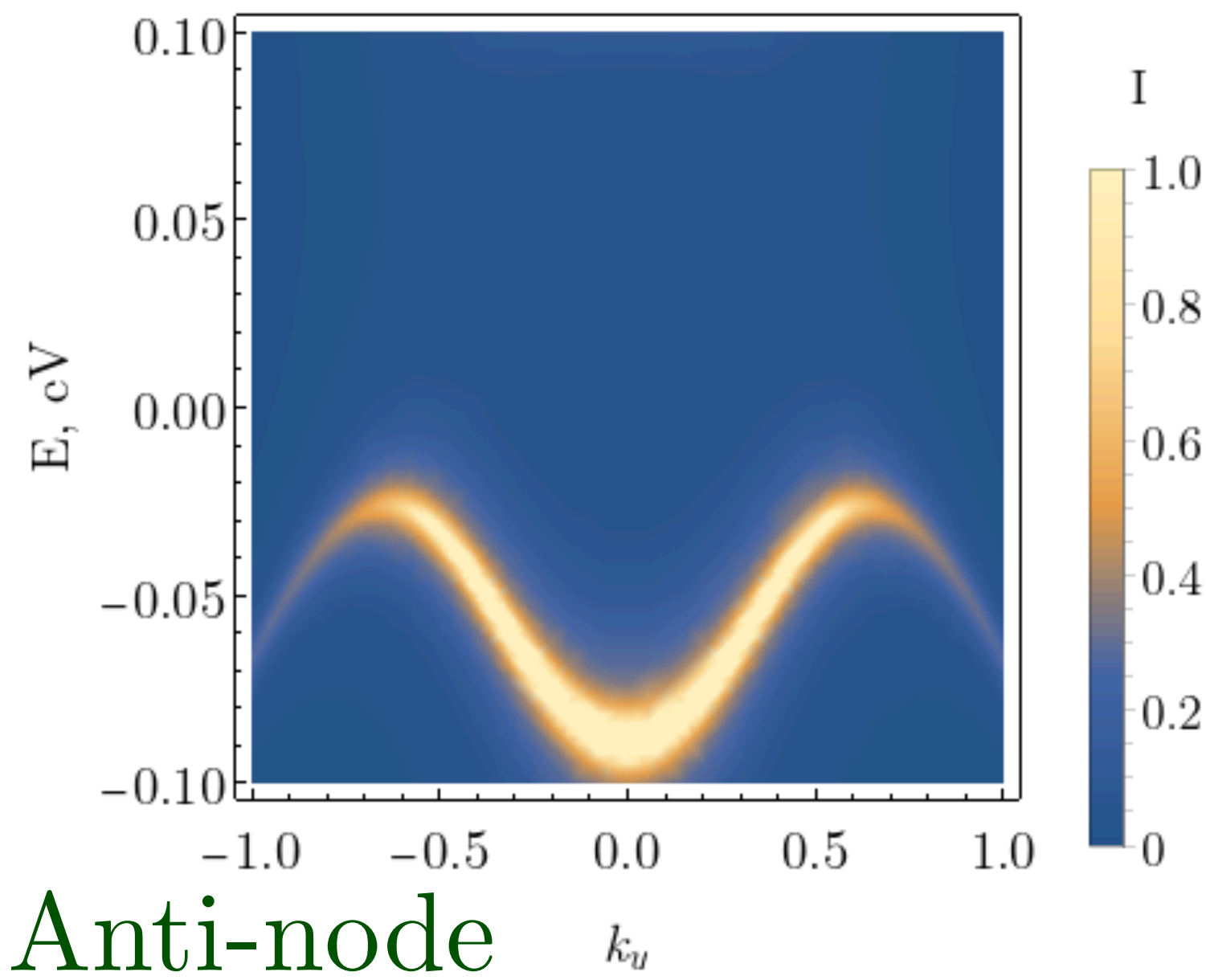


# Photoemission at small $p$

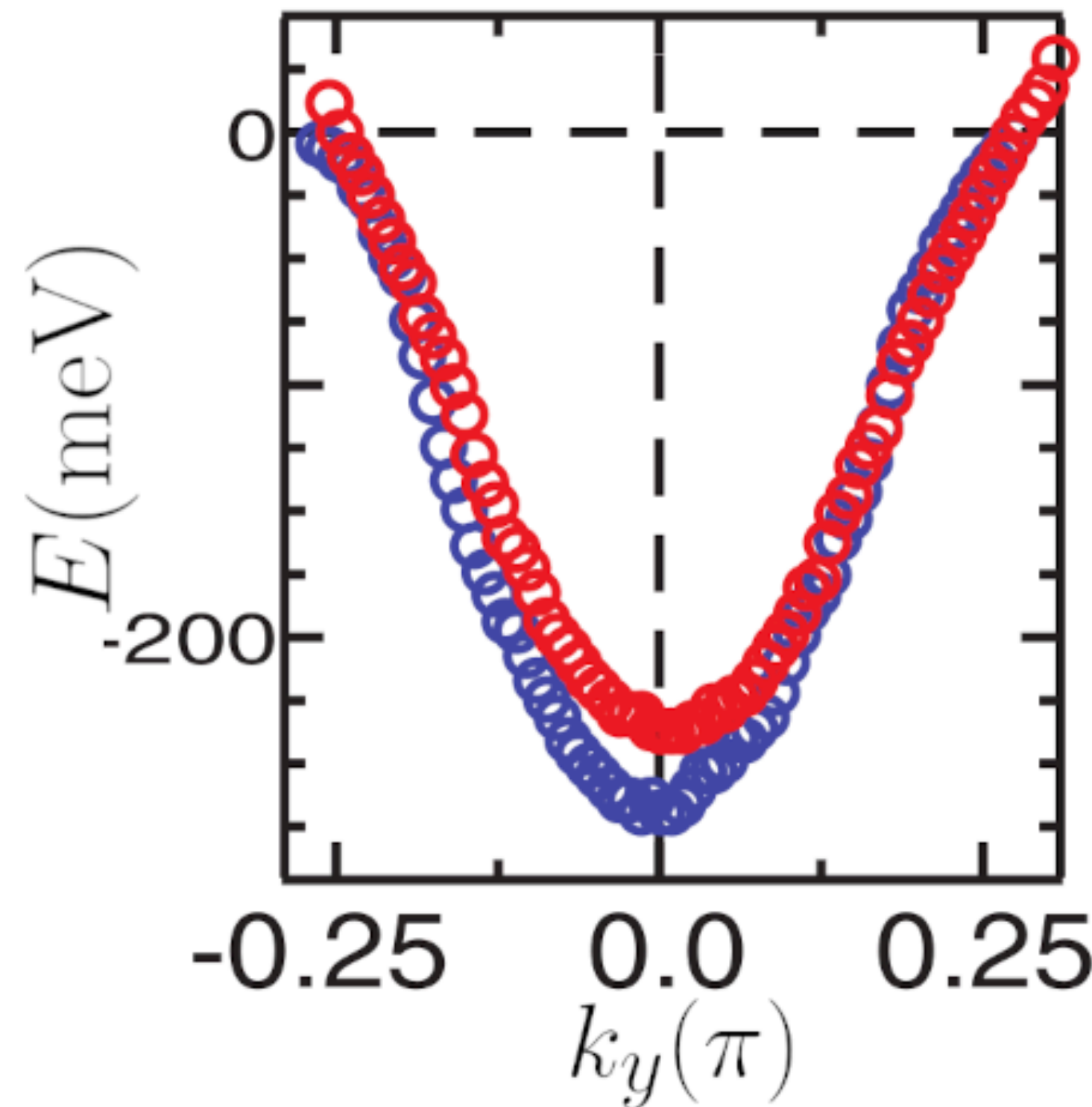
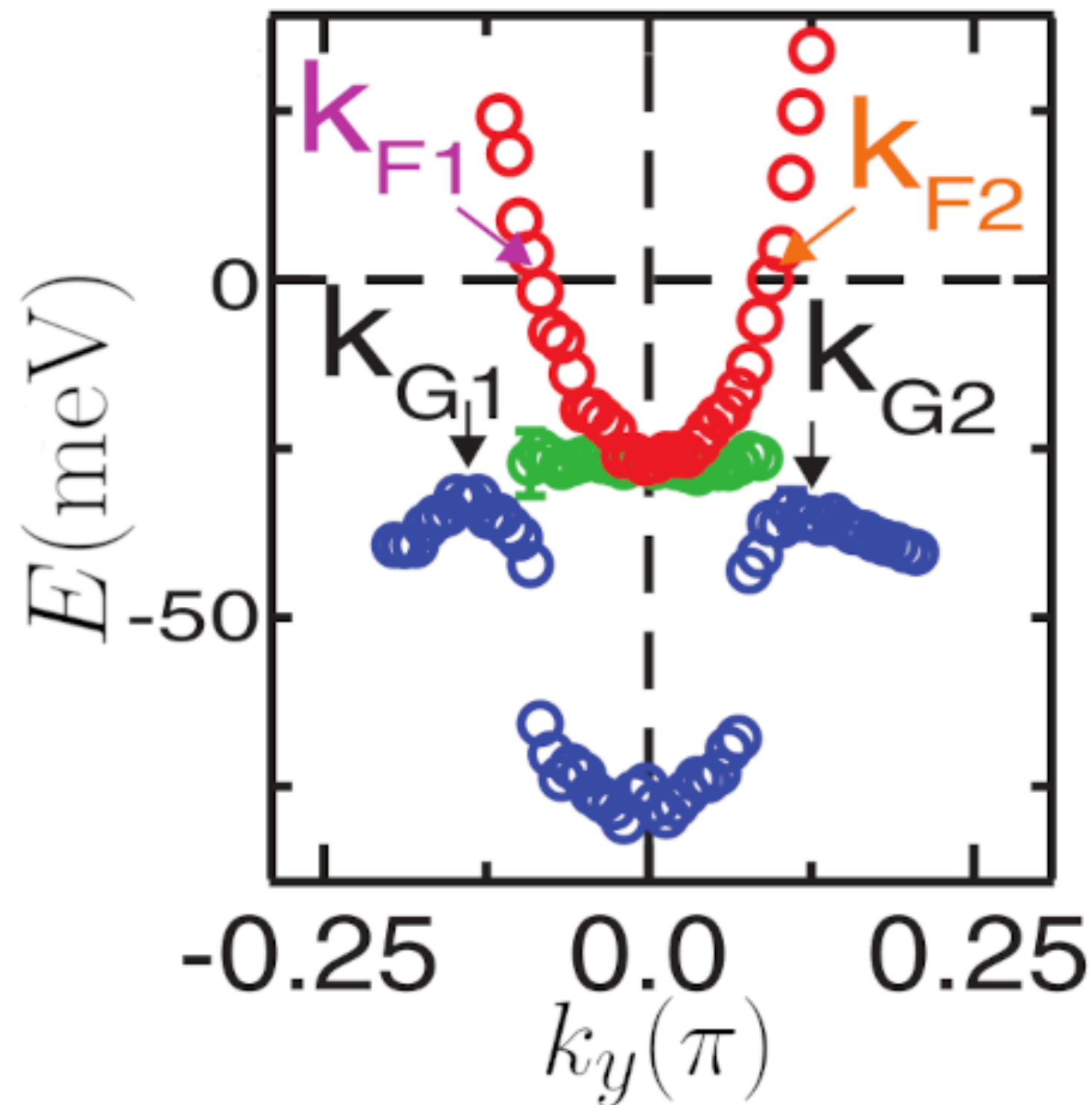


“Fermi pockets”

Reconstructed Fermi Surface of Underdoped  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  Cuprate Superconductors, H.-B. Yang, J. D. Rameau, Z.-H. Pan, G. D. Gu, P. D. Johnson, H. Claus, D. G. Hinks, and T. E. Kidd, PRL **107**, 047003 (2011).



FL\* in a  
one-band model



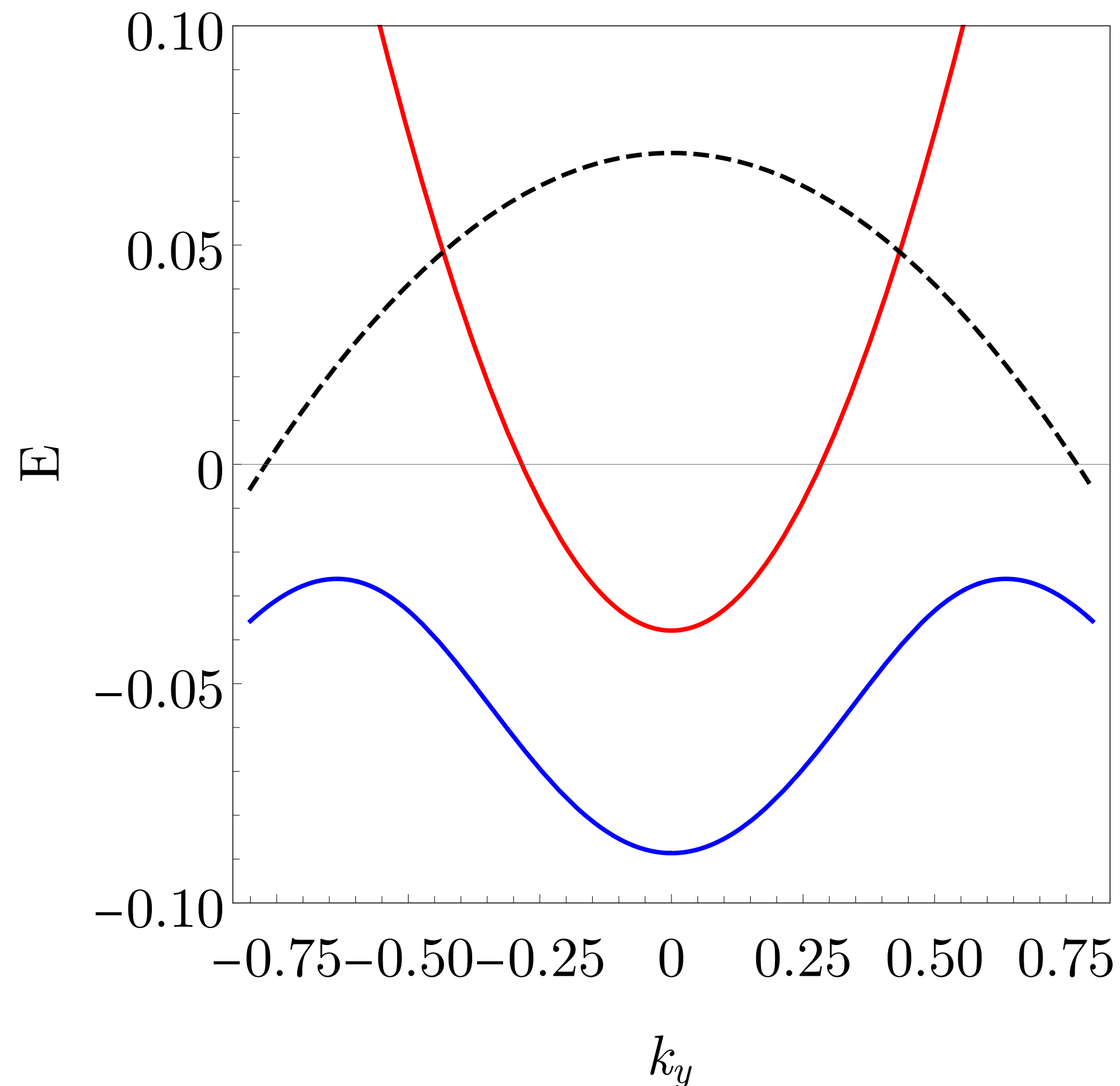
ARPES on Bi2201

R.-H. He, M. Hashimoto, H. Karapetyan, J. D. Koralek, J. P. Hinton, J. P. Testaud, V. Nathan, Y. Yoshida, H. Yao, K. Tanaka, W. Meevasana, R. G. Moore, D. H. Lu, S. K. Mo, M. Ishikado, H. Eisaki, Z. Hussain, T. P. Devereaux, S. A. Kivelson, J. Orenstein, A. Kapitulnik, and Z.-X. Shen, *Science* **331**, 1579 (2011)



