

Microstructure of charge order in the cuprates, and implications for the pseudogap

Strong Correlations and Unconventional Superconductivity:
Towards a Conceptual Framework
KITP, Santa Barbara

September 23, 2014
Subir Sachdev

Talk online: sachdev.physics.harvard.edu



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Kazuhiro Fujita
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Mohammad Hamidian
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Stephen Edkins
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Michael Lawler



J. C. Seamus Davis



Eun-Ah Kim

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See talk by
Kazuhiro Fujita
on Friday



Michael Lawler



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Eun-Ah Kim

Theorists at Harvard



Max Metlitski
(KITP, UCSB)



Rolando La Placa
(MIT)



Andrea Allais



Johannes
Bauer



Debanjan
Chowdhury



Jay Deep Sau
(Maryland)



Alexandra
Thomson

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Rohan



Lea Allais

See poster by
Debanjan Chowdhury



Johannes
Bauer



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Chowdhury

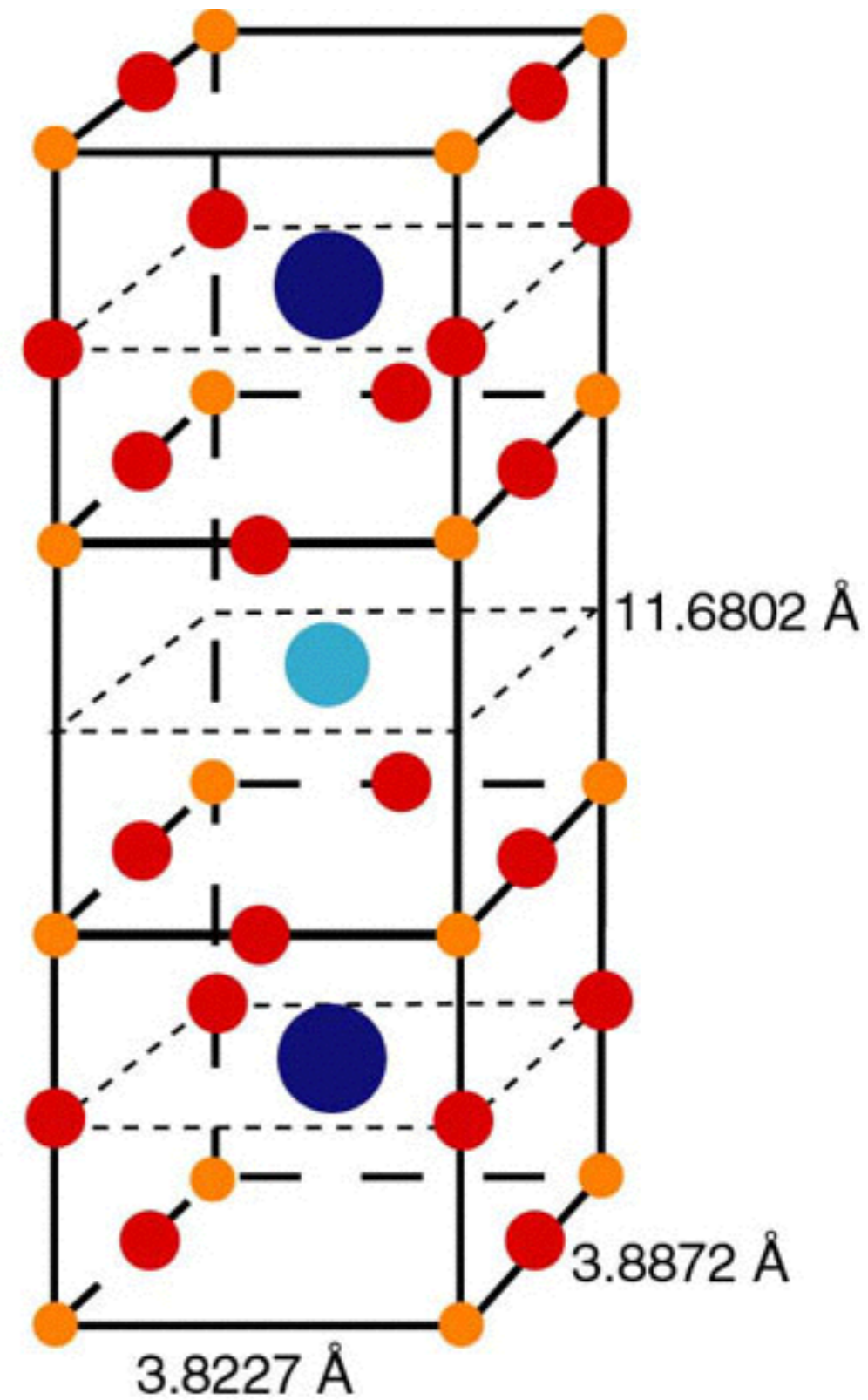
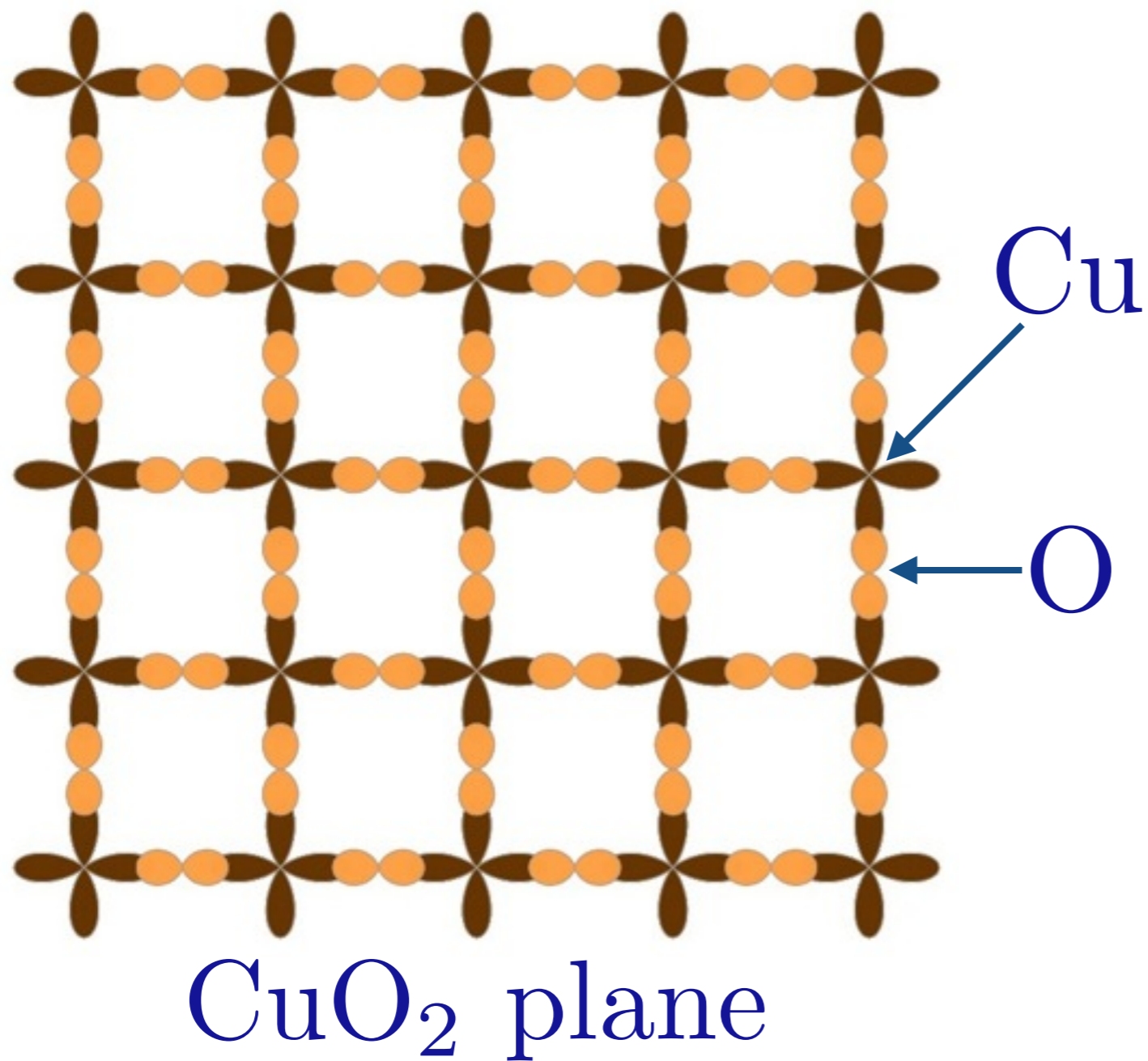


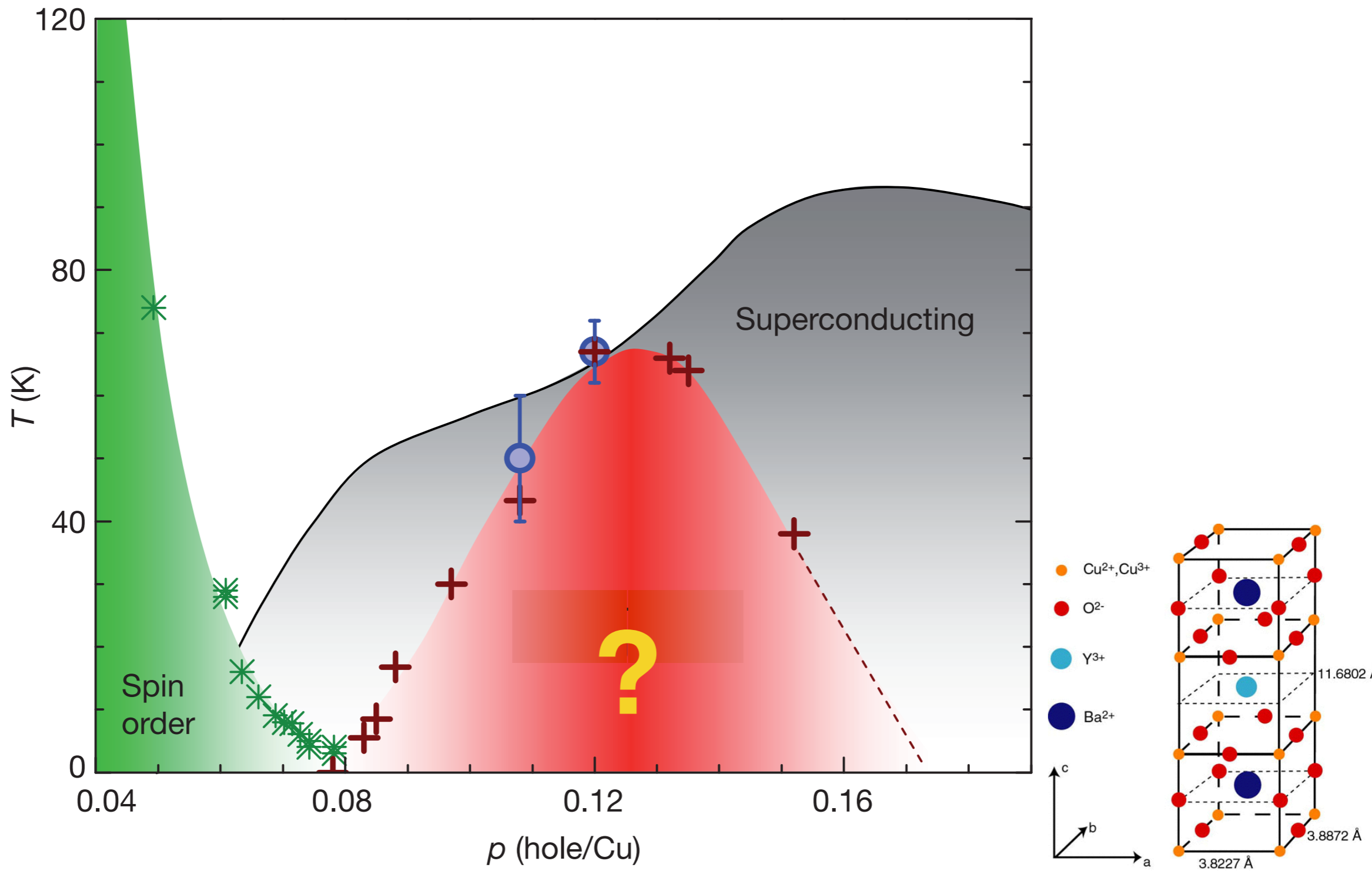
Jay Deep Sau
(Maryland)