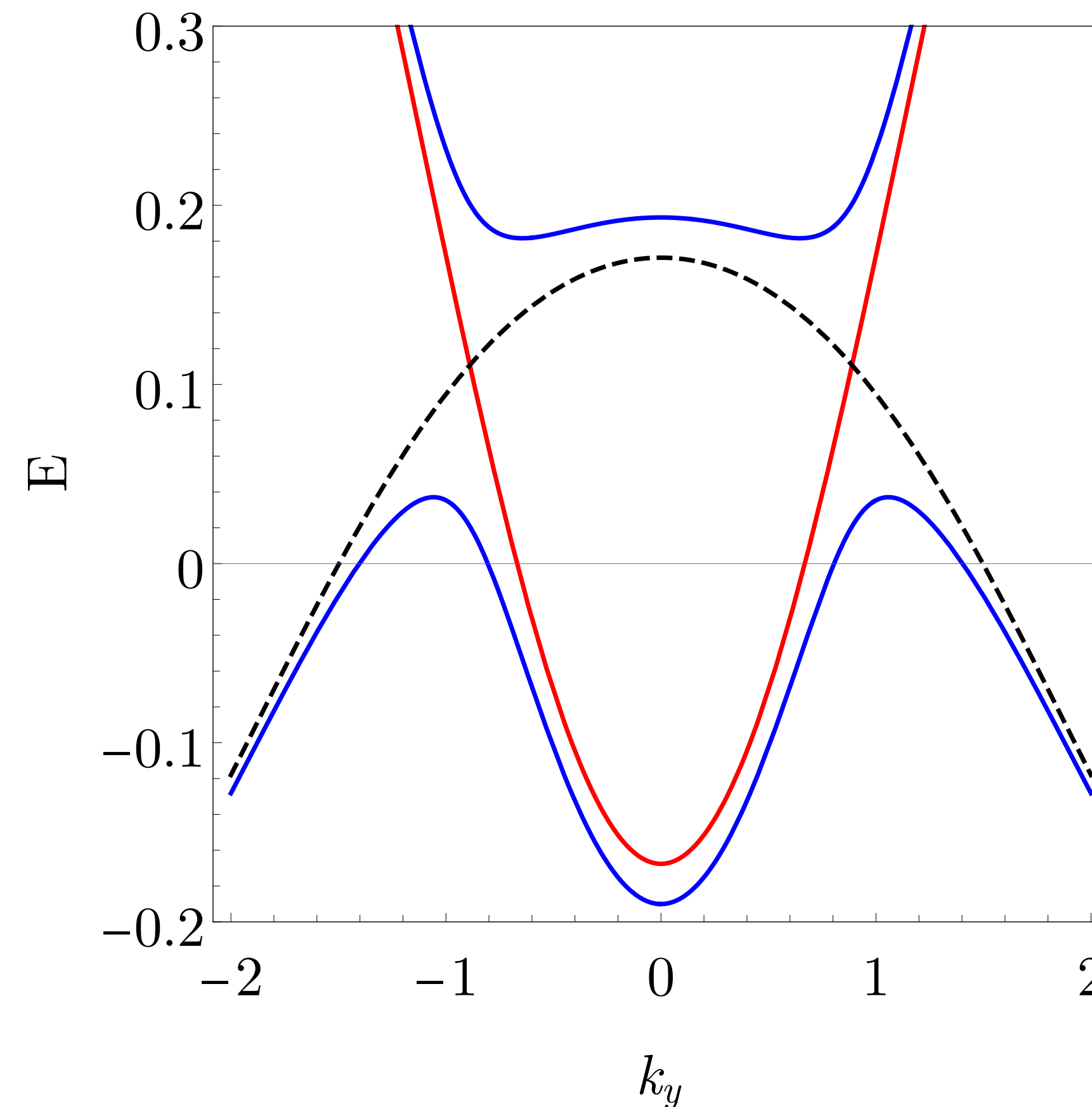
# FL\* in a **one-band** model

Anti-node:  $k_x = \pi$



# Electronic dispersion

Node:  $k_x = 2$

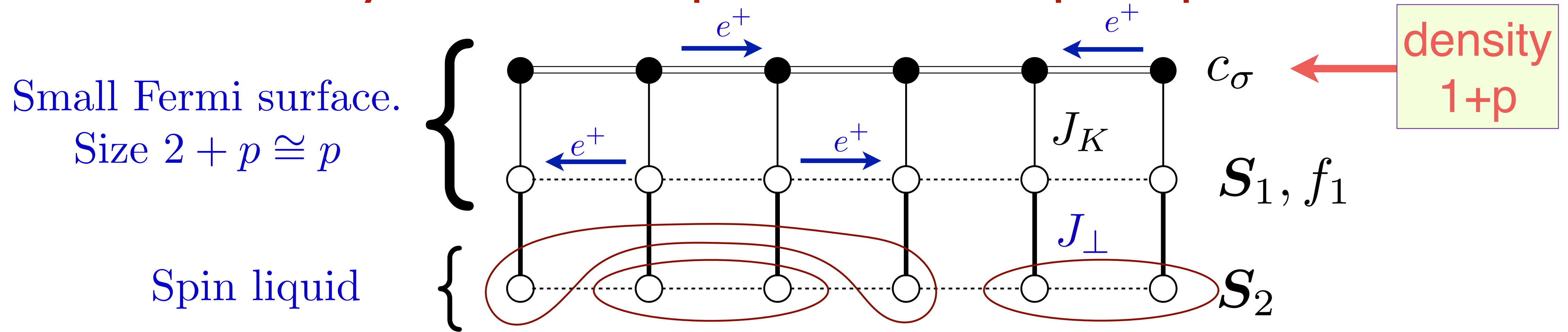


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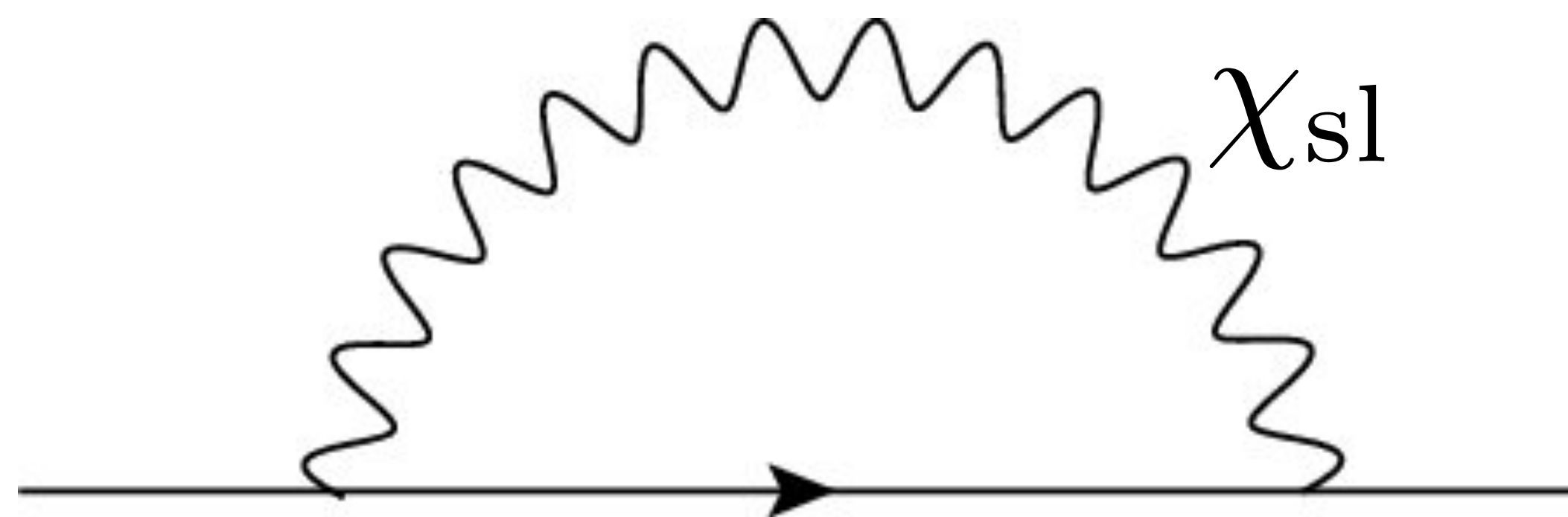
$$H = - \sum_{i,j} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,j} t_{1,ij} f_{1i\sigma}^\dagger f_{1j\sigma} + \sum_i B (c_{i\sigma}^\dagger f_{1i\sigma} + f_{1i\sigma}^\dagger c_{i\sigma})$$

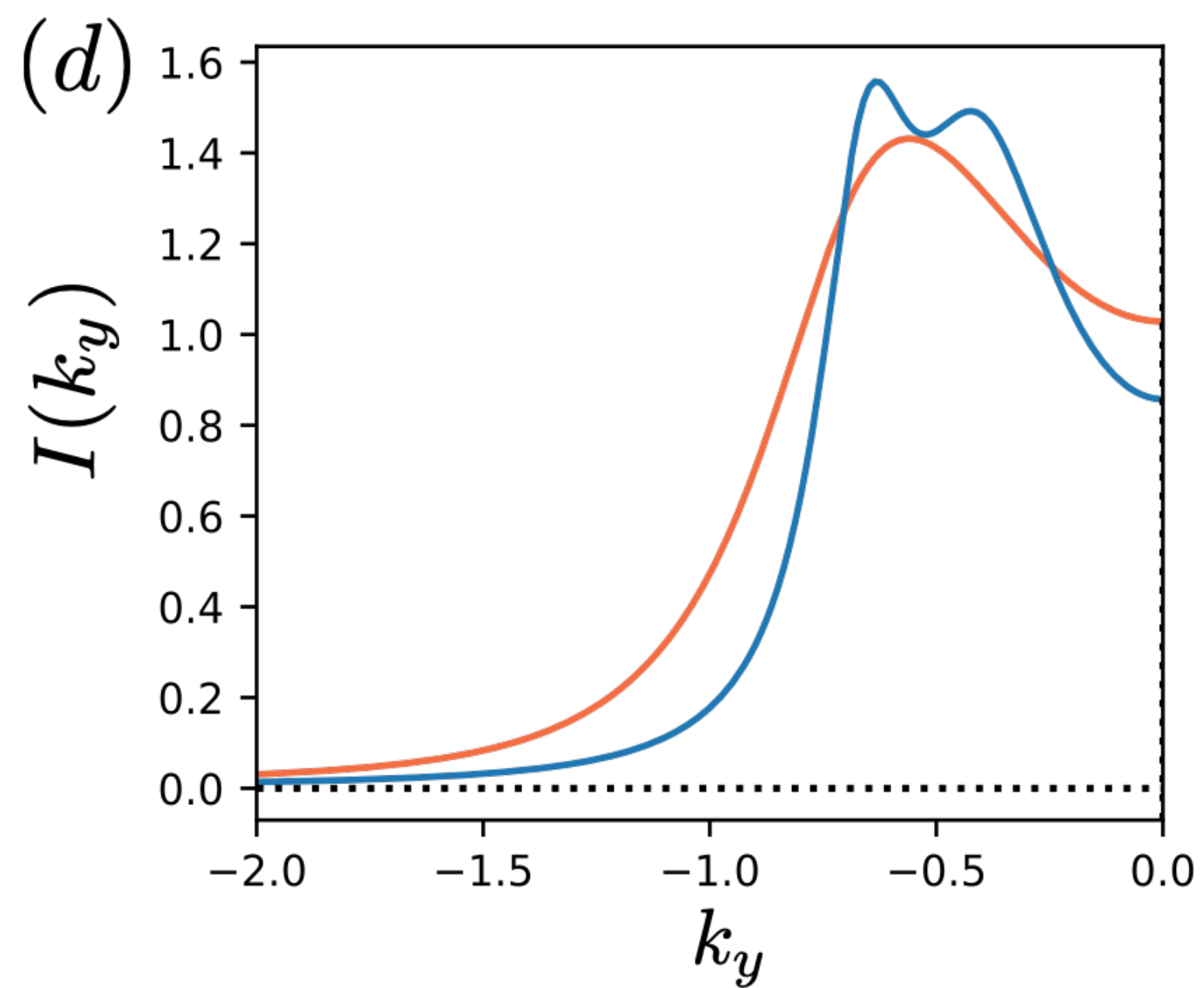
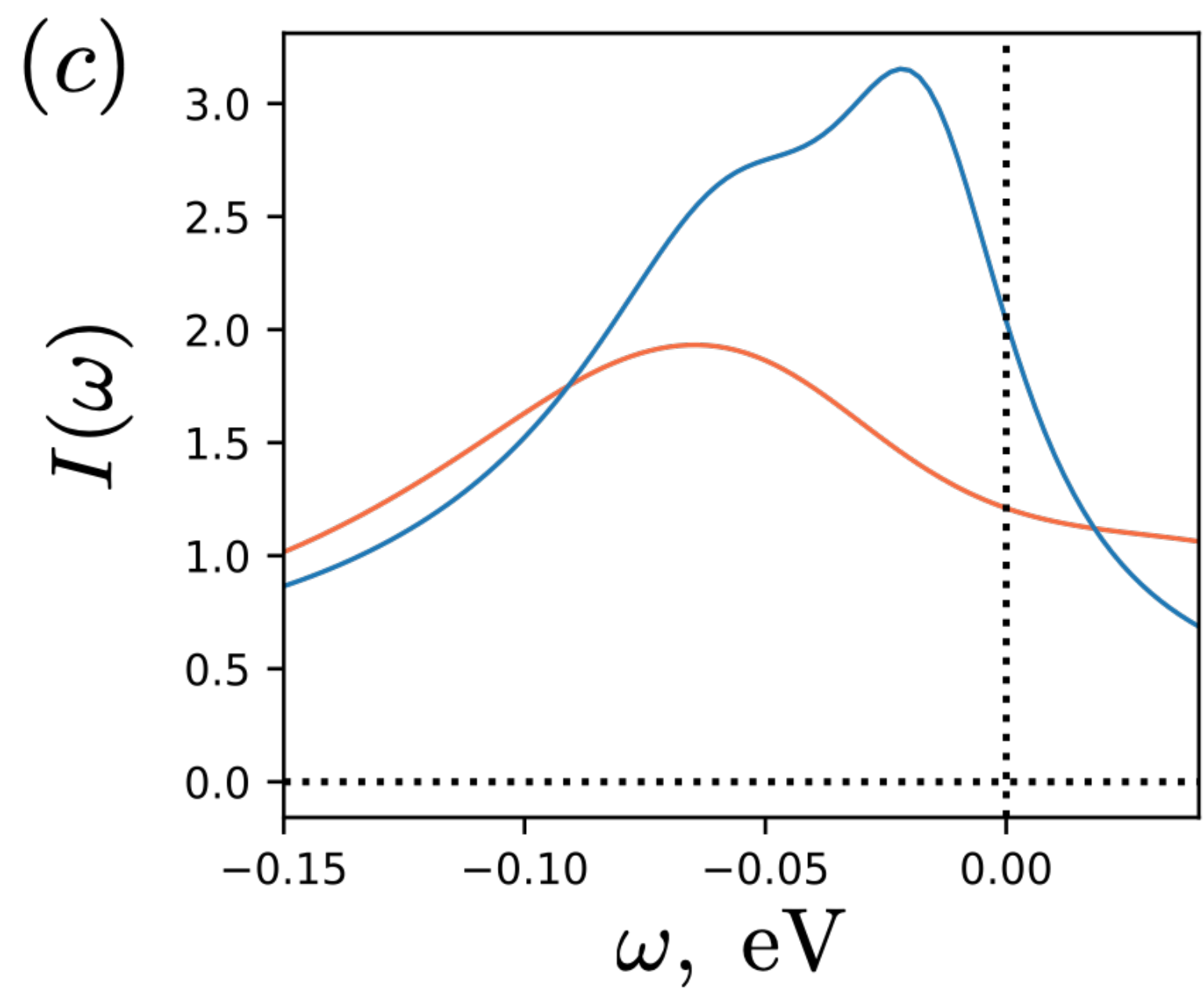
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 Eun-Gook Moon, SS,  
 PRB **83**, 224508 (2011)