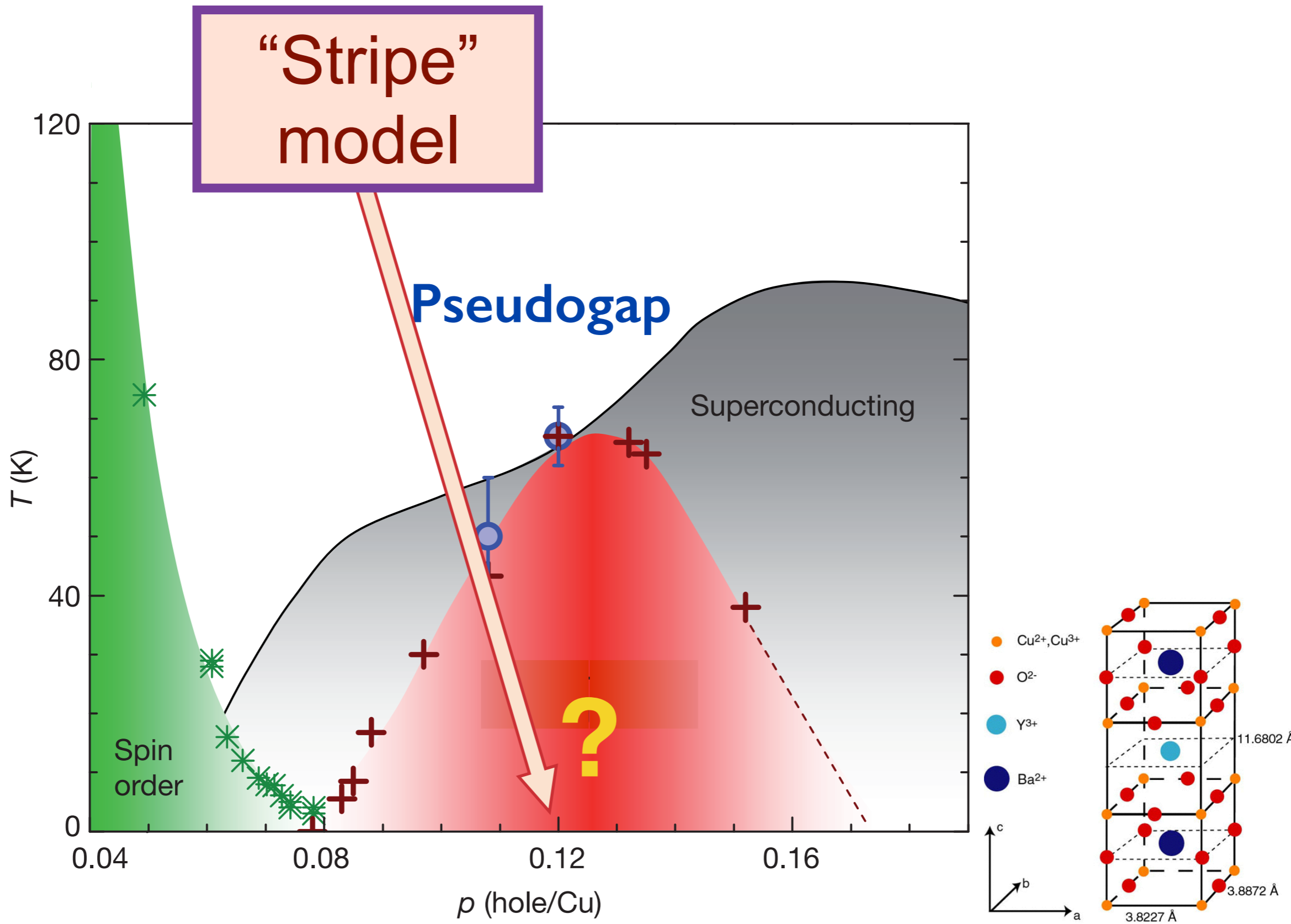
Alexandra
Thomson

High temperature superconductors



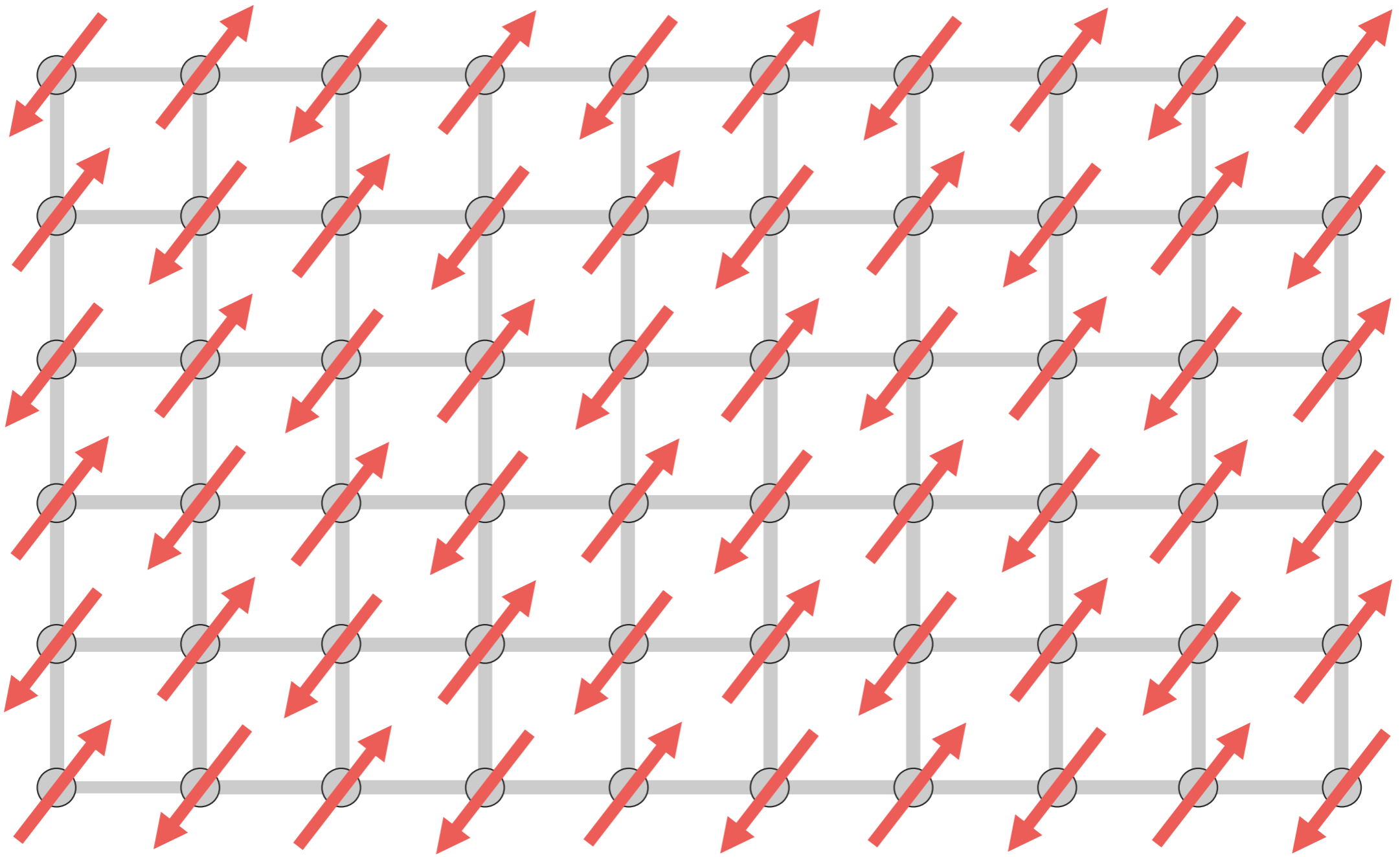


T. Wu, H. Mayaffre, S. Kramer, M. Horvatic, C. Berthier, W.N. Hardy, R. Liang, D.A. Bonn, and M.-H. Julien, *Nature* **477**, 191 (2011).



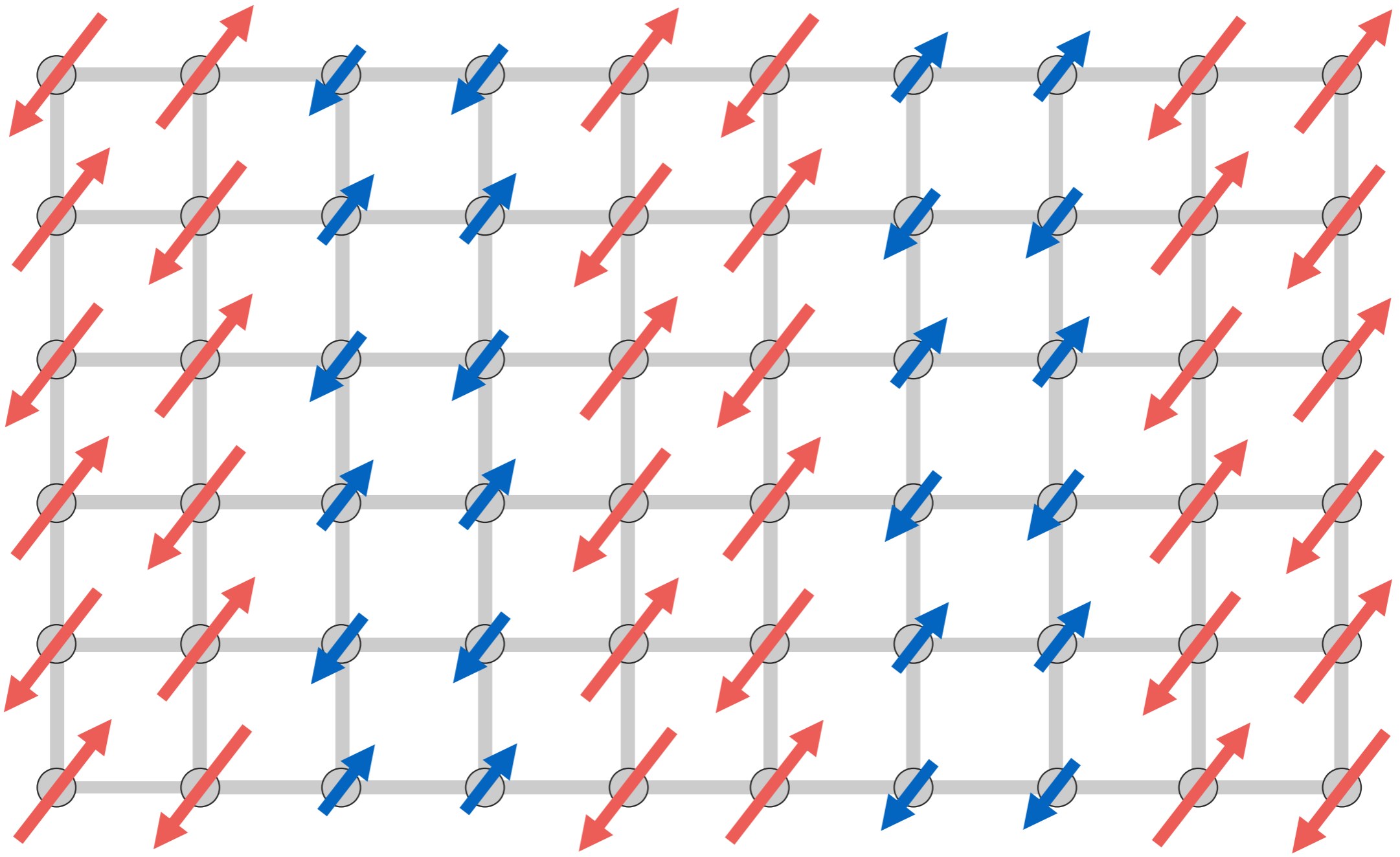
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“Stripe” model