# Dynamic consequences of the spin liquid



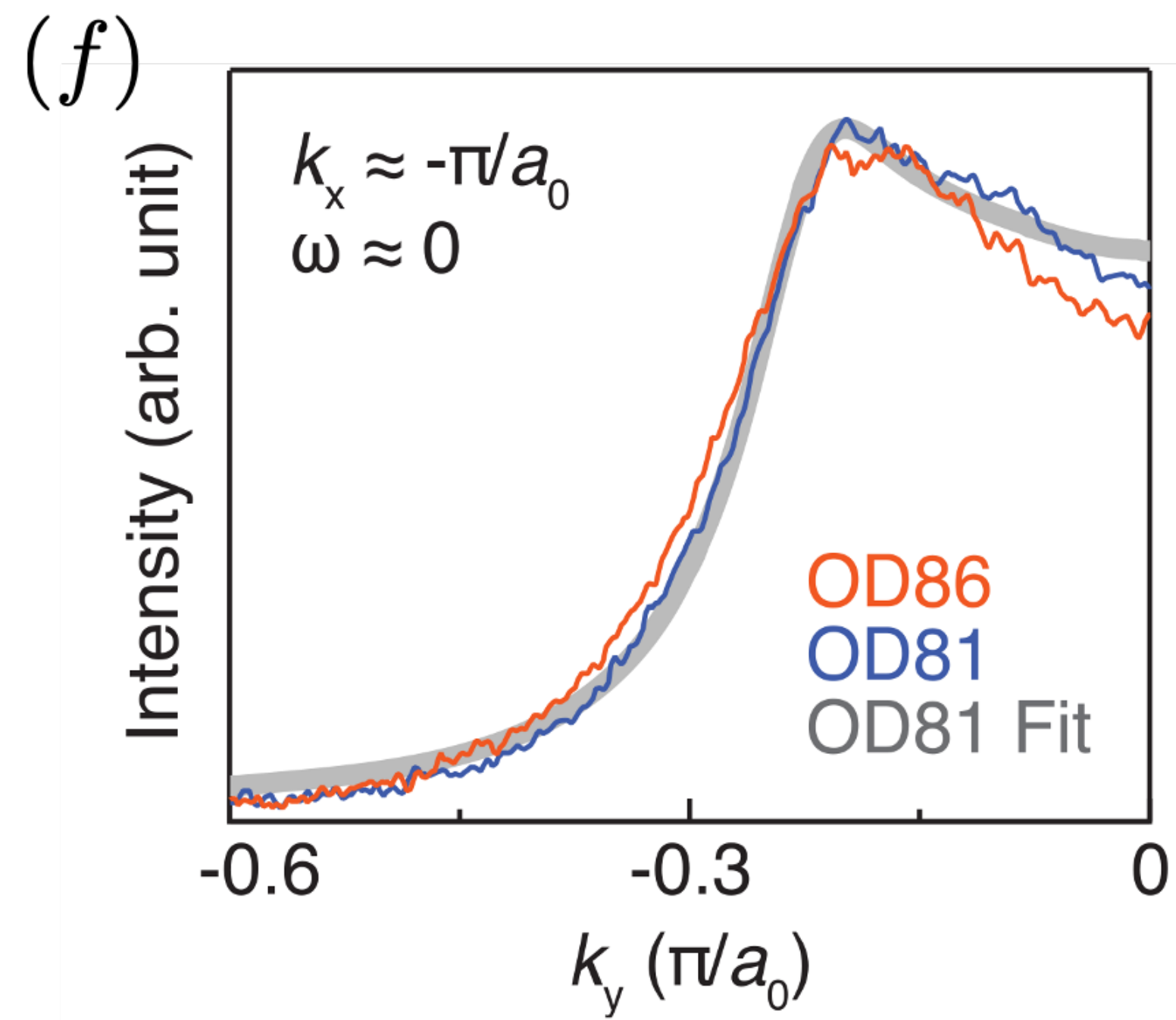
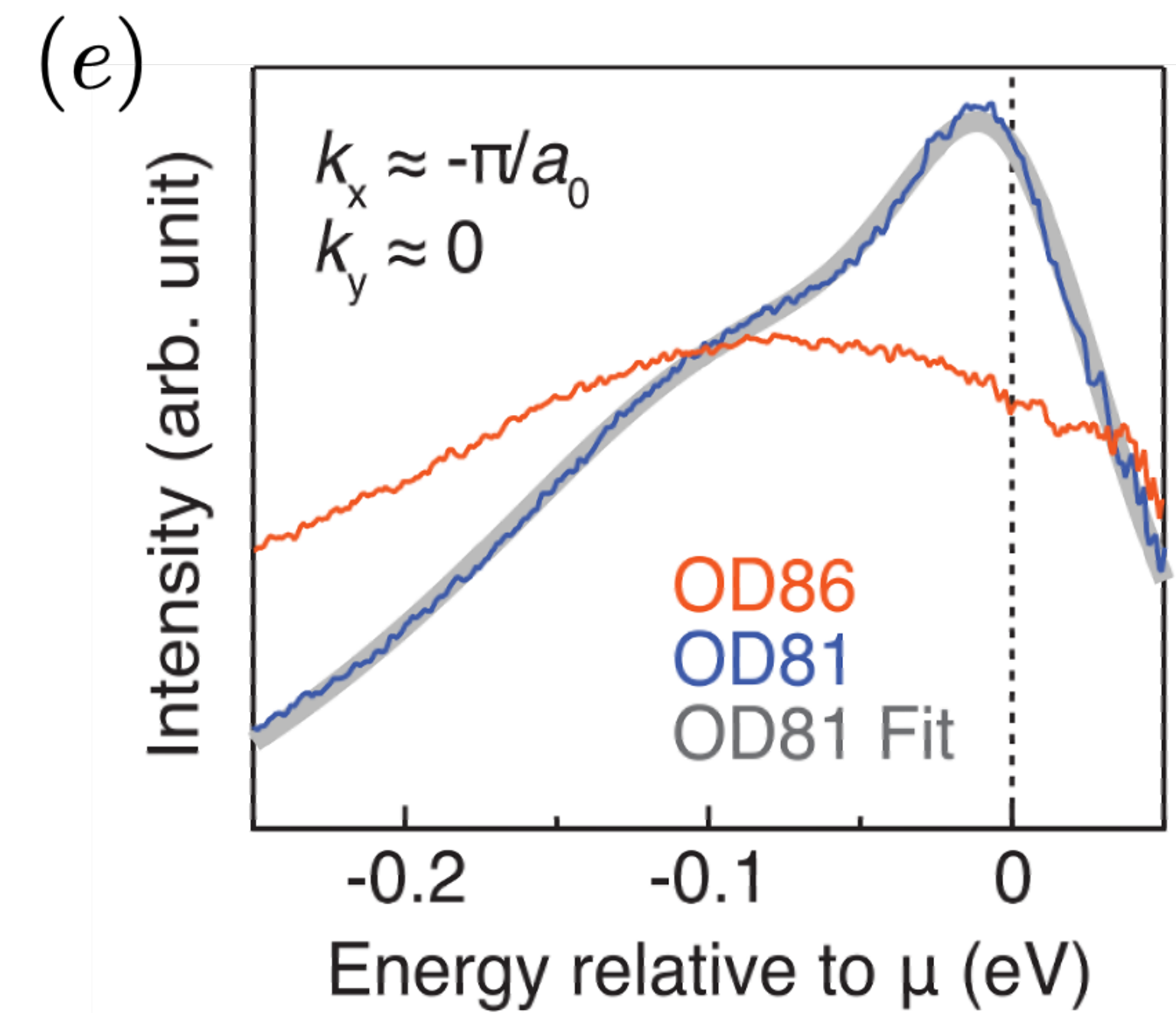
The only singular gauge fluctuations are those in the spin liquid of the  $S_2$ . We can compute their influence on the electronic spectrum perturbatively in the exchange couplings in terms of the dynamic spin susceptibility  $\chi_{sl}$ .





Antinodal EDC and MDC

(c,d) Theory with SYK spin liquid in  $\Psi_2$  layer. Similar EDC obtained by gapless  $\mathbb{Z}_2$  spin liquid



(e,f) Experiments on Bi2212 by S.-D. Chen, M. Hashimoto, Y. He, D. Song, K.-J. Xu, J.-F. He, T. P. Devereaux, H. Eisaki, D.-H. Lu, J. Zaanen, and Z.-X. Shen, Science **366**, 1099 (2019).

1. Paramagnon fractionalization theory of the Hubbard model
2. Photoemission in the cuprates
3. Confinement transitions from the pseudogap metal





**Alexander  
Nikolaenko**



**Darshan Joshi**



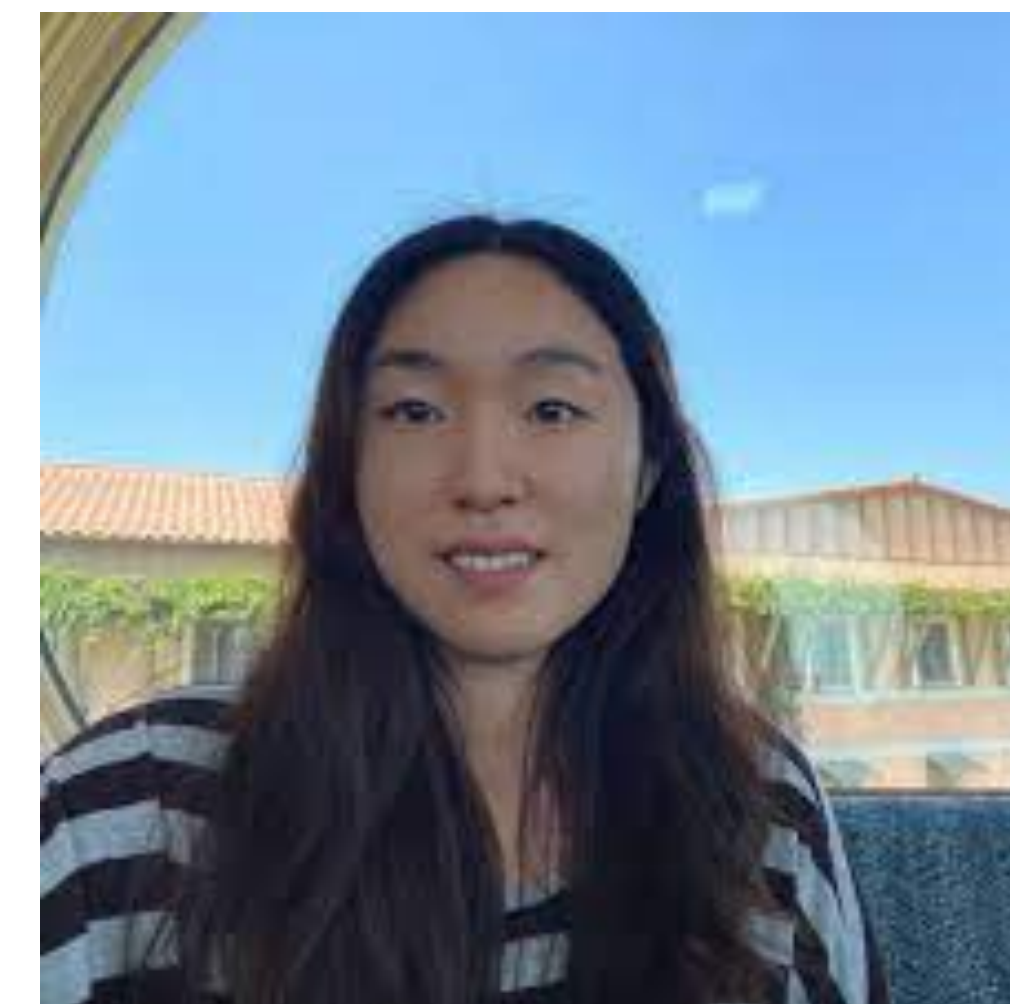
**Jonas von Milczewski**



**Henry Shackleton**

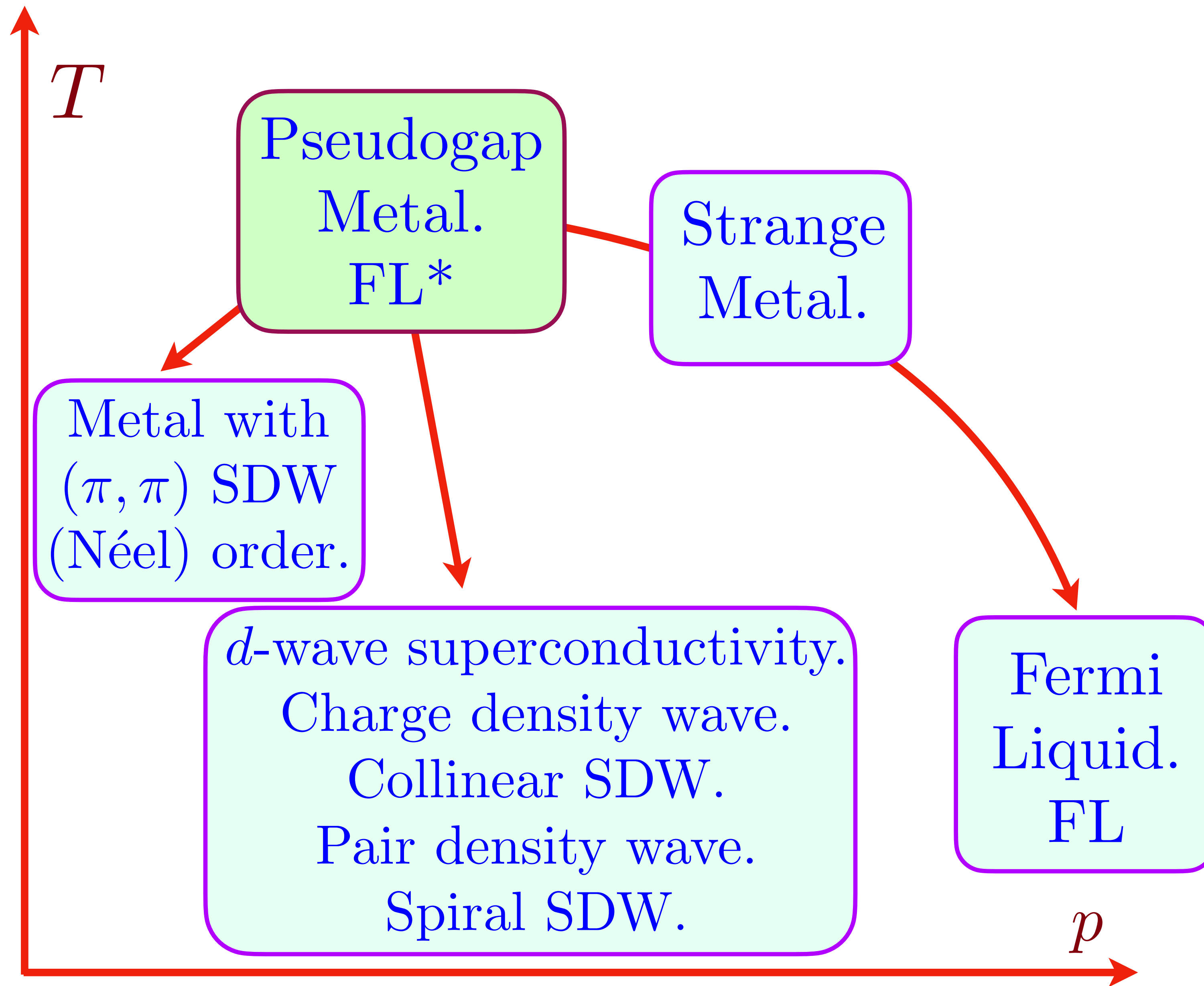


**Maine Christos**



**Zhu-Xi Luo**



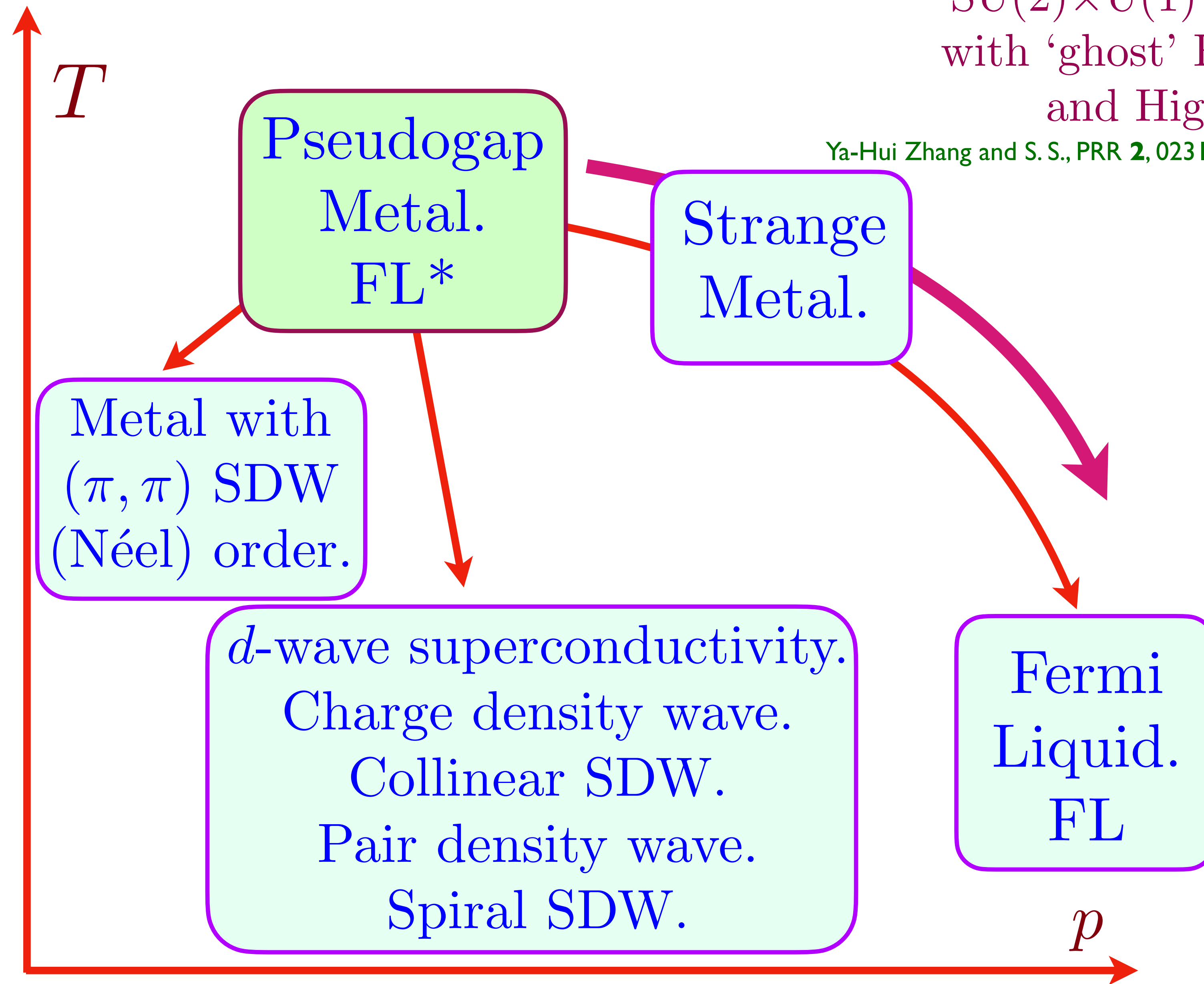




Yahui  
Zhang

$SU(2) \times U(1)$  gauge theory  
with 'ghost' Fermi surfaces  
and Higgs fields.

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

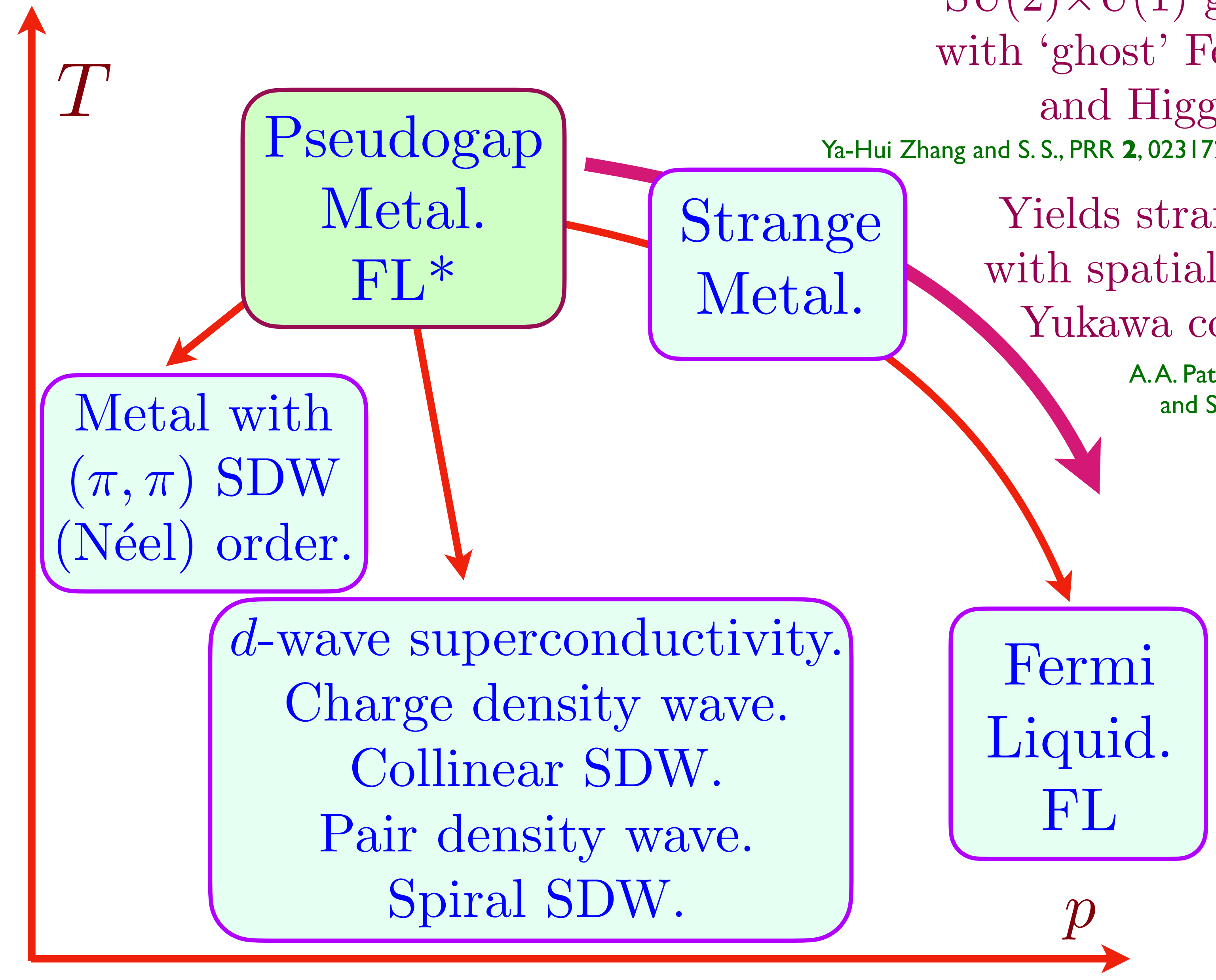


SU(2)×U(1) gauge theory with ‘ghost’ Fermi surfaces and Higgs fields.

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

Yields strange metal with spatially random Yukawa couplings.