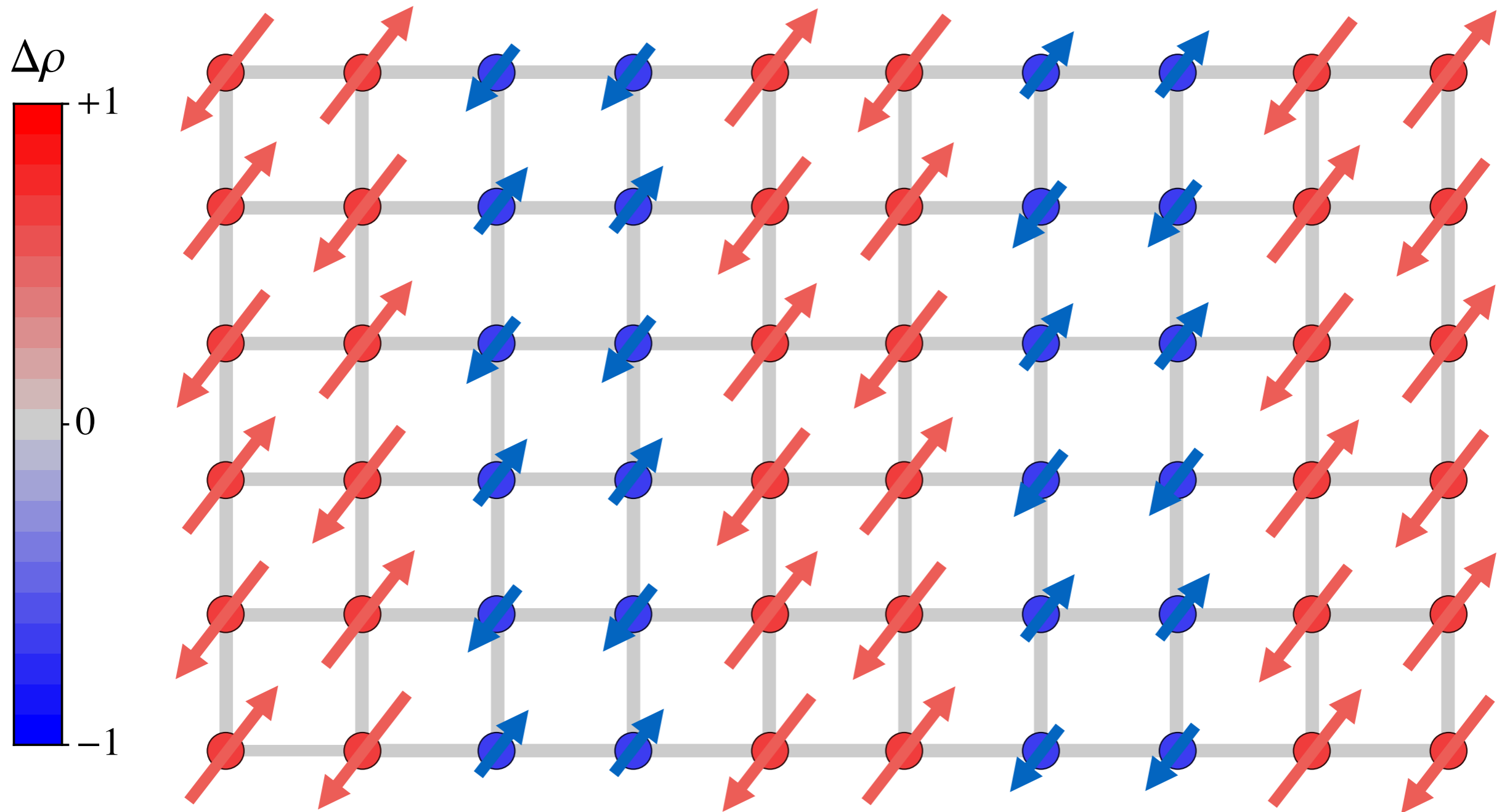
Start with an antiferromagnet

“Stripe” model



Domain walls 4 lattice spacings apart

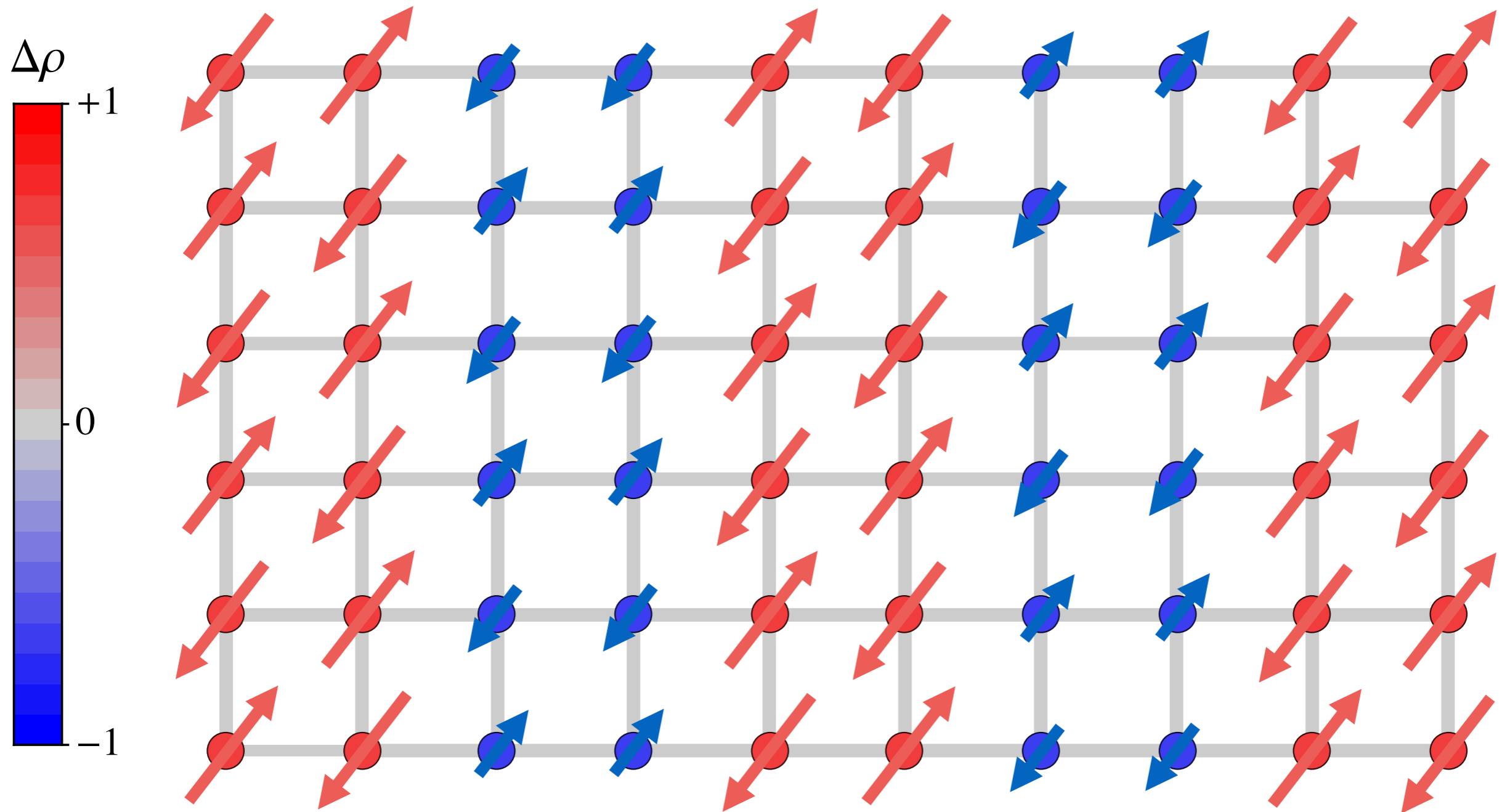
“Stripe” model



Put the holes in the domain walls

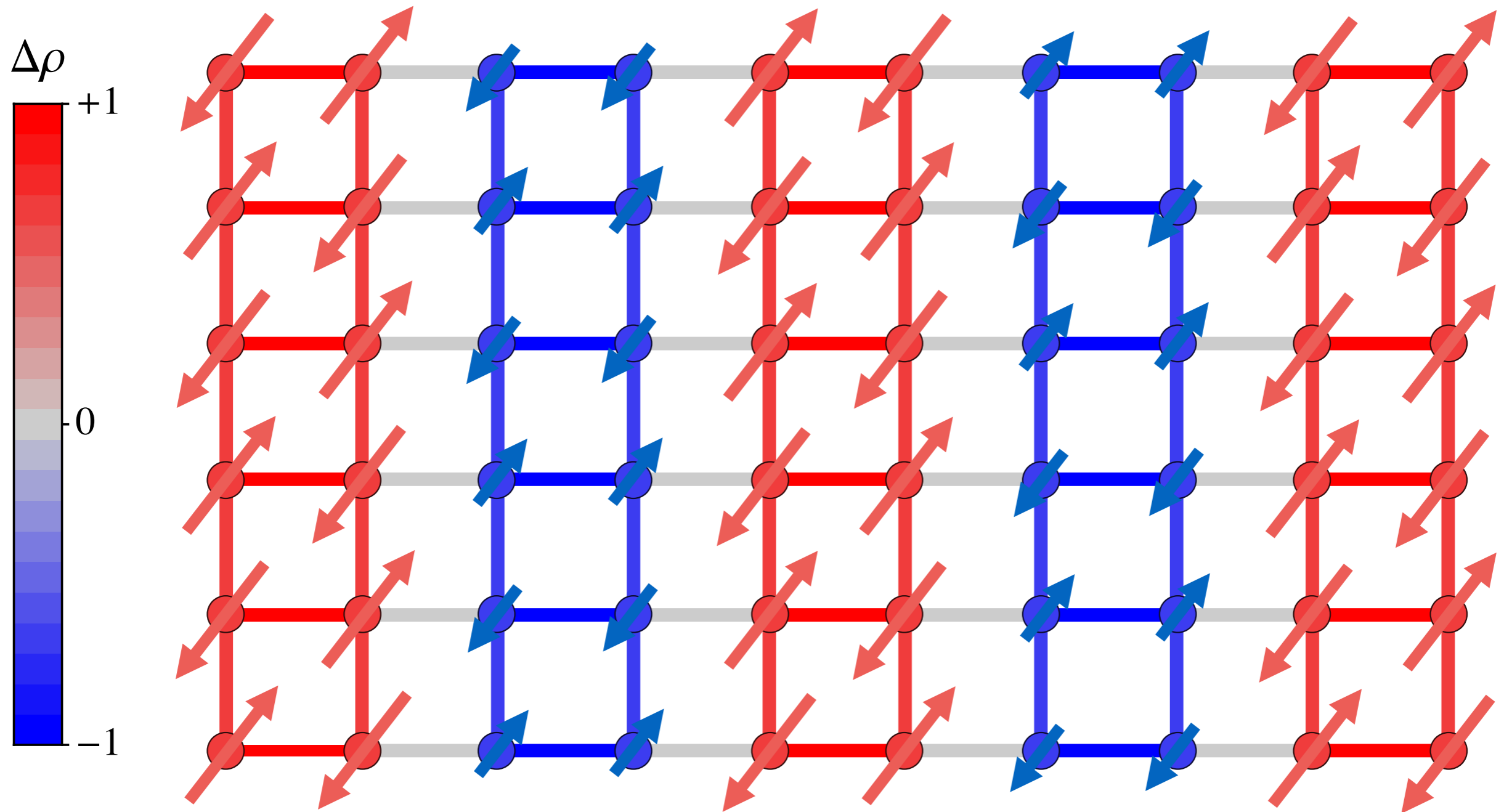
“Stripe”
model

Observed in La-based
compounds (Tranquada..)