A.A. Patel, Haoyu Guo, I. Esterlis, and S. S., arXiv:2203.04990

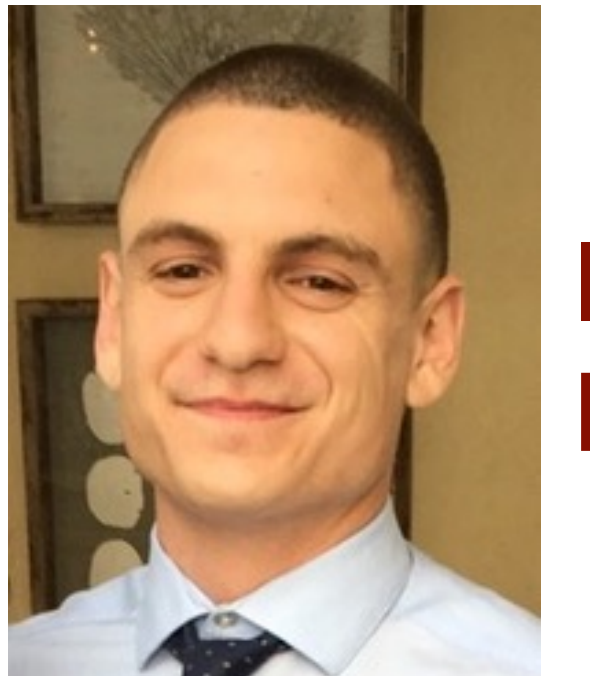


Yahui Zhang

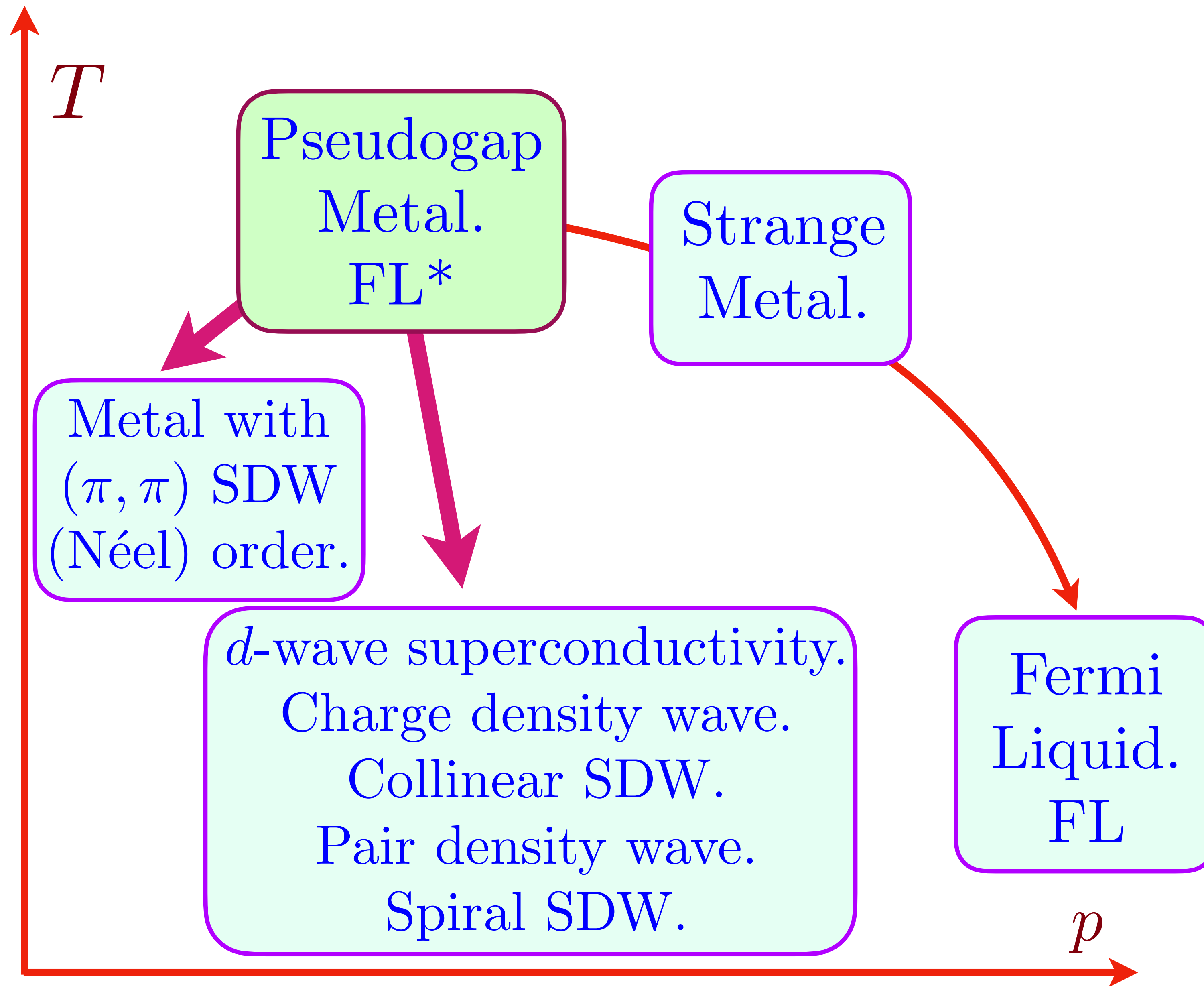
Aavishkar Patel

Haoyu Guo

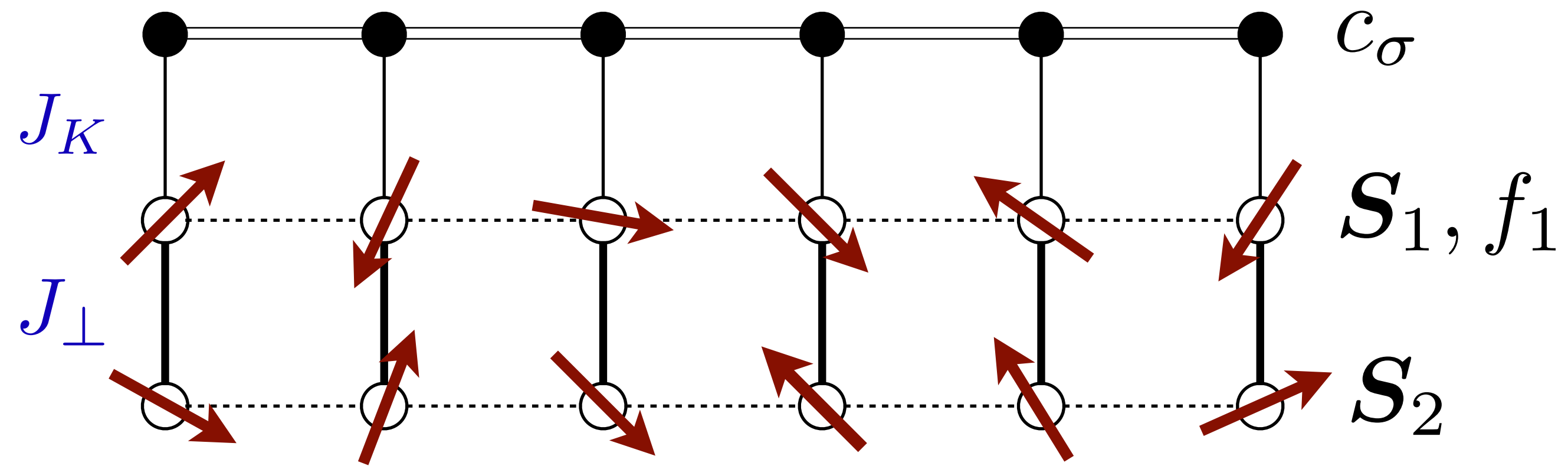
Ilya Esterlis





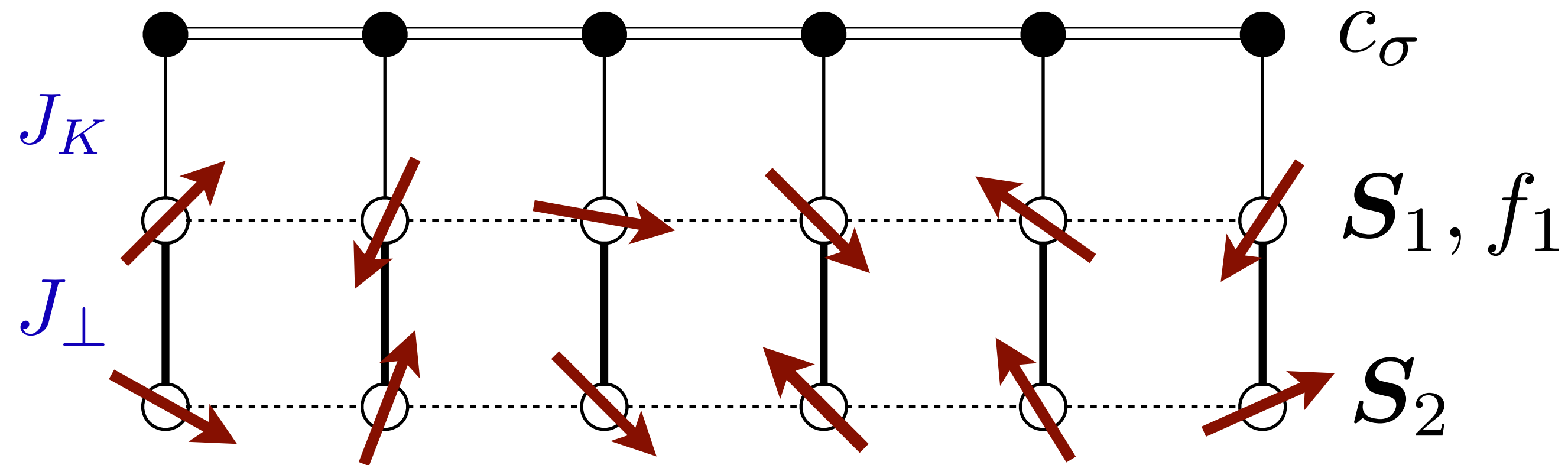


Spin liquid of  $\mathcal{S}_2$ :



(A) Schwinger boson representation ( $\mathcal{S}_{2i} = b_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} b_{i\beta}$ ) leads to spin liquid described by  $\mathbb{C}\mathbb{P}^1$  field theory:  $N_f = 2$  relativistic complex scalars,  $Z$ , coupled to a  $U(1)$  gauge field.

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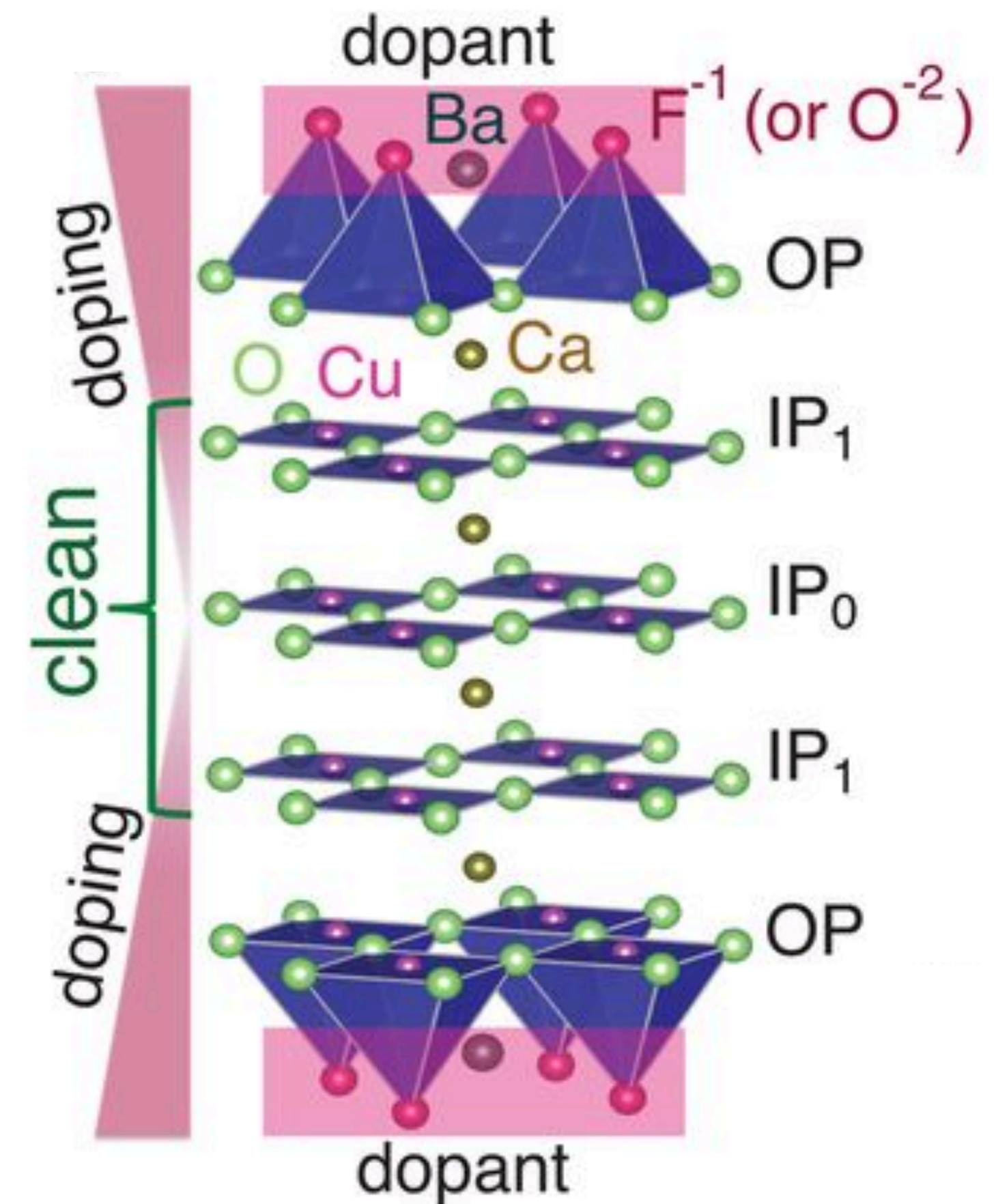
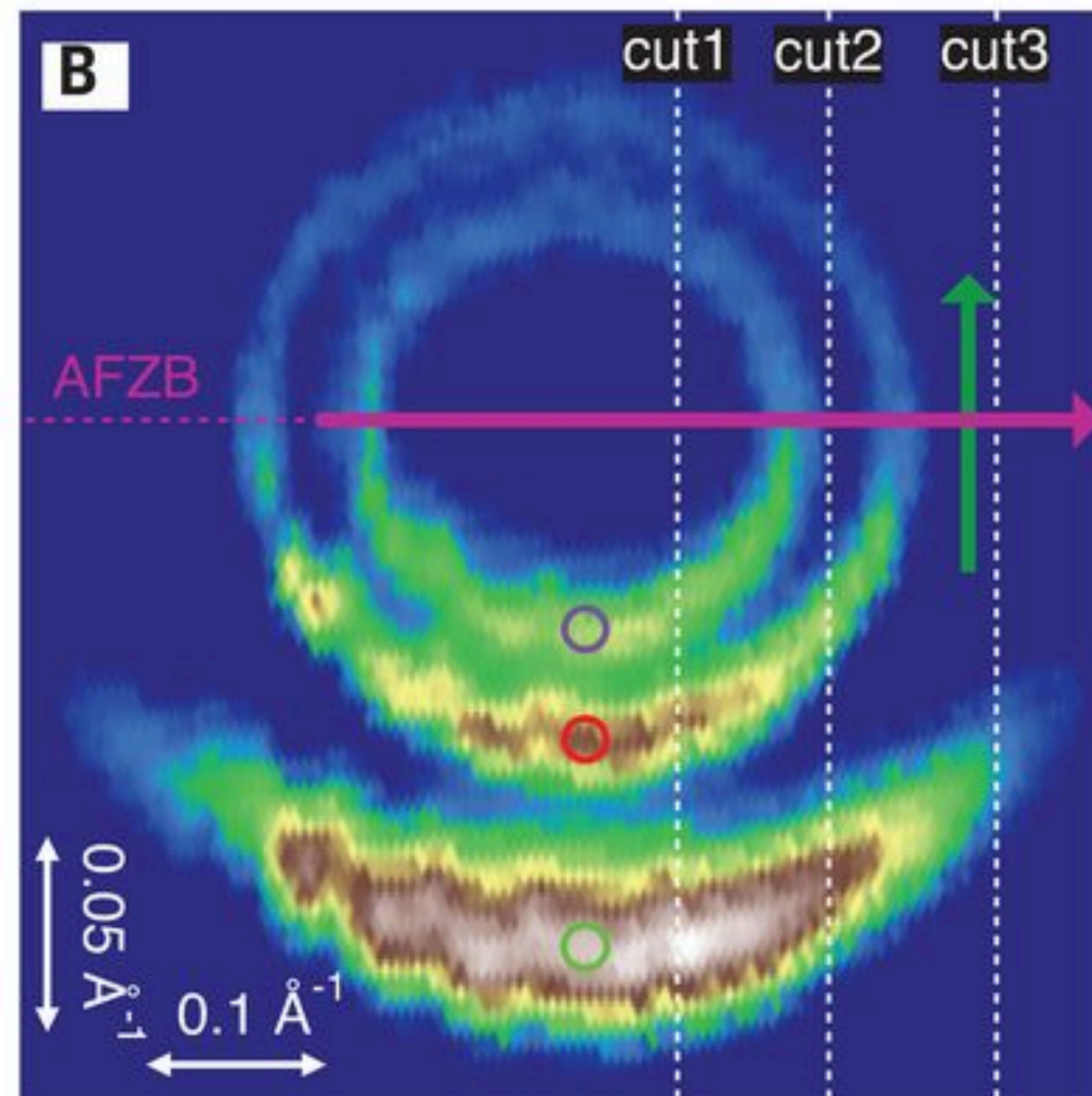
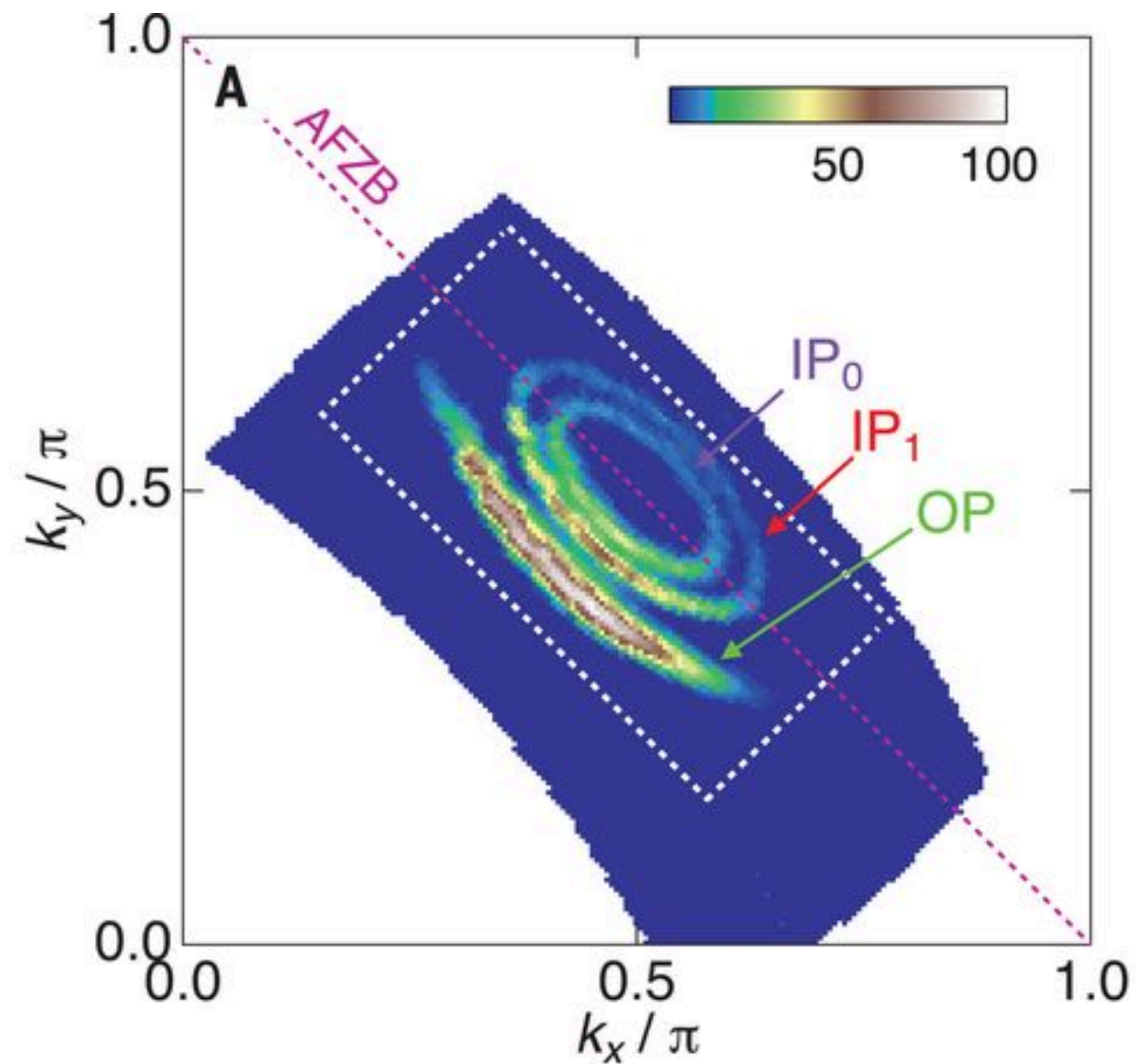
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Confinement transition: Condensation of  $Z$  leads to  $(\pi, \pi)$  Néel order, or incommensurate spiral spin density waves.



# Observation of small Fermi pockets protected by clean $\text{CuO}_2$ sheets of a high- $T_c$ superconductor

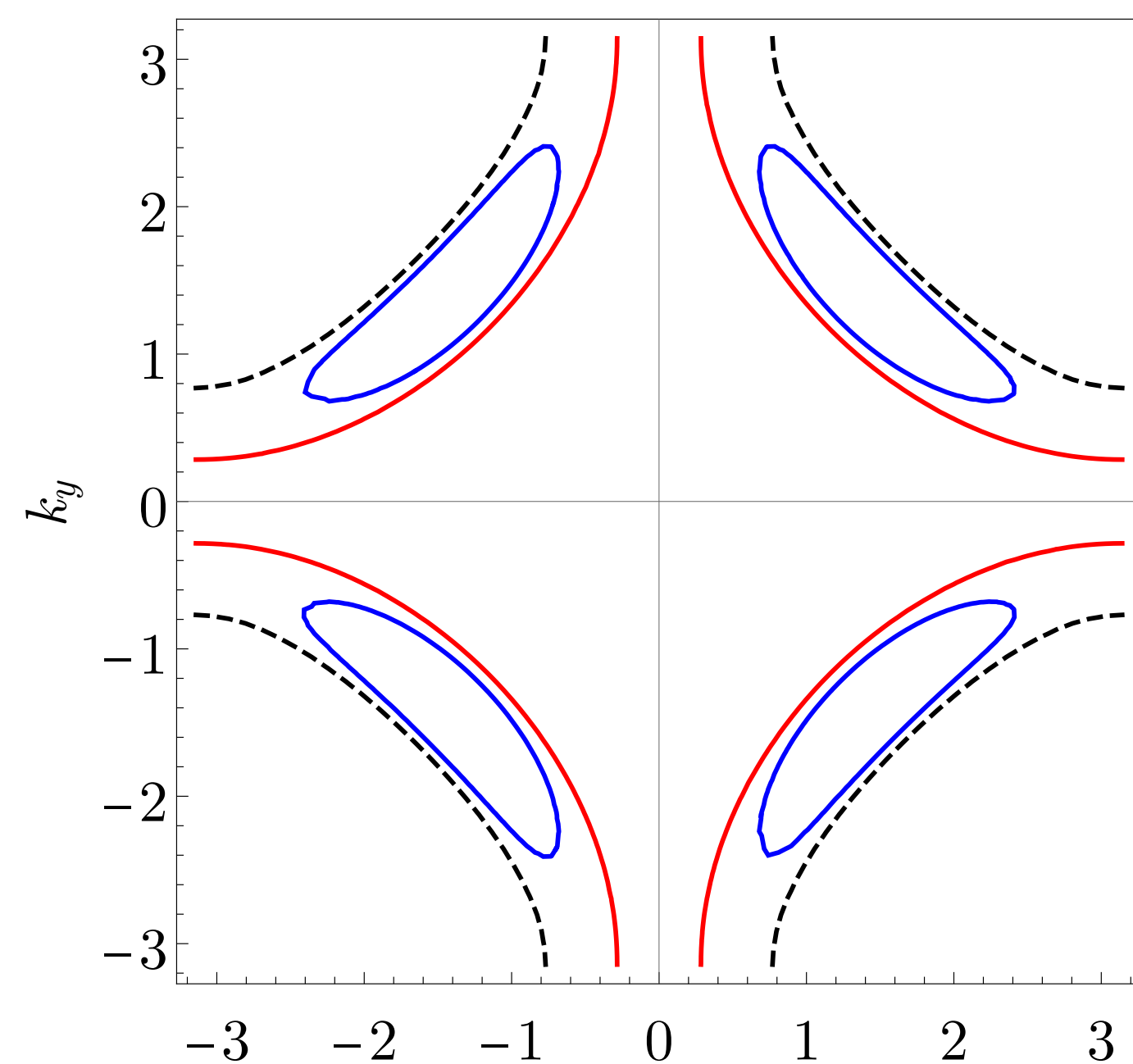
So Kunisada<sup>1</sup>, Shunsuke Isono<sup>2</sup>, Yoshimitsu Kohama<sup>1,3</sup>, Shiro Sakai<sup>4</sup>, Cédric Bareille<sup>1</sup>, Shunsuke Sakuragi<sup>1</sup>, Ryo Noguchi<sup>1</sup>, Kifu Kurokawa<sup>1</sup>, Kenta Kuroda<sup>1</sup>, Yukiaki Ishida<sup>1</sup>, Shintaro Adachi<sup>5</sup>, Ryotaro Sekine<sup>2</sup>, Timur K. Kim<sup>6</sup>, Cephise Cacho<sup>6</sup>, Shik Shin<sup>1,7</sup>, Takami Tohyama<sup>8</sup>, Kazuyasu Tokiwa<sup>2\*</sup>, Takeshi Kondo<sup>1,3\*</sup>



Hole pockets  
in a metallic SDW state  
with Néel order at  $(\pi, \pi)$ .

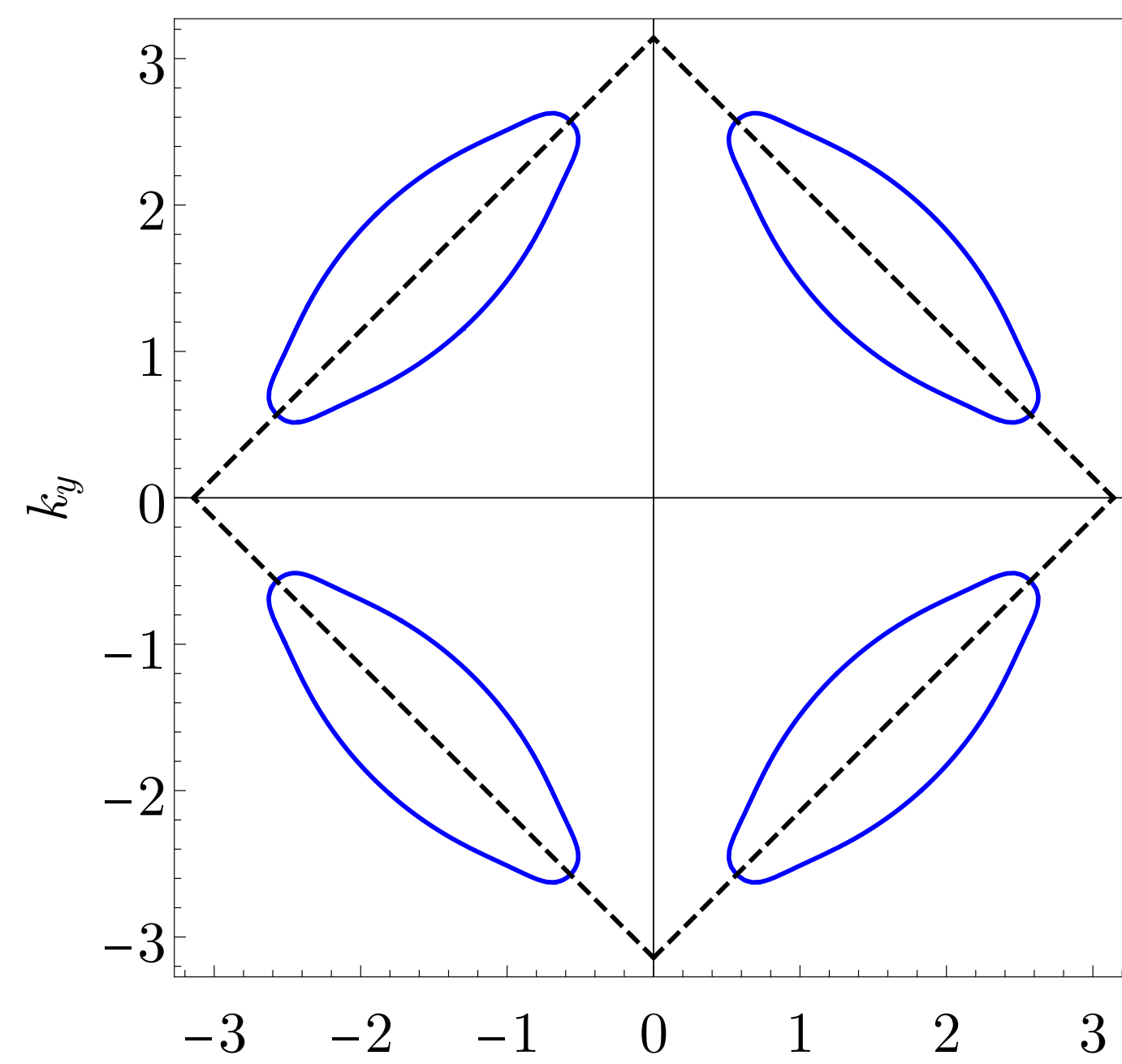
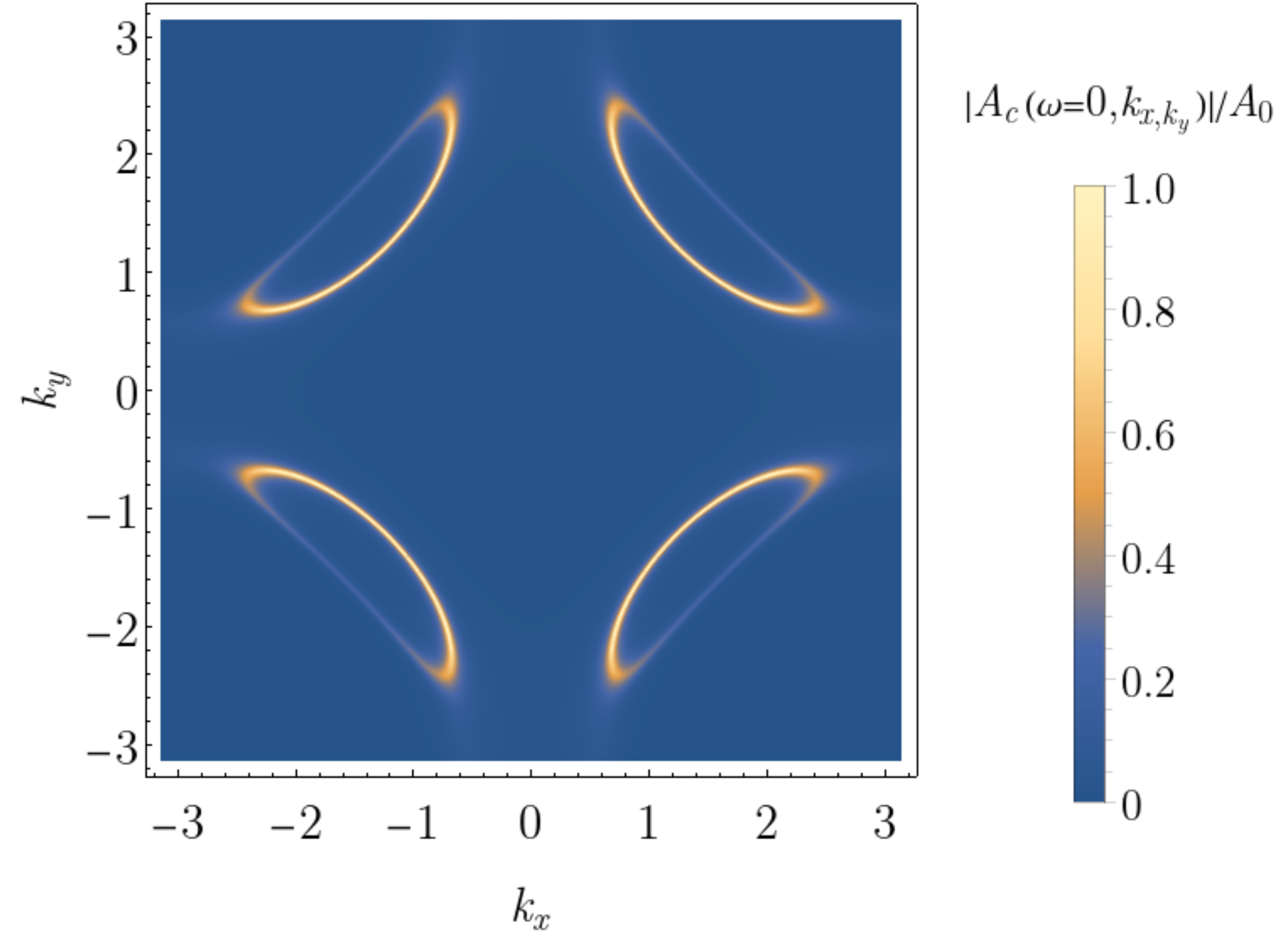
Science **369**, 833 (2020).