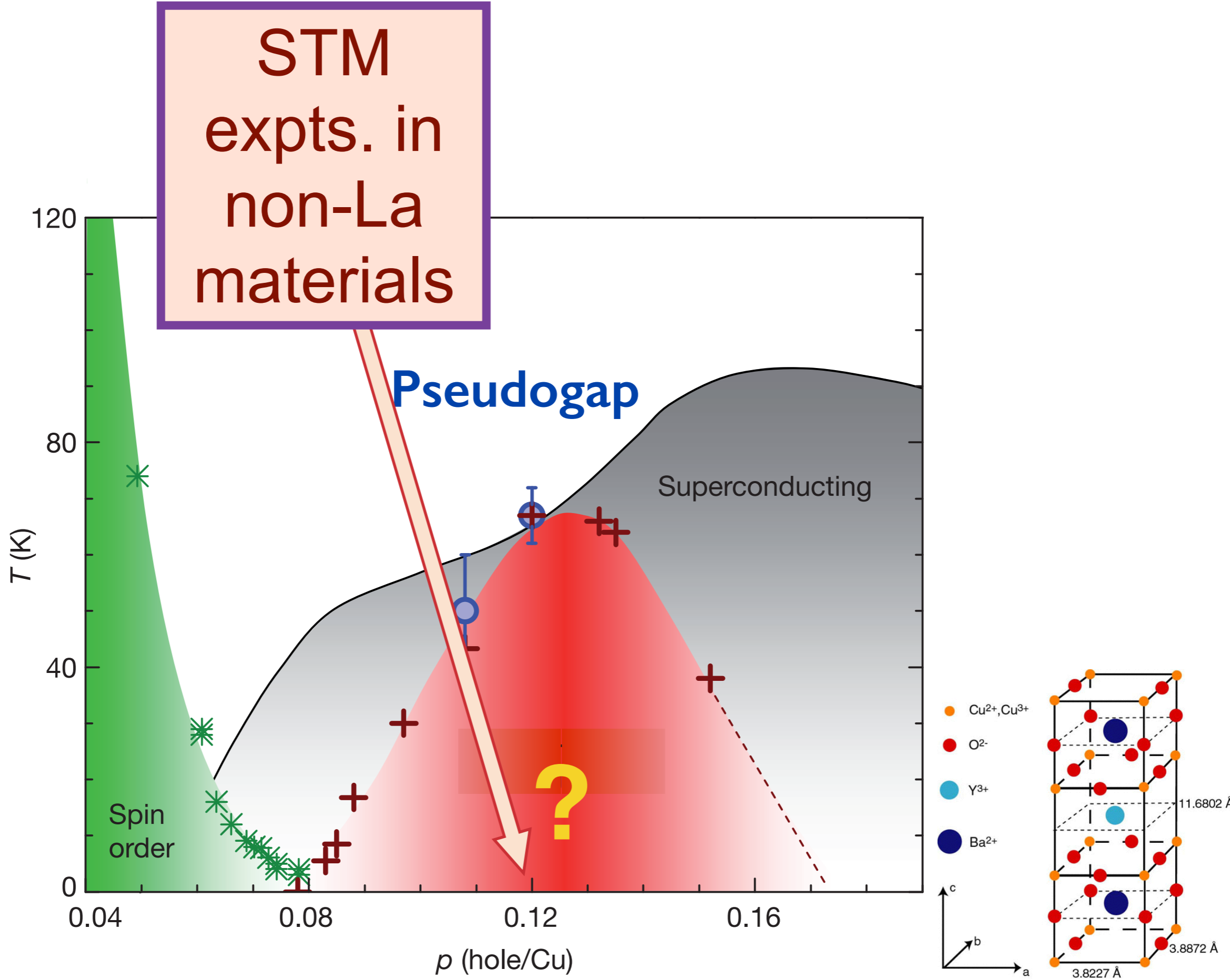


Put the holes in the domain walls

“Stripe” model



Colors on the bonds map the local exchange energy



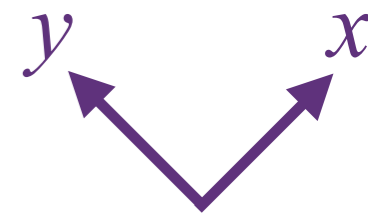
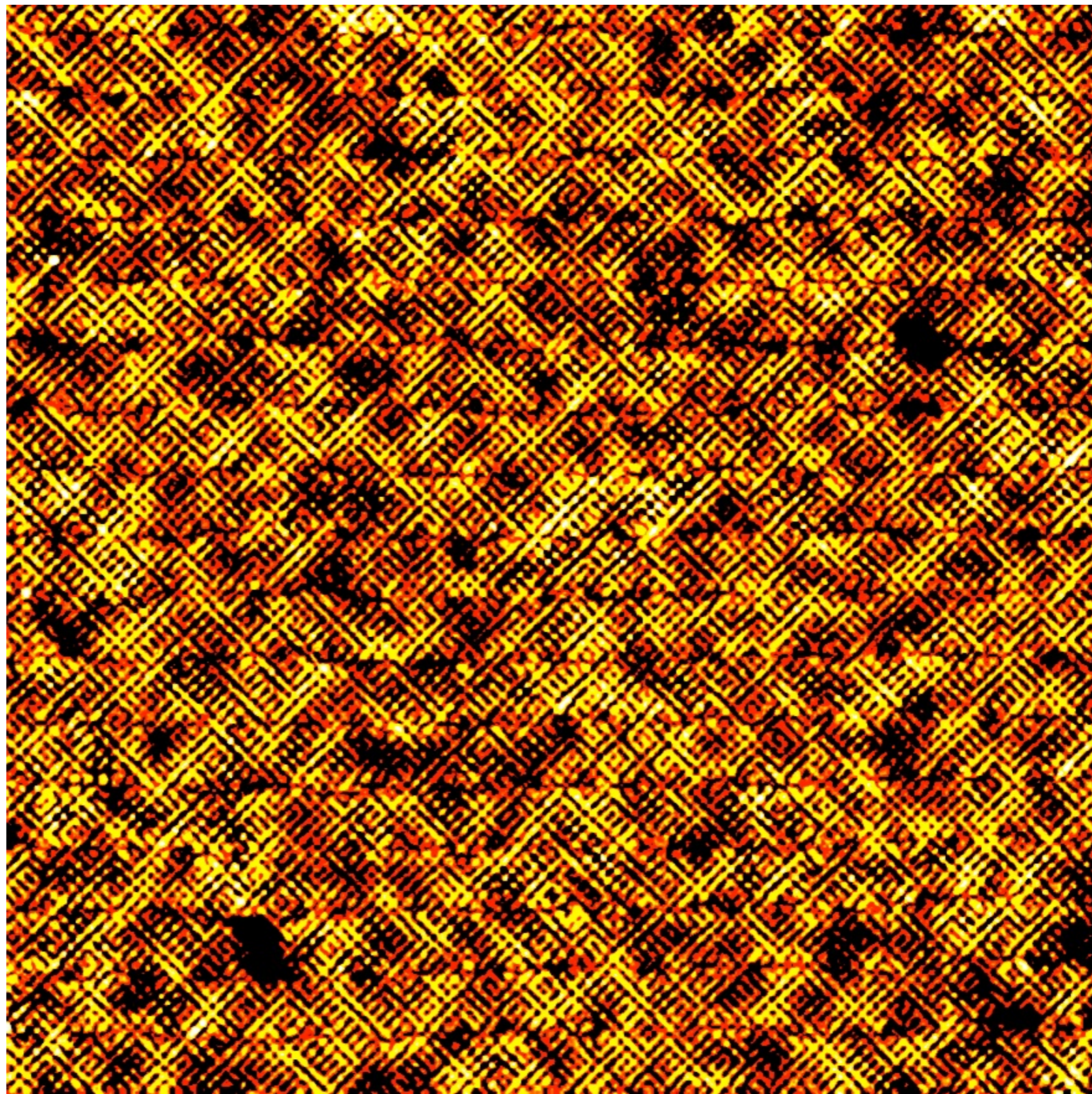
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See also

C. Howald, H. Eisaki,
N. Kaneko, M. Greven,
and A. Kapitulnik,
Phys. Rev. B **67**,
014533 (2003);

M. Vershinin, S. Misra,
S. Ono, Y. Abe, Yoichi
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A. Yazdani, *Science*
303, 1995 (2004).

W. D. Wise, M. C. Boyer,
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Nature Phys. **4**, 696
(2008).



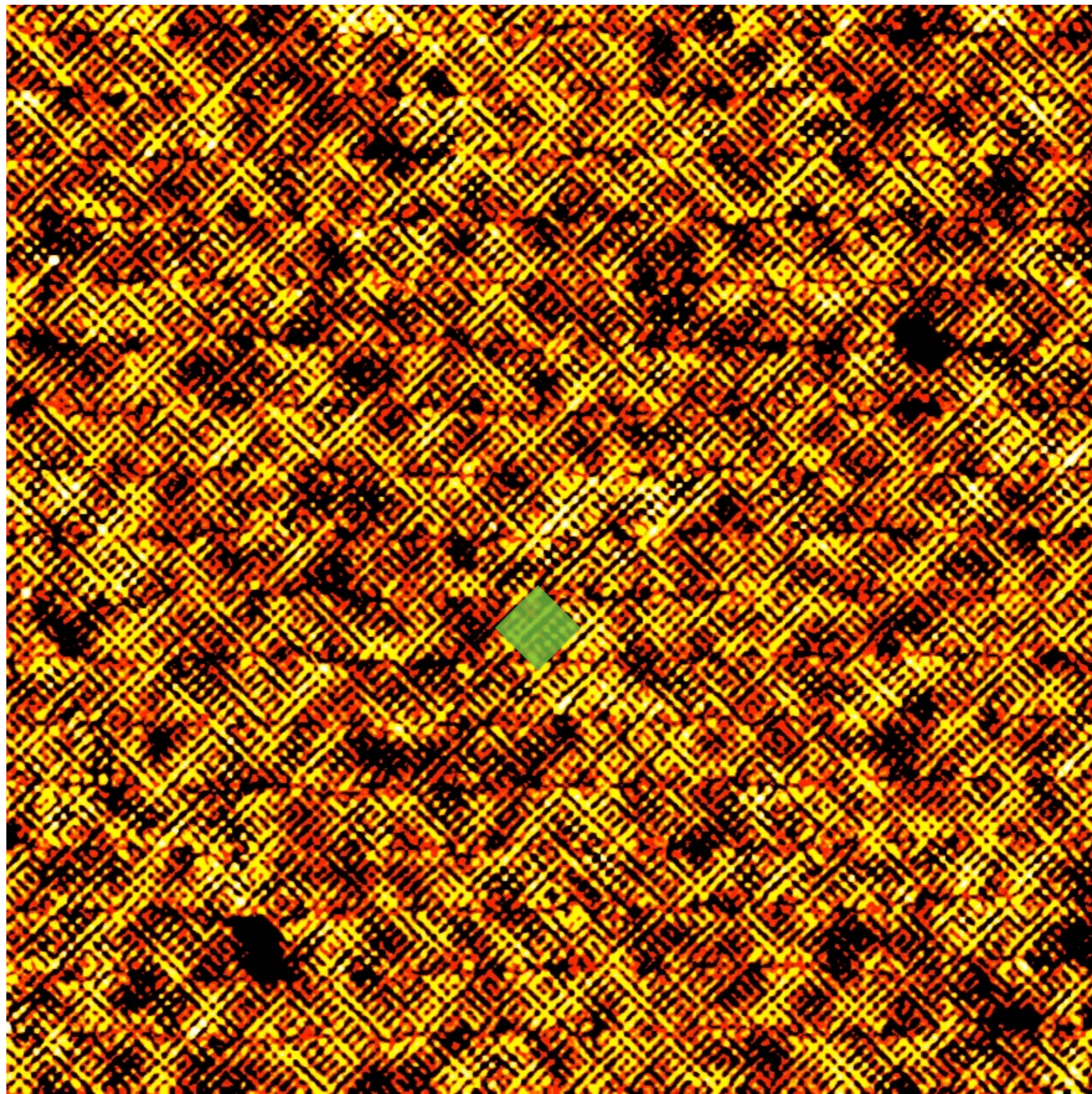
“R-map” of BSCCO in zero magnetic field, similar to those published in Y. Kohsaka, C. Taylor, K. Fujita, A. Schmidt, C. Lupien, T. Hanaguri, M. Azuma, M. Takano, H. Eisaki, H. Takagi, S. Uchida, and J. C. Davis, *Science* **315**, 1380 (2007). Davis group has sub-angstrom resolution capabilities, with lattice drift corrections, which make sublattice phase-resolved STM possible.

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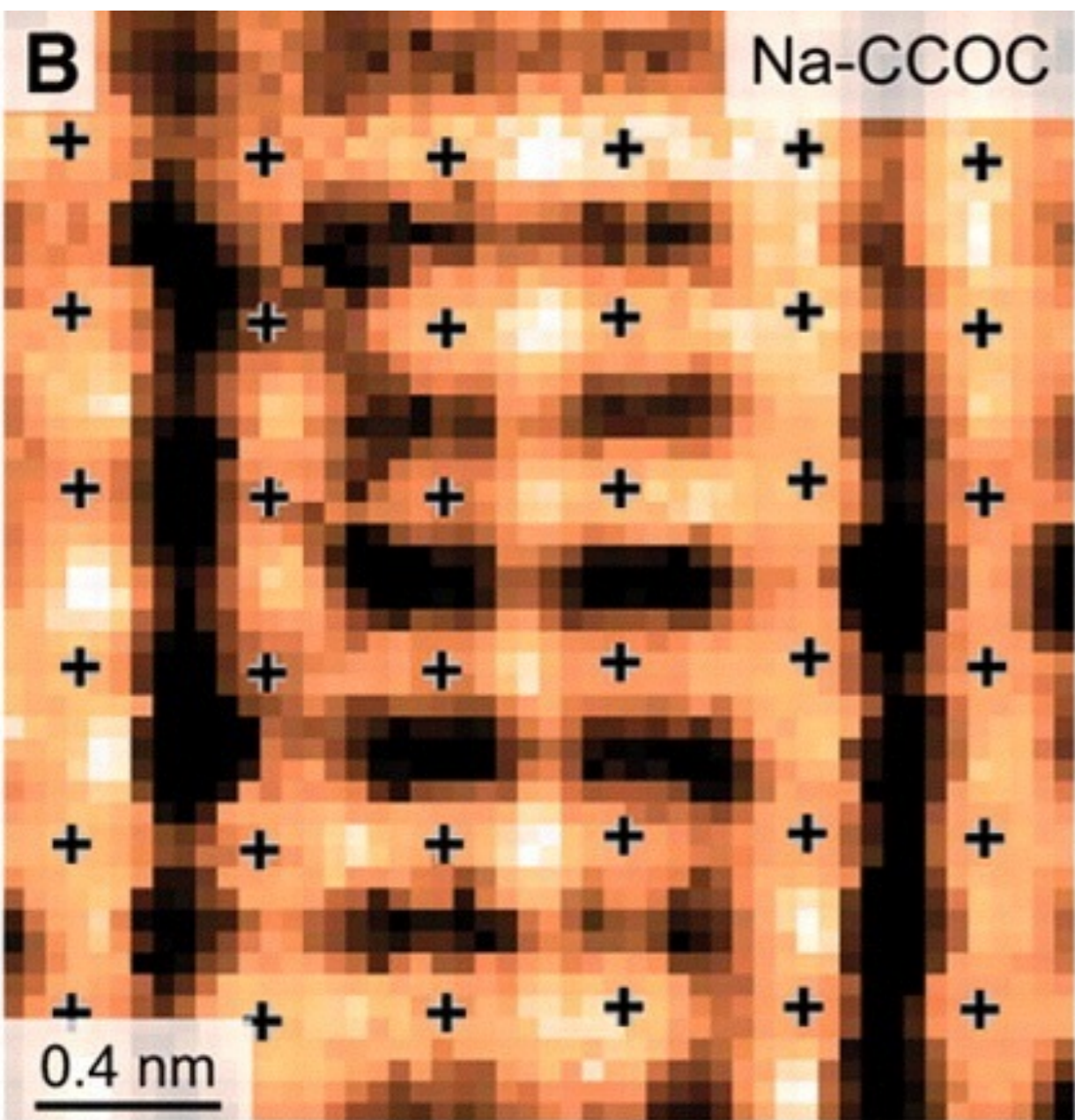
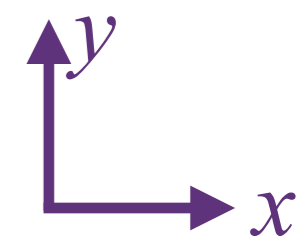
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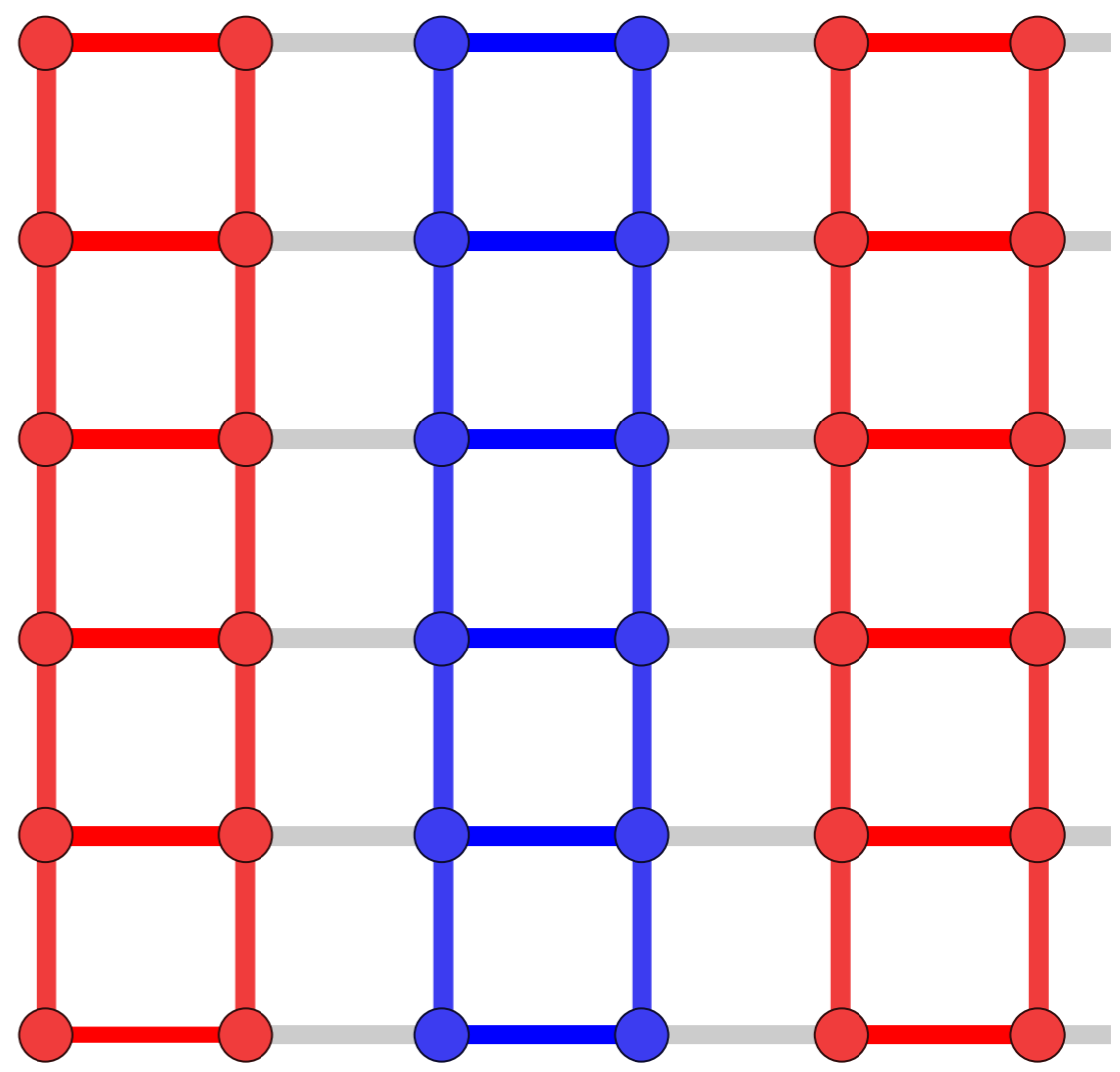
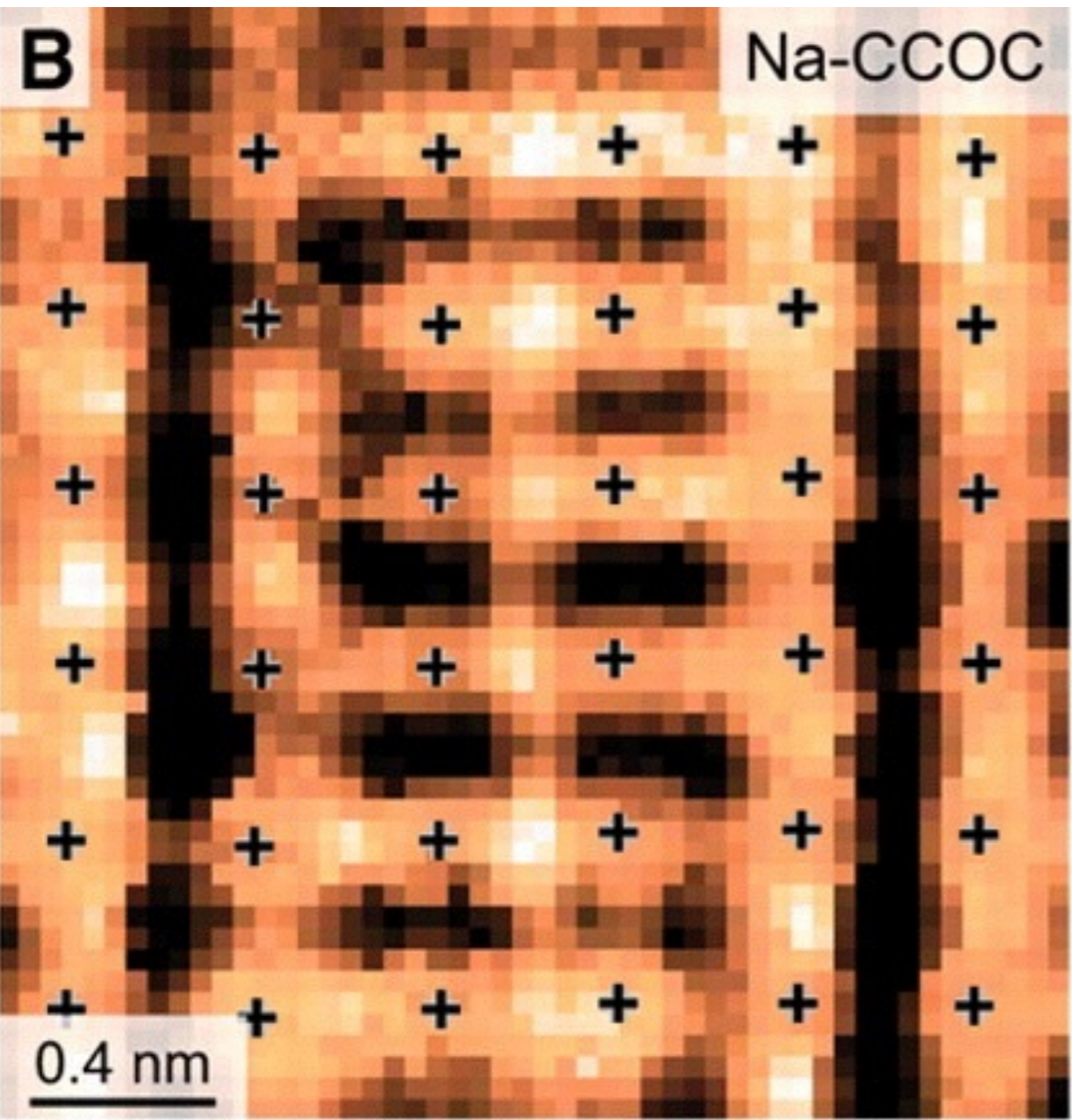
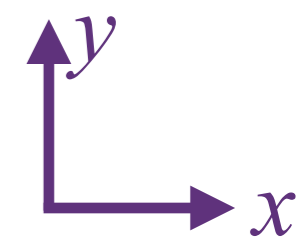
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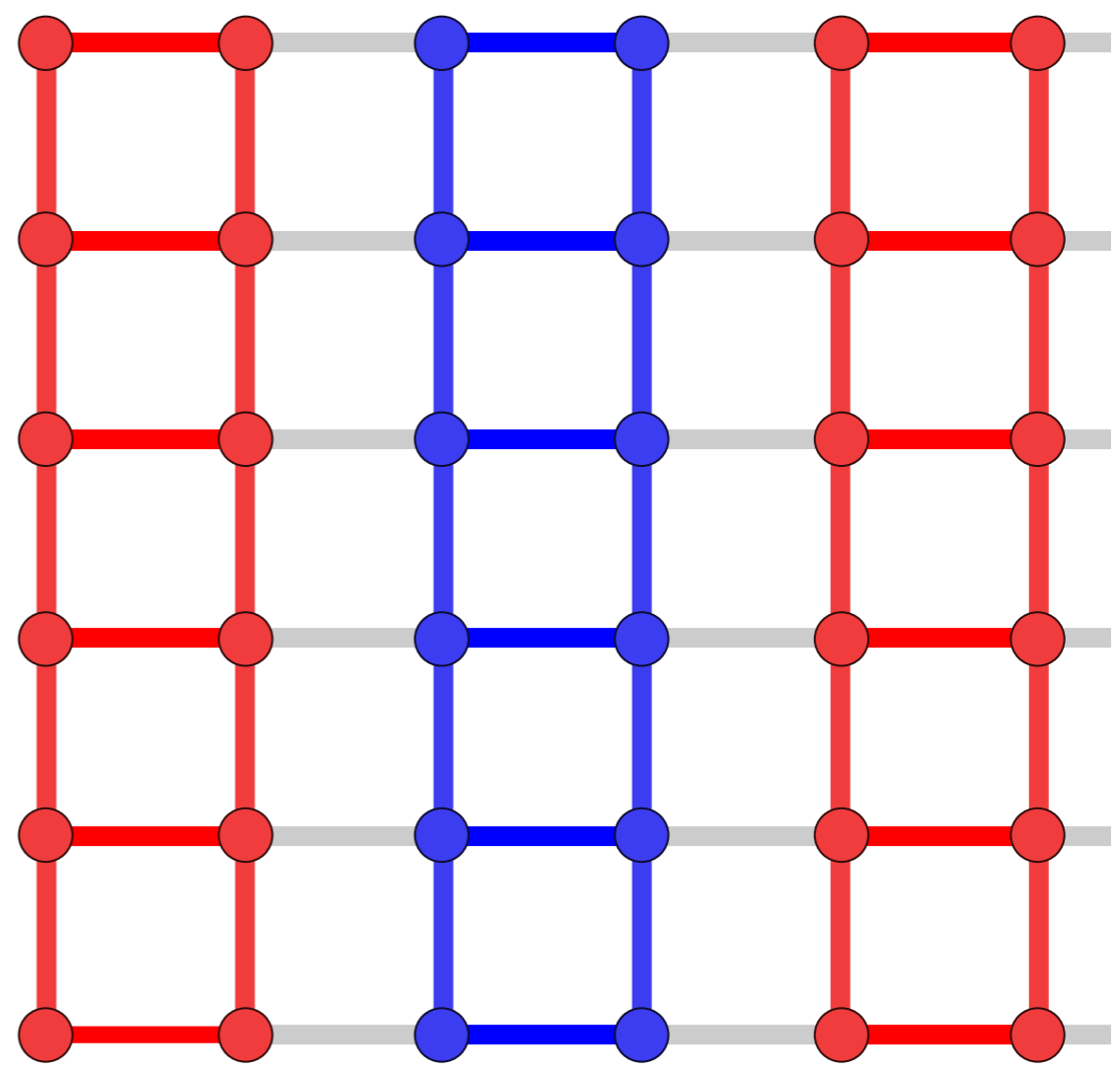
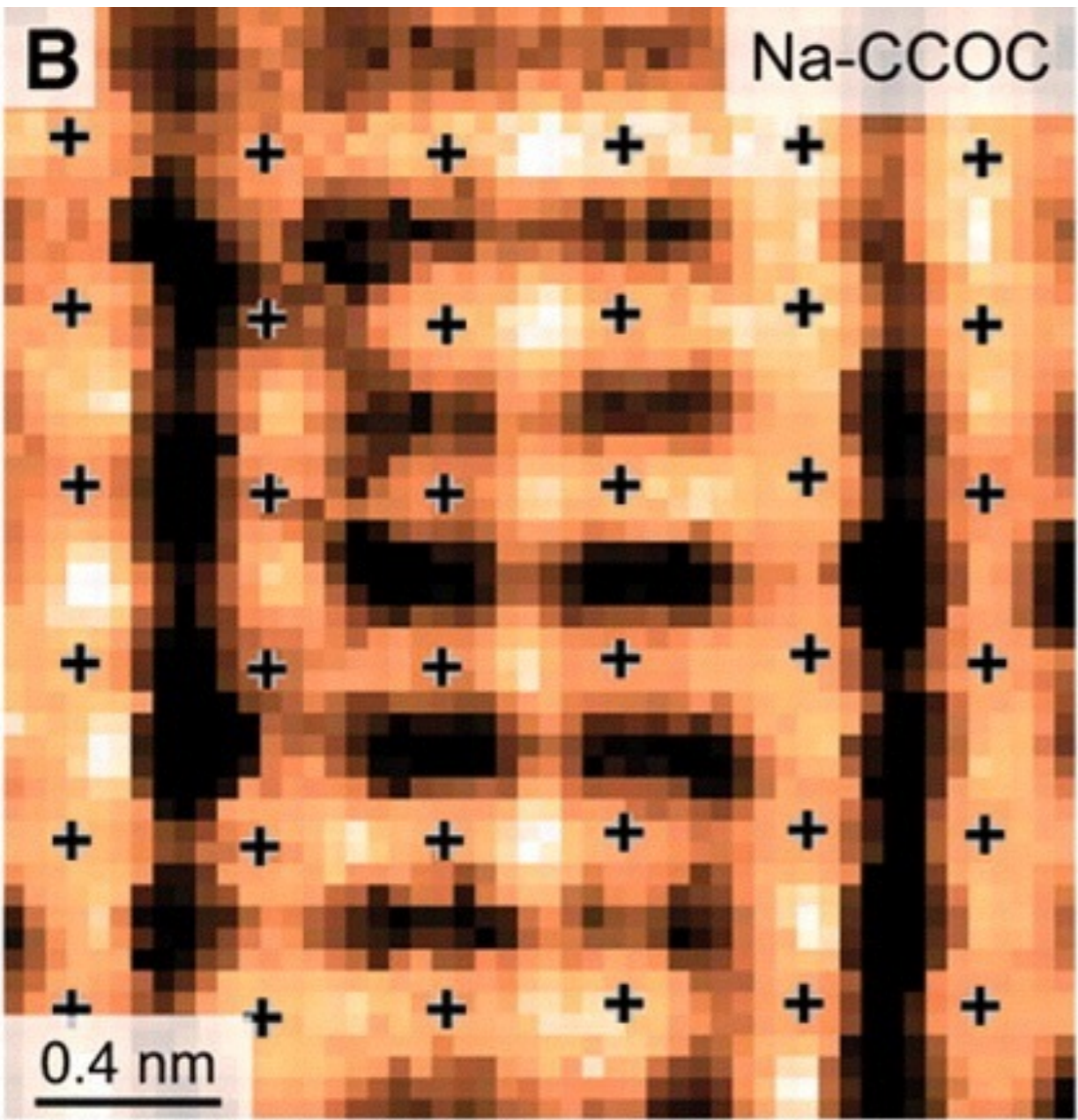
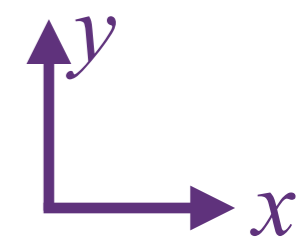