FL\*

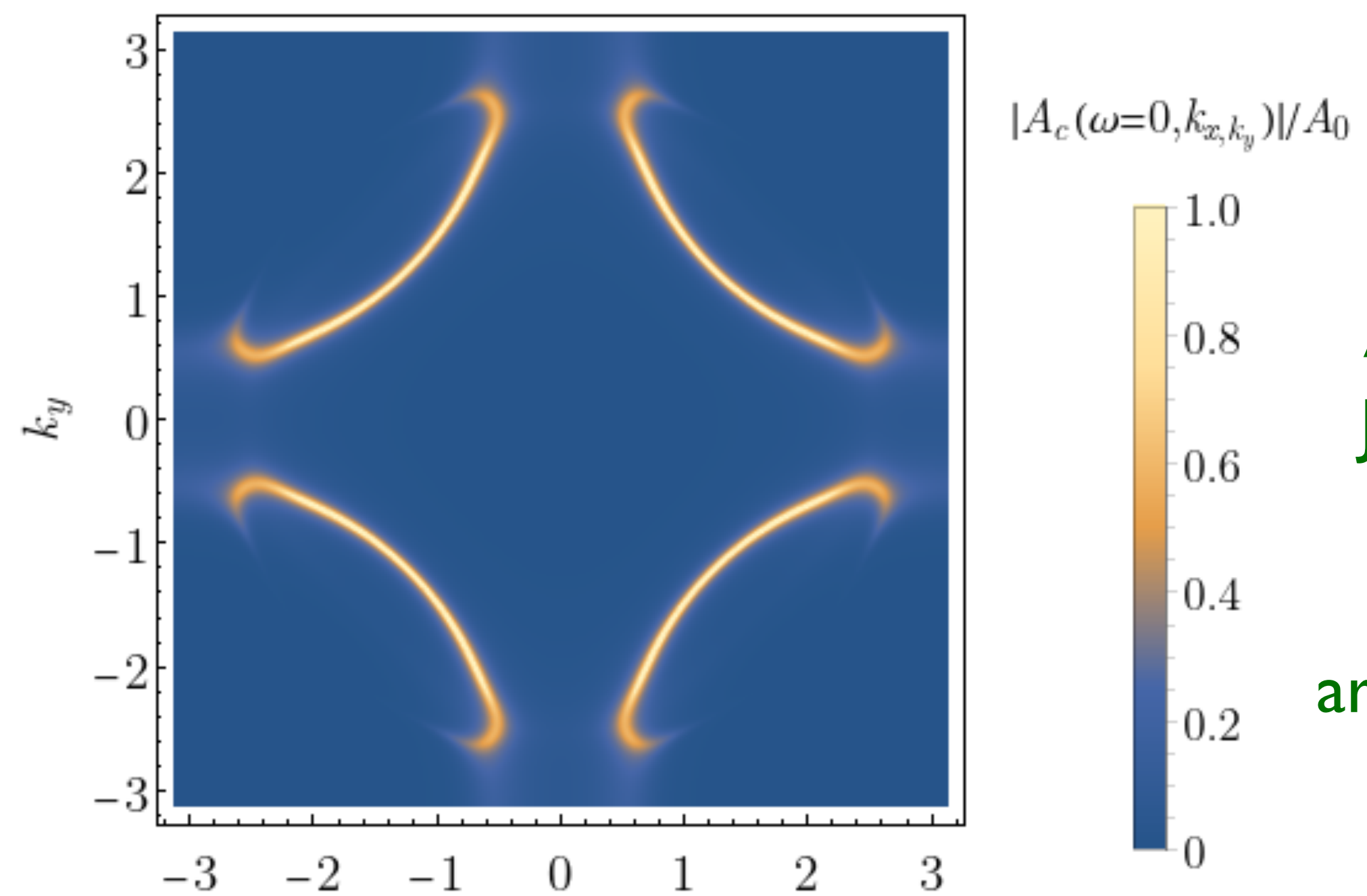
$\langle Z \rangle = 0$



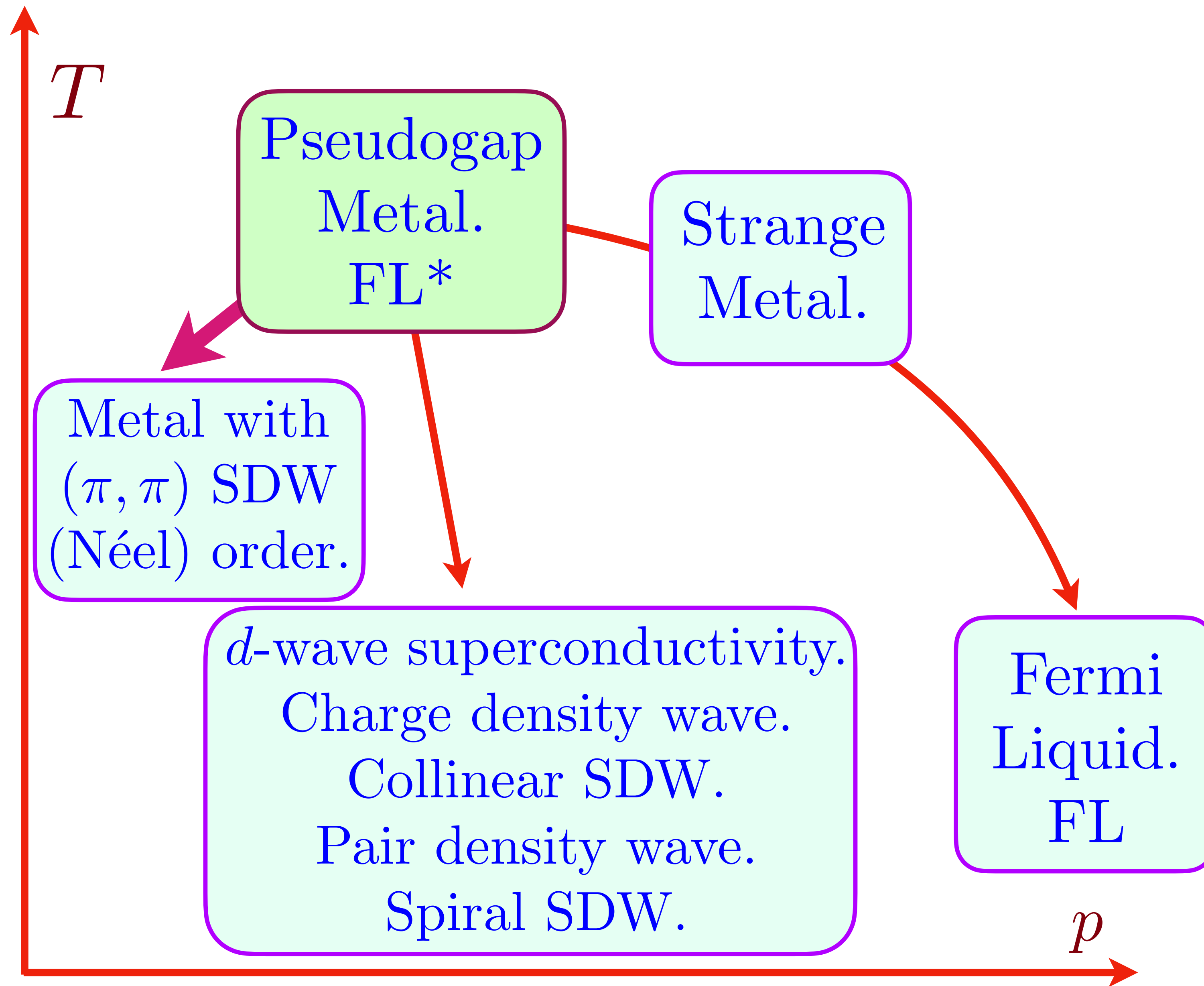
Néel

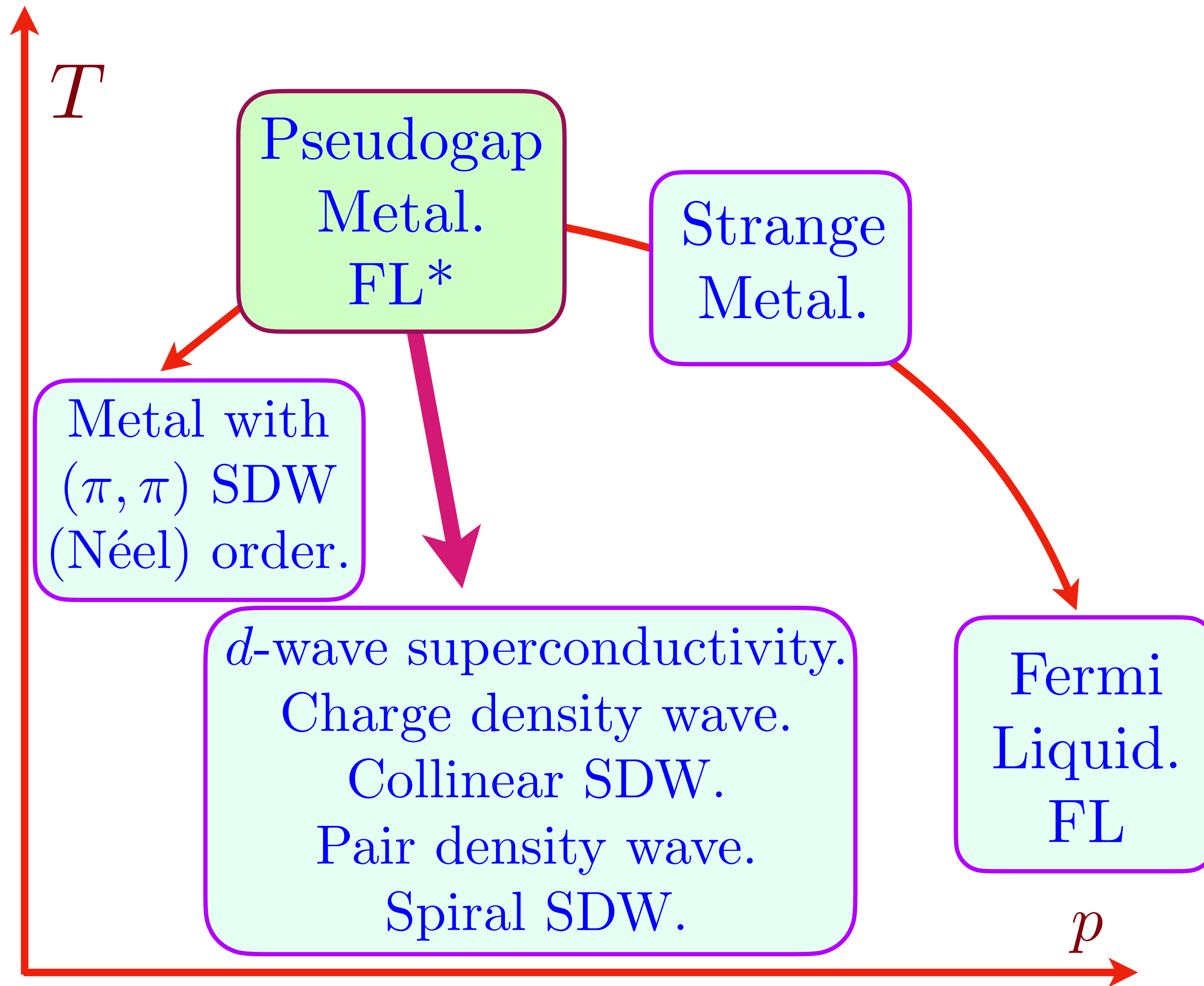
$(\pi, \pi)$  SDW

$\langle Z \rangle \neq 0$



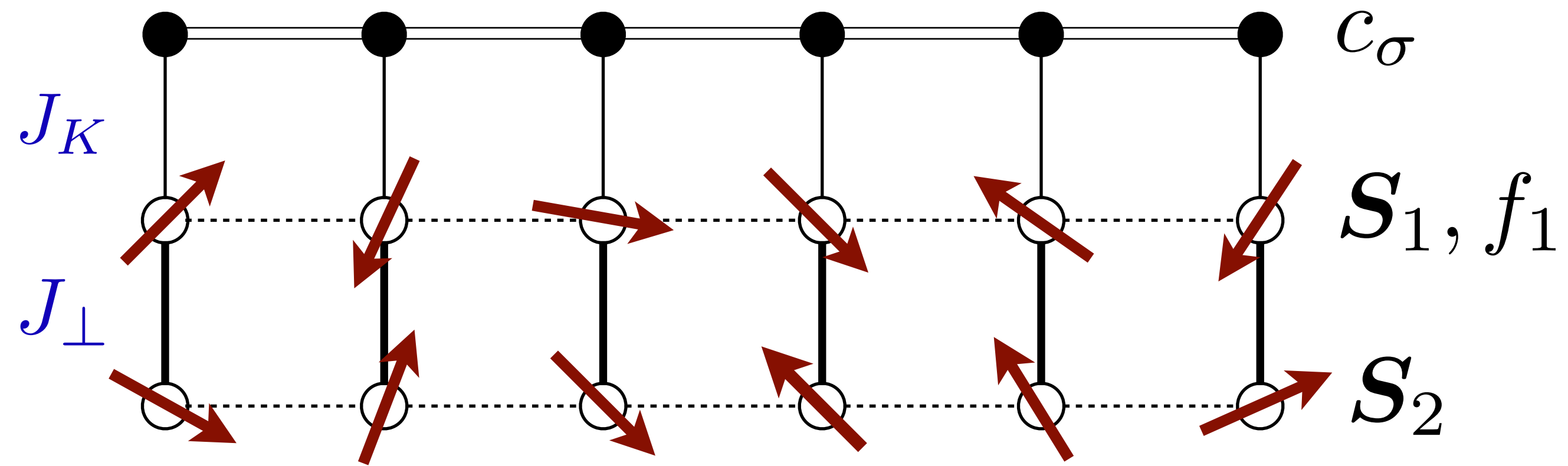
A. Nikolaenko,  
 J. v. Milczewski,  
 D. G. Joshi,  
 S.S.,  
 arXiv:2211.xxxxx