Y. Kohsaka *et al.*, SCIENCE **315**, 1380 (2007)



“Stripe” model

Y. Kohsaka *et al.*, SCIENCE **315**, 1380 (2007)



“Stripe” model

Microstructure of STM picture does not match this simple “stripe” model

Y. Kohsaka *et al.*, SCIENCE 315, 1380 (2007)

Charge density wave (CDW) order

$$\langle c_{\alpha}^{\dagger}(\mathbf{r})c_{\alpha}(\mathbf{r}) \rangle = \Psi_{CDW}(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} + \text{c.c.}$$



Nearly constant CDW order parameter

Unconventional density wave (DW) :
Bose condensation of particle-hole pairs

$$\langle c_{\alpha}^{\dagger}(\mathbf{r}_1)c_{\alpha}(\mathbf{r}_2) \rangle$$
$$= \left[\mathcal{P}(\mathbf{r}_1 - \mathbf{r}_2) \right] \times \Psi_{DW} \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \right) e^{i\mathbf{Q} \cdot (\mathbf{r}_1 + \mathbf{r}_2)/2} + \text{c.c.}$$

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Crucial “center-of-mass” co-ordinate.
(Not used in previous work)
Simplifies action of time-reversal

Unconventional density wave (DW) :
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Density wave form factor (internal particle-hole pair wavefunction)

$$\mathcal{P}(\mathbf{r}) = \int \frac{d^2k}{4\pi^2} \mathcal{P}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{r}}$$

Time-reversal symmetry requires $\mathcal{P}(\mathbf{k}) = \mathcal{P}(-\mathbf{k})$.

We expand (using reflection symmetry for \mathbf{Q} along axes or diagonals)

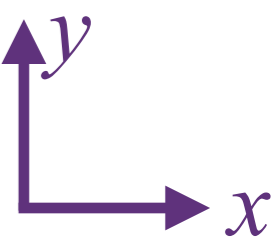
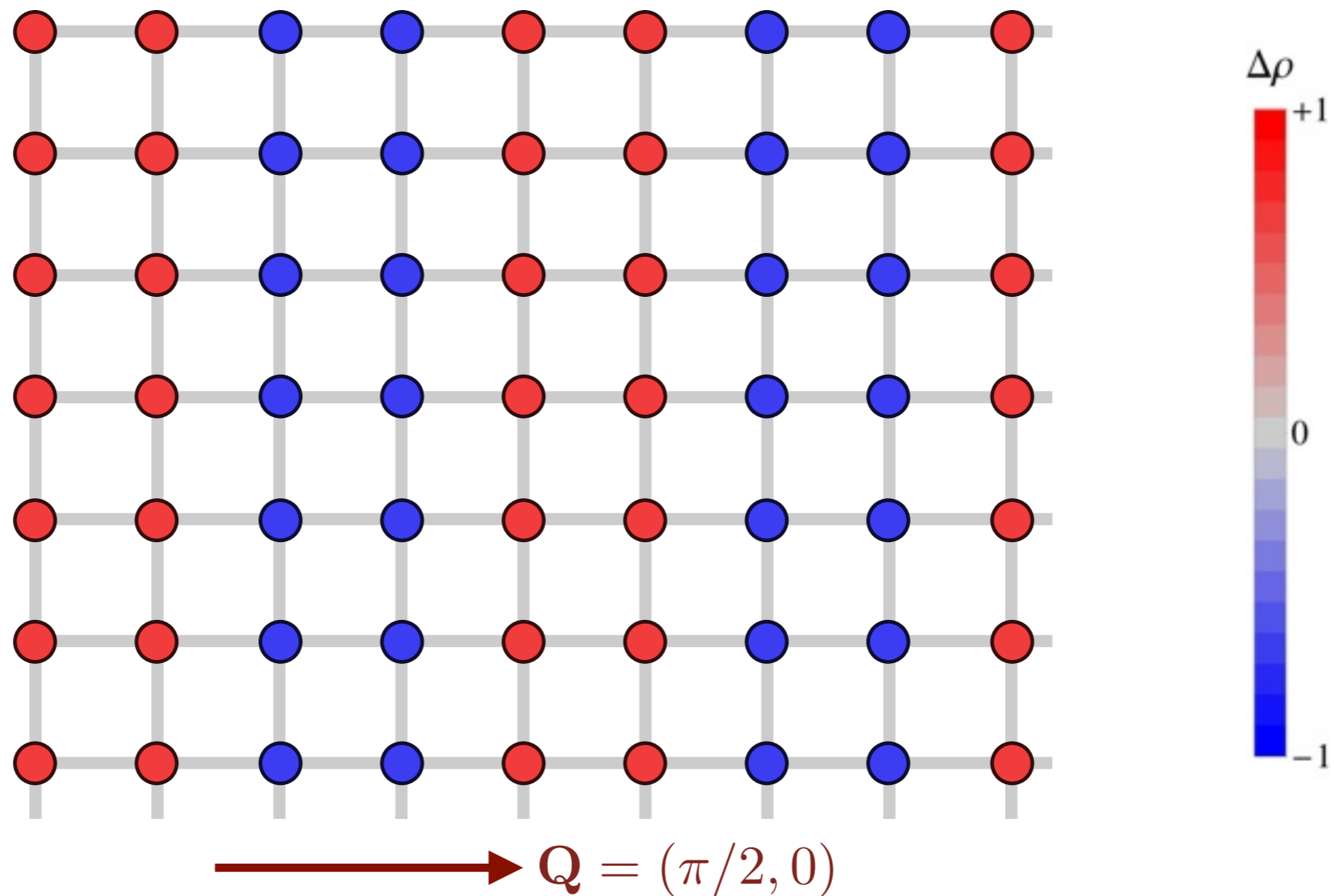
$$\mathcal{P}(\mathbf{k}) = \mathcal{P}_s + \mathcal{P}_{s'}(\cos k_x + \cos k_y) + \mathcal{P}_d(\cos k_x - \cos k_y)$$

Conventional CDW order: s -form factor

Plot of $P_{ij} = \langle c_{i\alpha}^\dagger c_{j\alpha} \rangle$ for $i = j$, and i, j nearest neighbors.

$$P_{ij} = \left[\int_{\mathbf{k}} \mathcal{P}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right] e^{i\mathbf{Q}\cdot(\mathbf{r}_i + \mathbf{r}_j)/2} + \text{c.c.}$$

$$\mathcal{P}(\mathbf{k}) = 1 \quad \text{and} \quad \mathbf{Q} = 2\pi(1/4, 0)$$

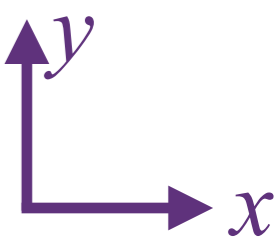
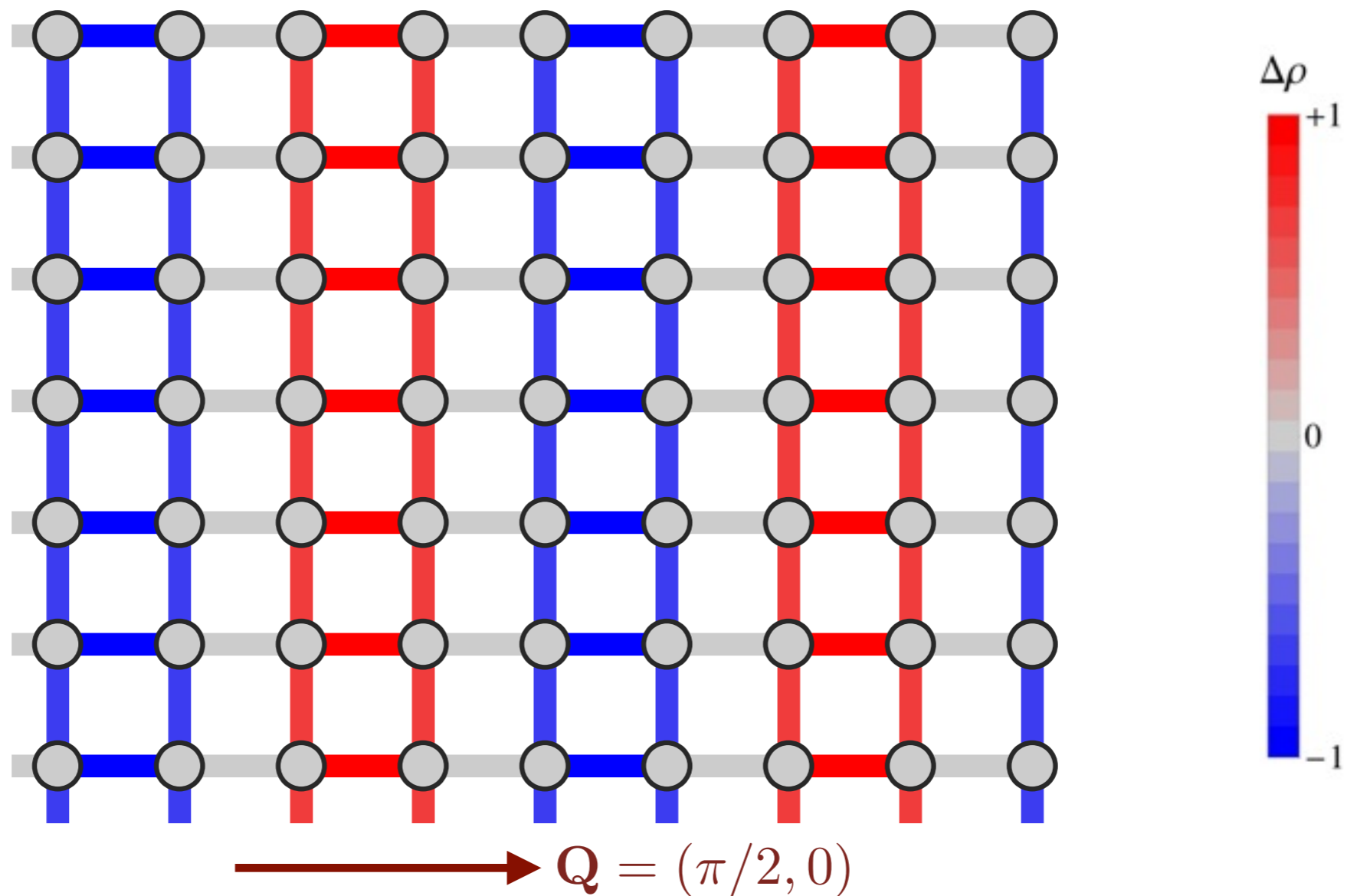


Unconventional DW order: s' -form factor

Plot of $P_{ij} = \langle c_{i\alpha}^\dagger c_{j\alpha} \rangle$ for $i = j$, and i, j nearest neighbors.

$$P_{ij} = \left[\int_{\mathbf{k}} \mathcal{P}(\mathbf{k}) e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right] e^{i\mathbf{Q} \cdot (\mathbf{r}_i + \mathbf{r}_j)/2} + \text{c.c.}$$

$$\mathcal{P}(\mathbf{k}) = e^{i\phi} [\cos(k_x) + \cos(k_y)] \quad \text{and} \quad \mathbf{Q} = 2\pi(1/4, 0)$$

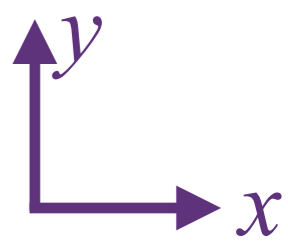


Unconventional DW order: s' -form factor

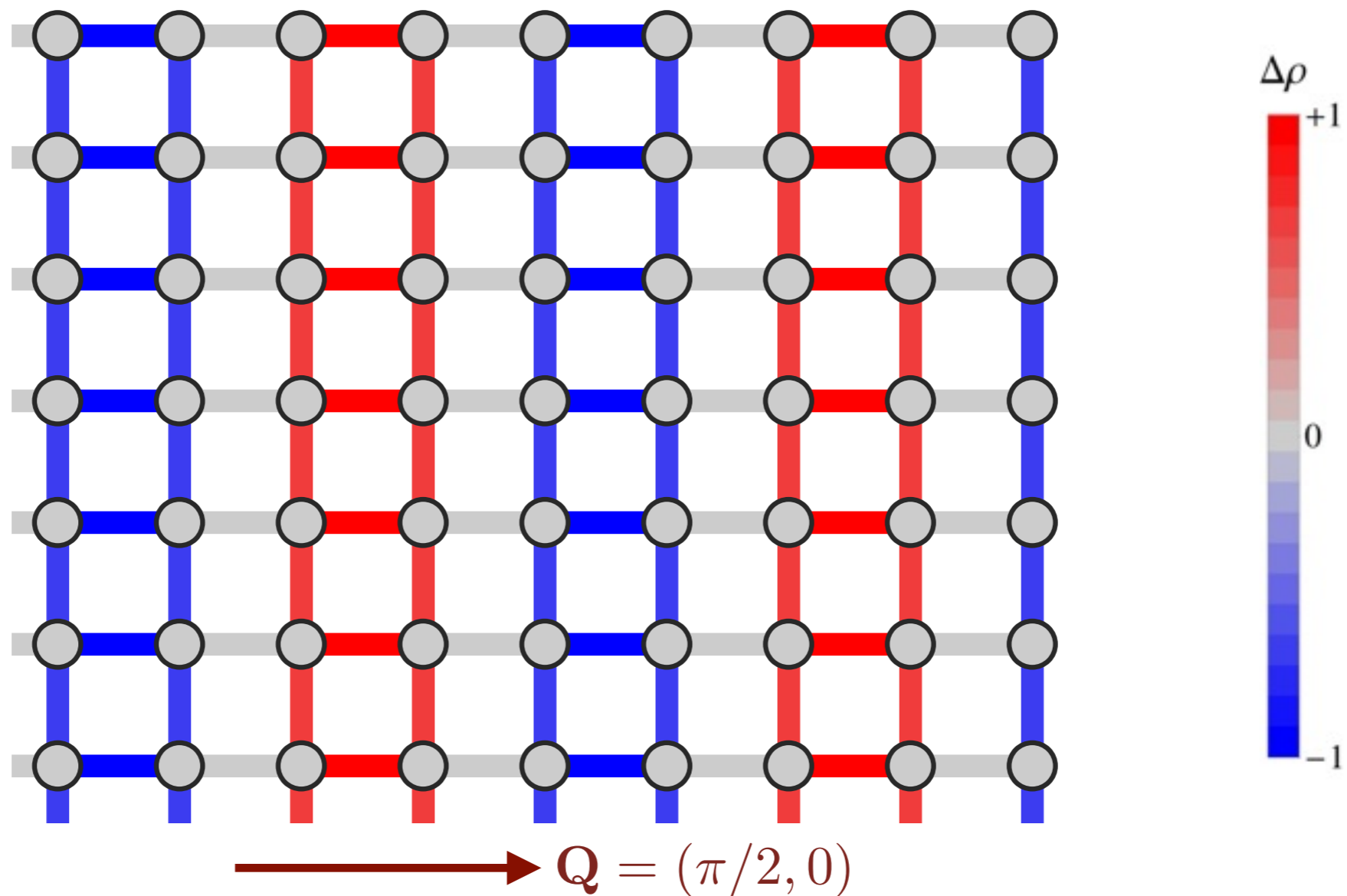
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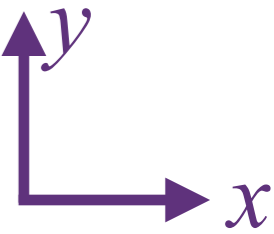


“Stripe”
model !



Unconventional DW order: s' -form factor

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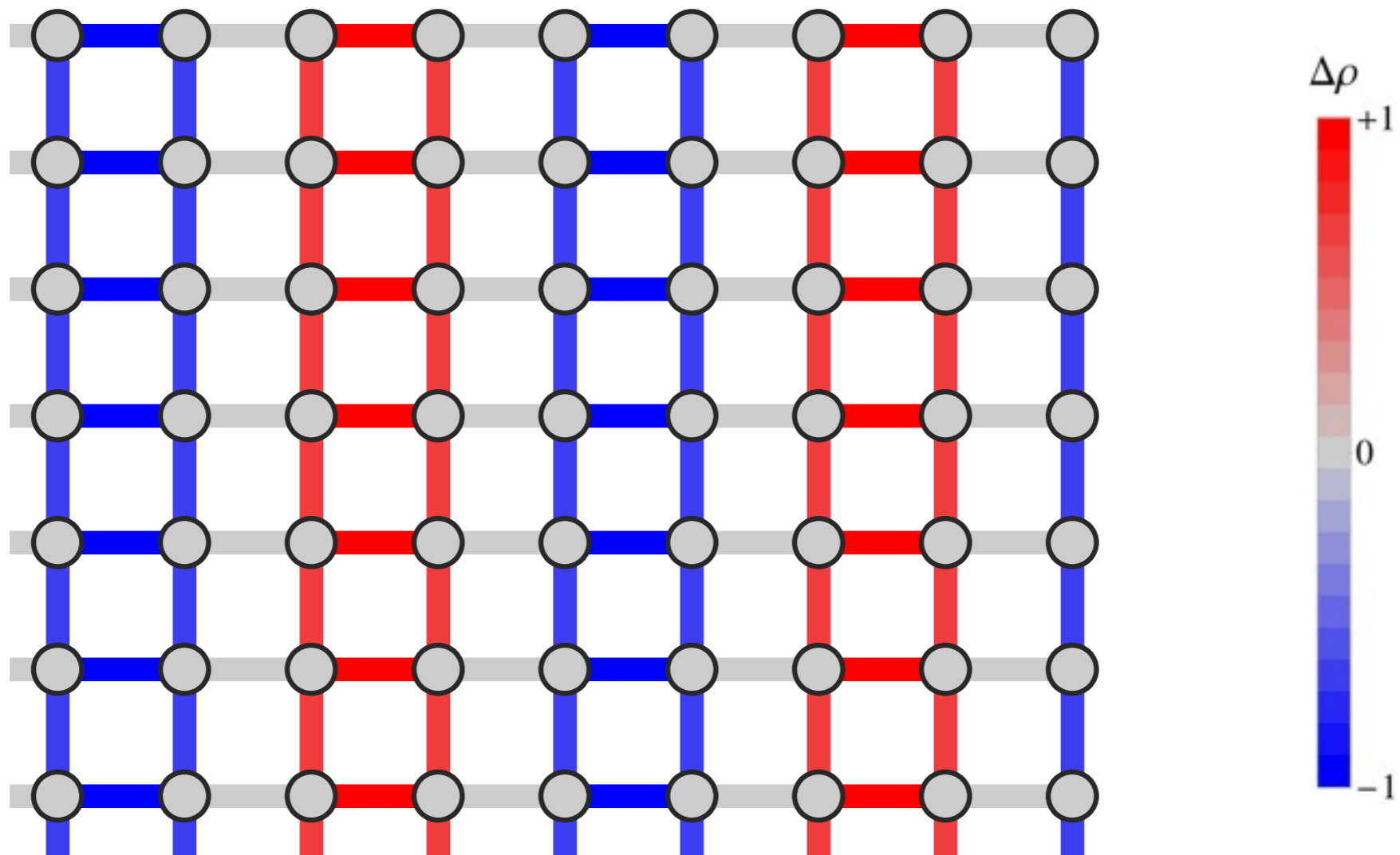


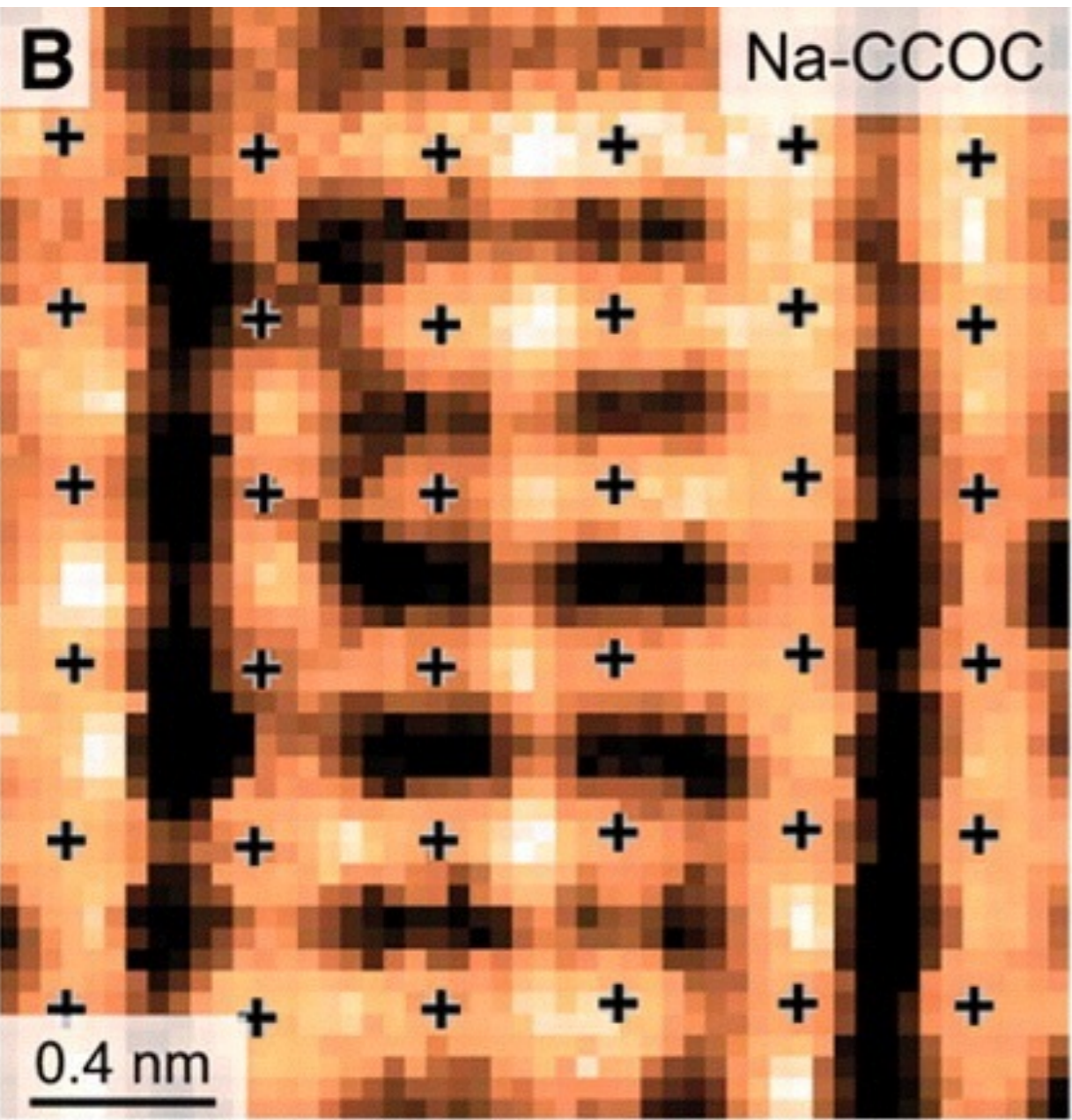
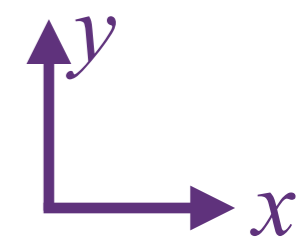
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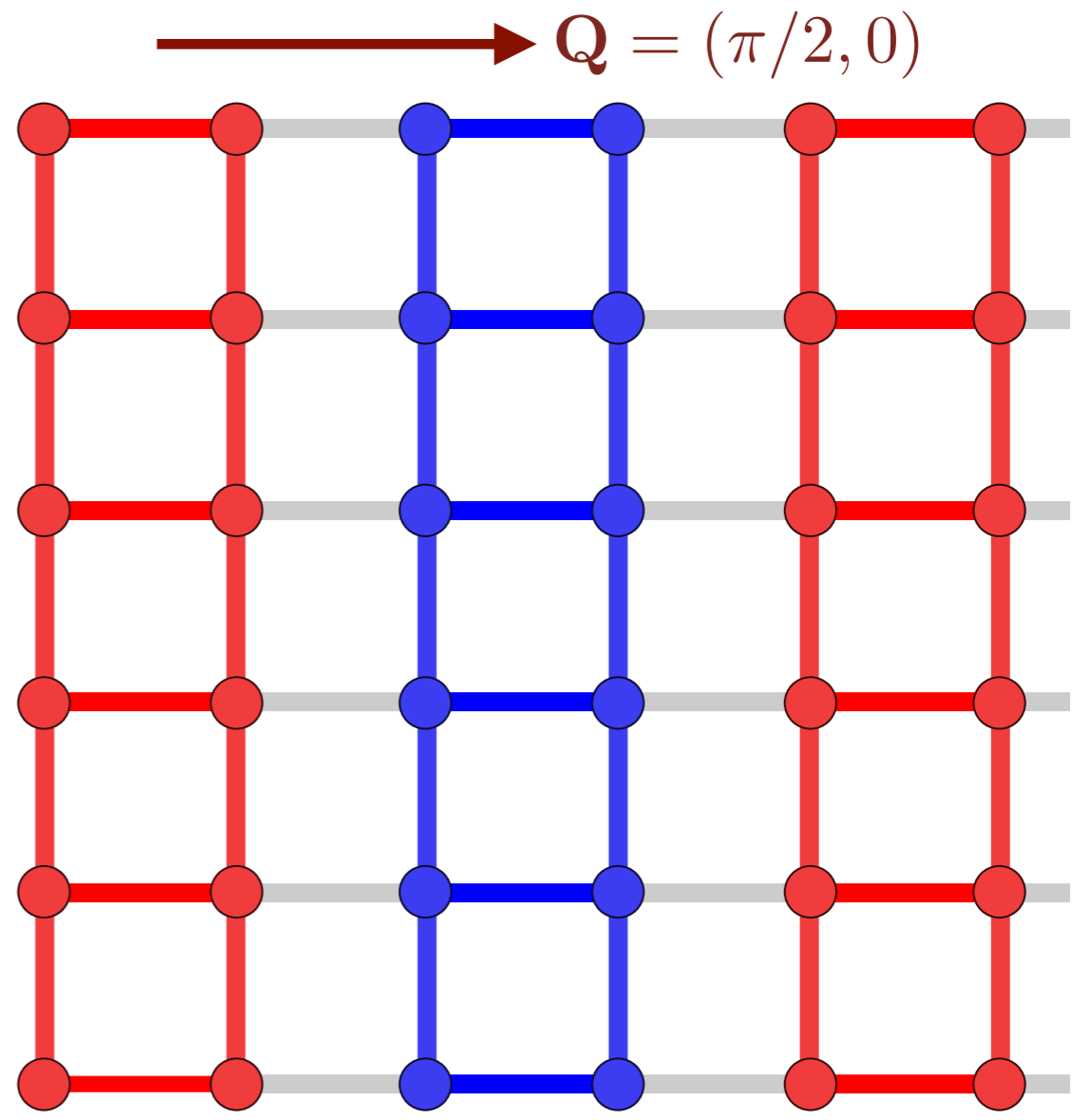
“Stripe”
model !