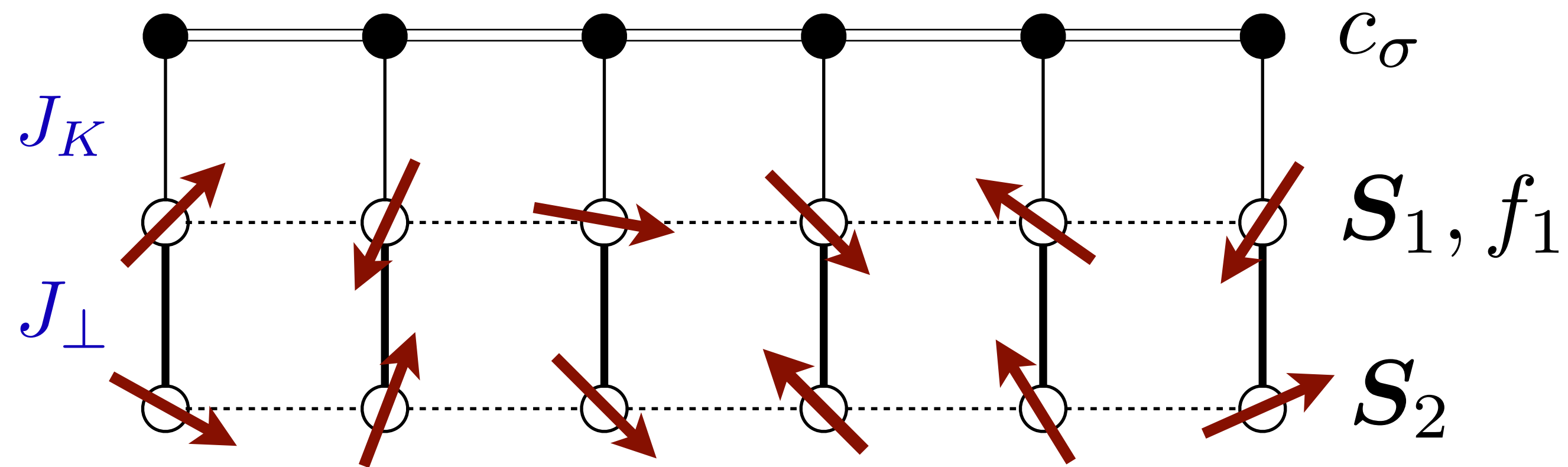
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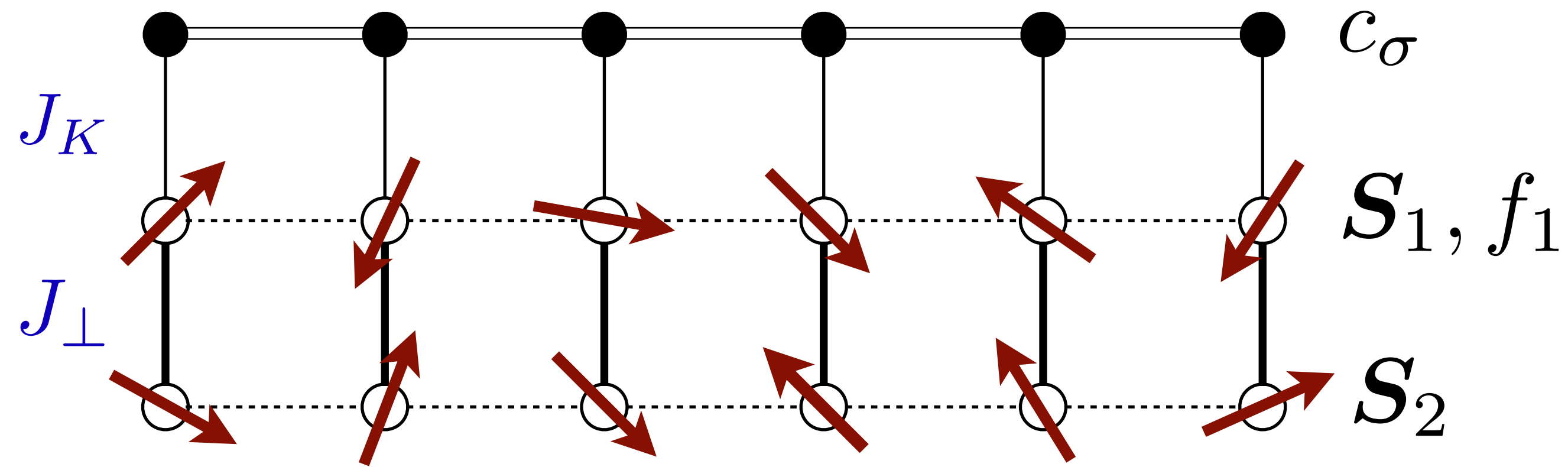


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(B) Schwinger fermion representation ( $\mathbf{S}_{2i} = f_{2i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_{2i\beta}$ ) and  $\pi$ -flux mean field theory leads to spin liquid described by a  $SU(2)$  gauge theory with  $N_f = 2$  massless Dirac fermions,  $\Psi$ .

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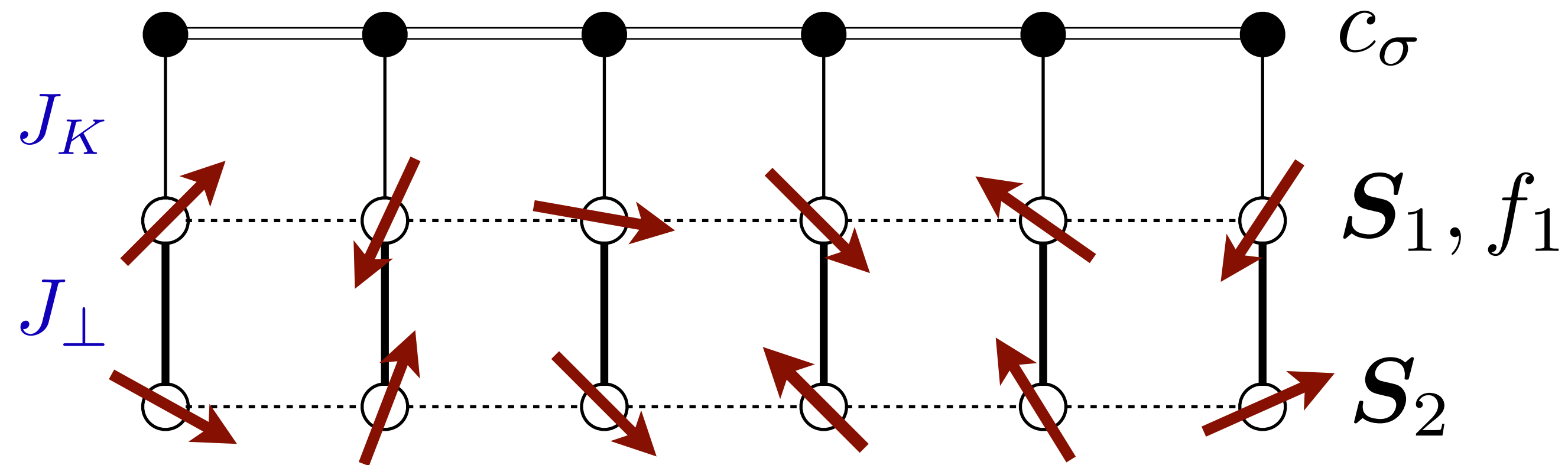
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**Boson-fermion duality**

Chong Wang,  
A. Nahum,  
M.A. Metlitski,  
Cenke Xu, and  
T. Senthil, PRX **7**,  
031051 (2017)



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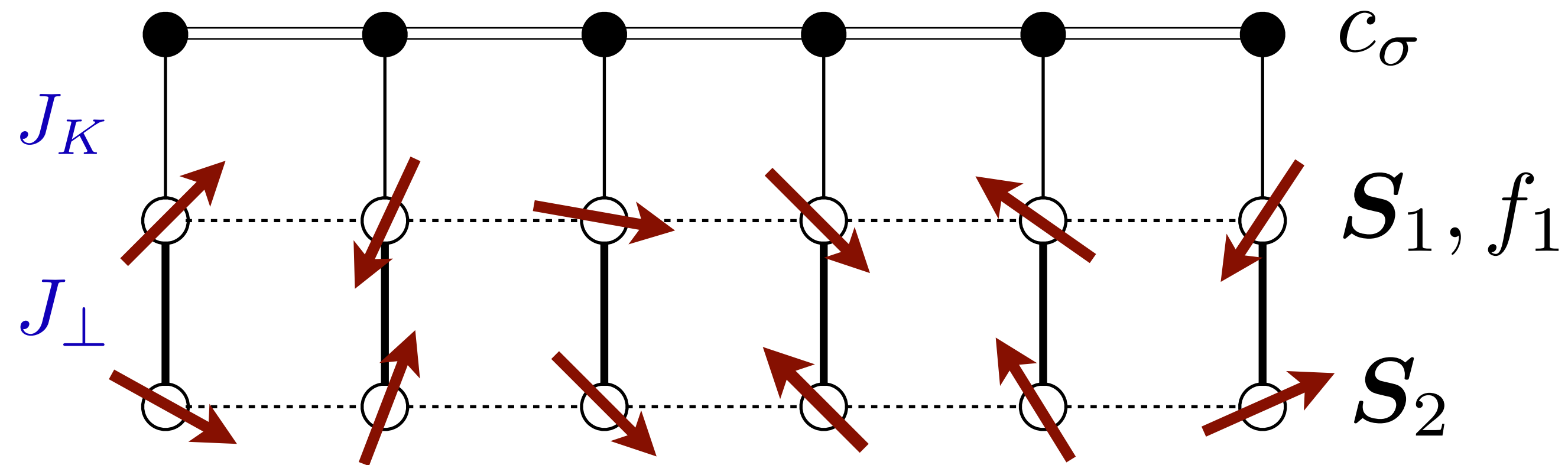
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There is now good evidence that the  $N_f = 2$   $SU(2)$ -QCD CFT is not stable.

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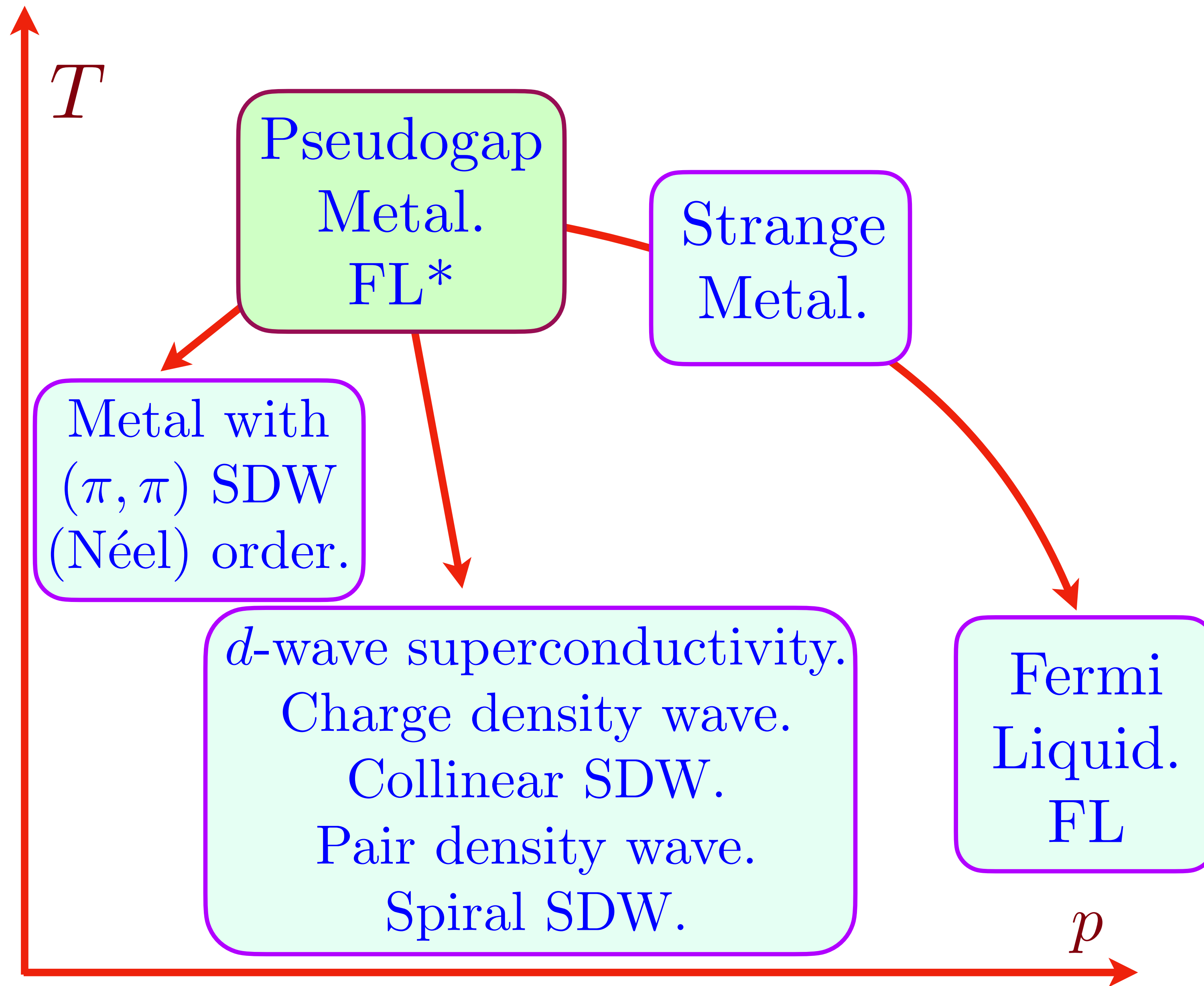
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Confinement transition: Condensation of  $\langle \Psi f_1 \rangle$ ,  $\langle \Psi f_1^\dagger \rangle$ , leads to  $d$ -wave superconductivity, charge density wave, pair density wave.

Boson-fermion duality

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A. Nahum,  
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## Summary

- Paramagnon fractionalization theory of FL\* for the pseudogap metal of the cuprate high temperature superconductors:

**Don't fractionalize the mobile electron, but fractionalize the paramagnon into 'ancilla qubits'.**

Predicts electronic spectra in good agreement with observations in *both* nodal and anti-nodal regions.

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Predicts electronic spectra in good agreement with observations in *both* nodal and anti-nodal regions.

- **Outlook:**

- 'Back side' of hole pockets in FL\* phase may be observable in cleaner samples.
- Theory for multi-point correlators in cold atom experiments.
- Theory for FL\*-FL transition leads to strange metal with spatially random couplings.
- Theory of quantum oscillations in underdoped cuprates at high fields.