X-ray
observations
indicate
strong s'
component in
LBCO





Y. Kohsaka *et al.*, SCIENCE **315**, 1380 (2007)



$s + s'$ -form factor density wave

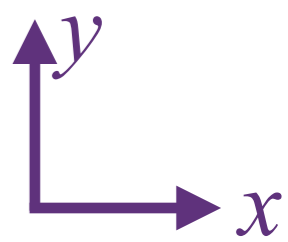
$s + s'$ form factor does not match STM measurements on BSCCO, Na-CCOC.

Unconventional DW order: d -form factor

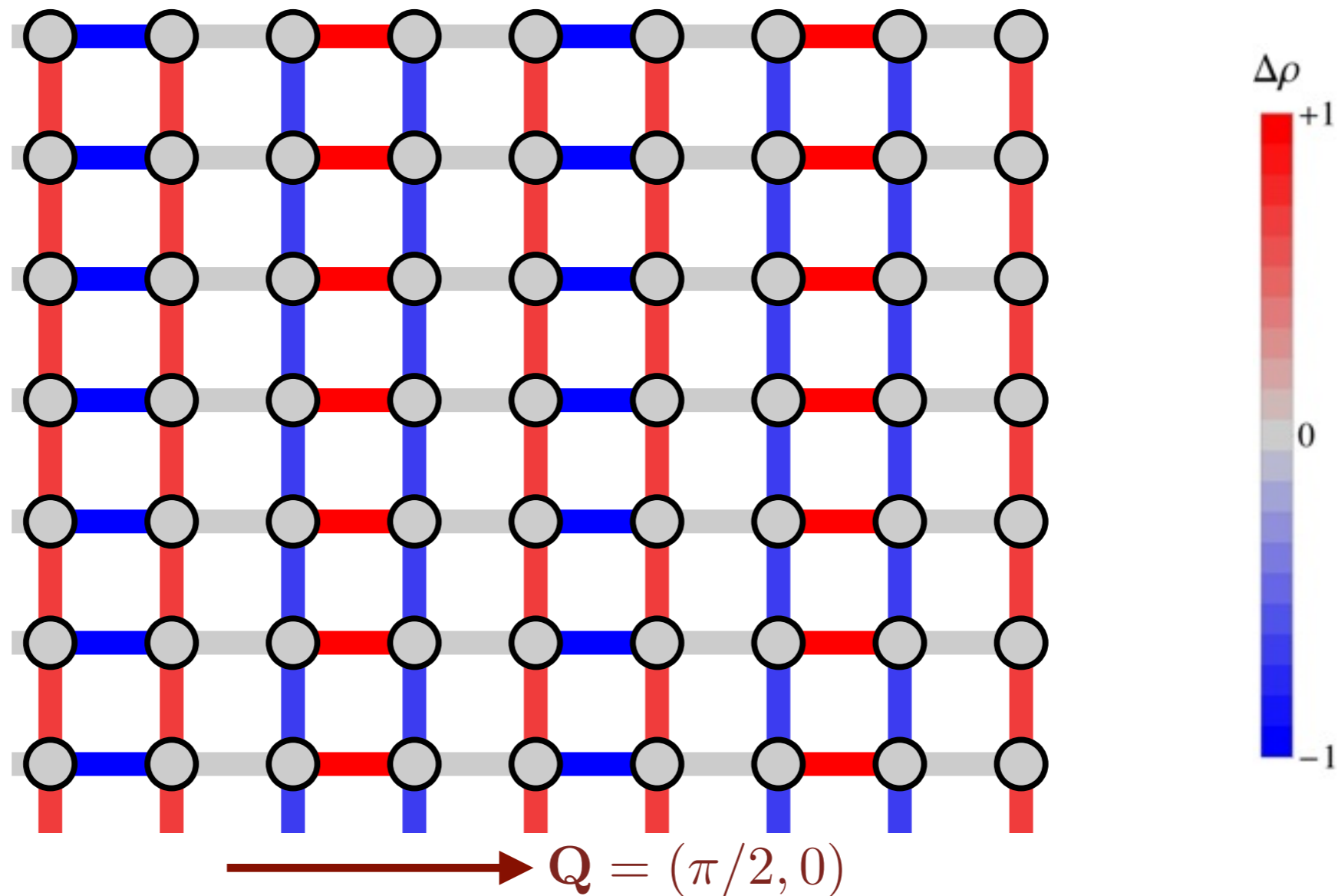
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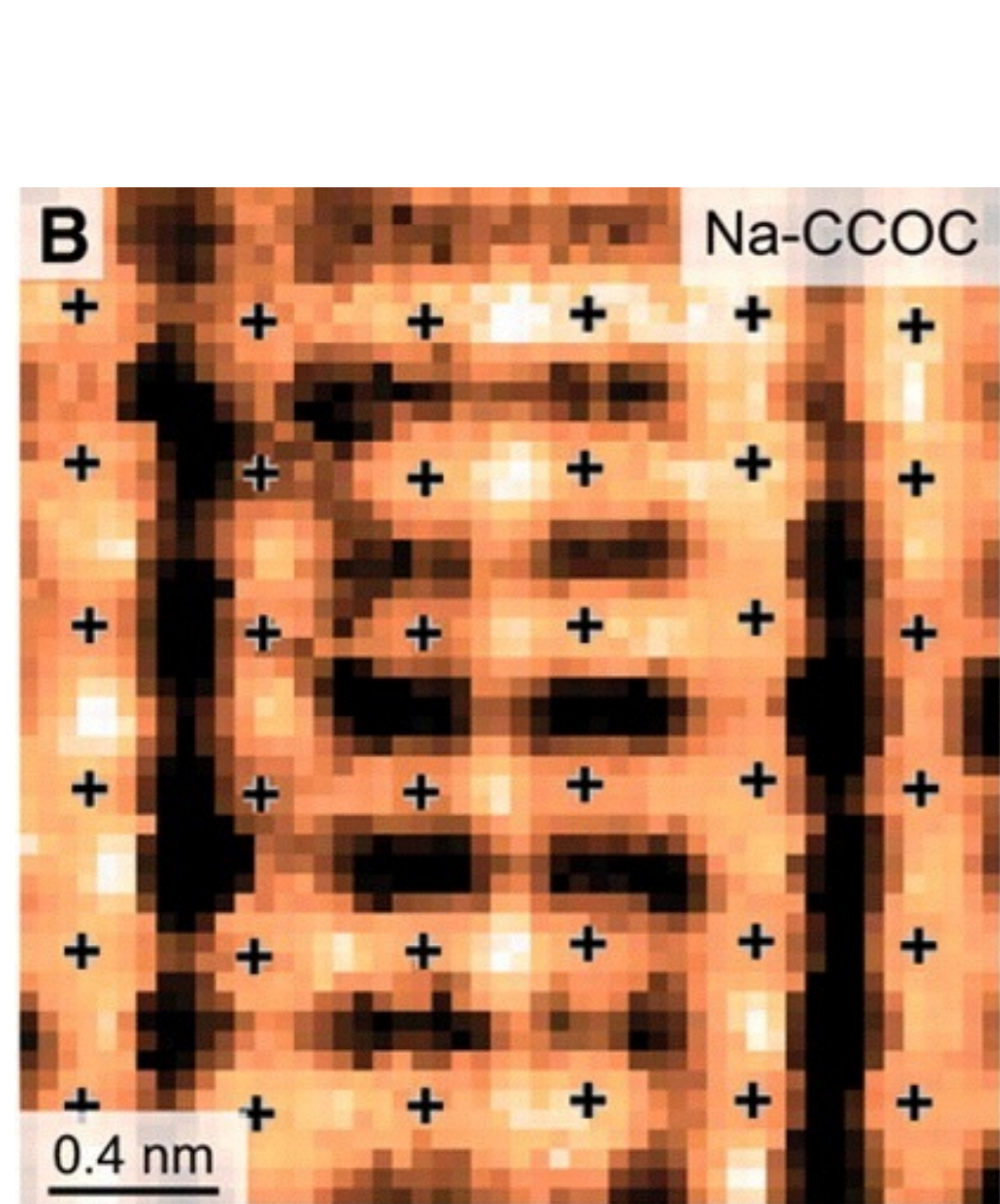
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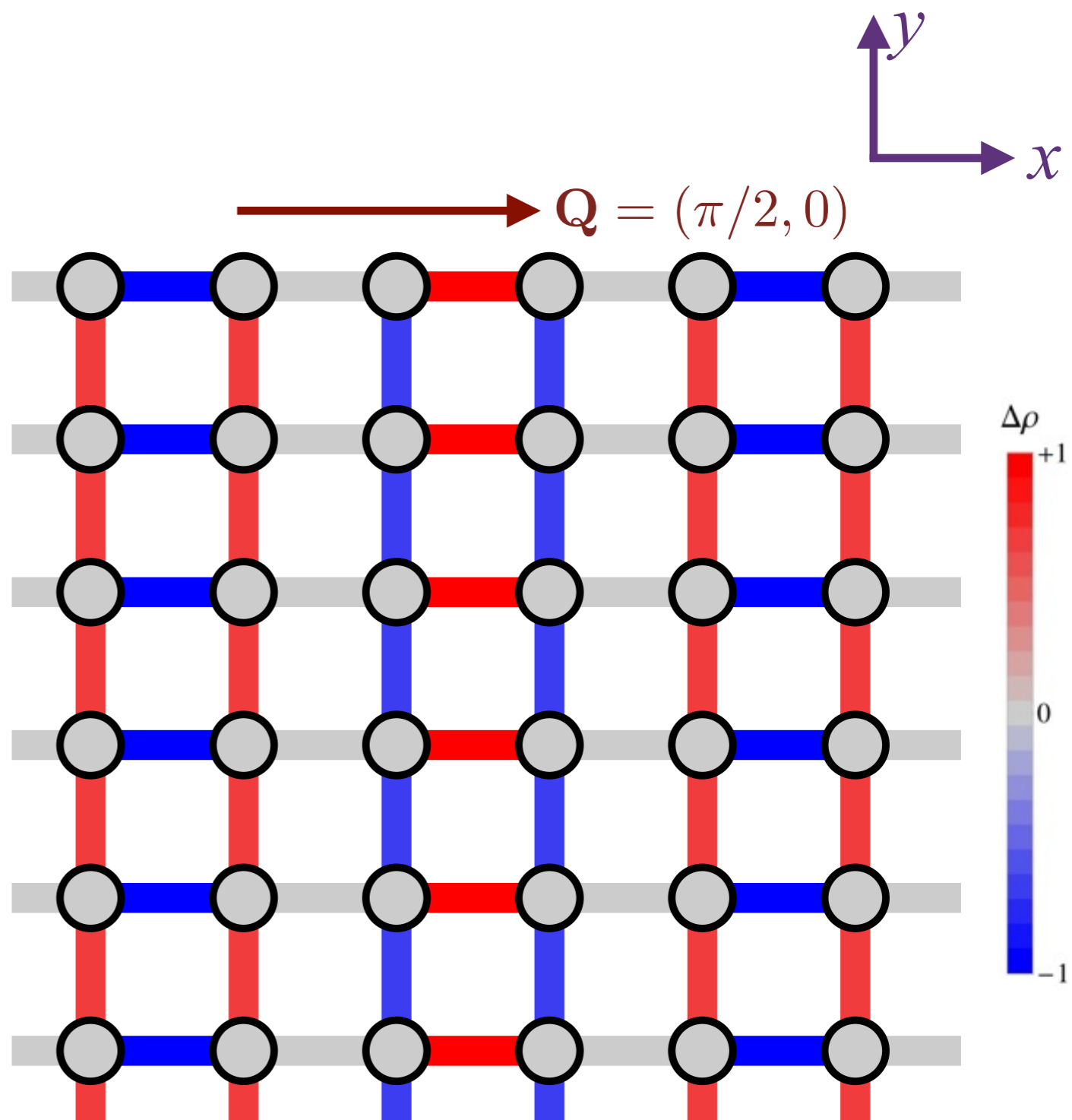
Density wave on horizontal bonds has a phase-shift of π relative to the wave on vertical bonds



M. A. Metlitski and S. Sachdev, Phys. Rev. B **82**, 075128 (2010).
 S. Sachdev and R. LaPlaca, Phys. Rev. Lett. **111**, 027202 (2013).

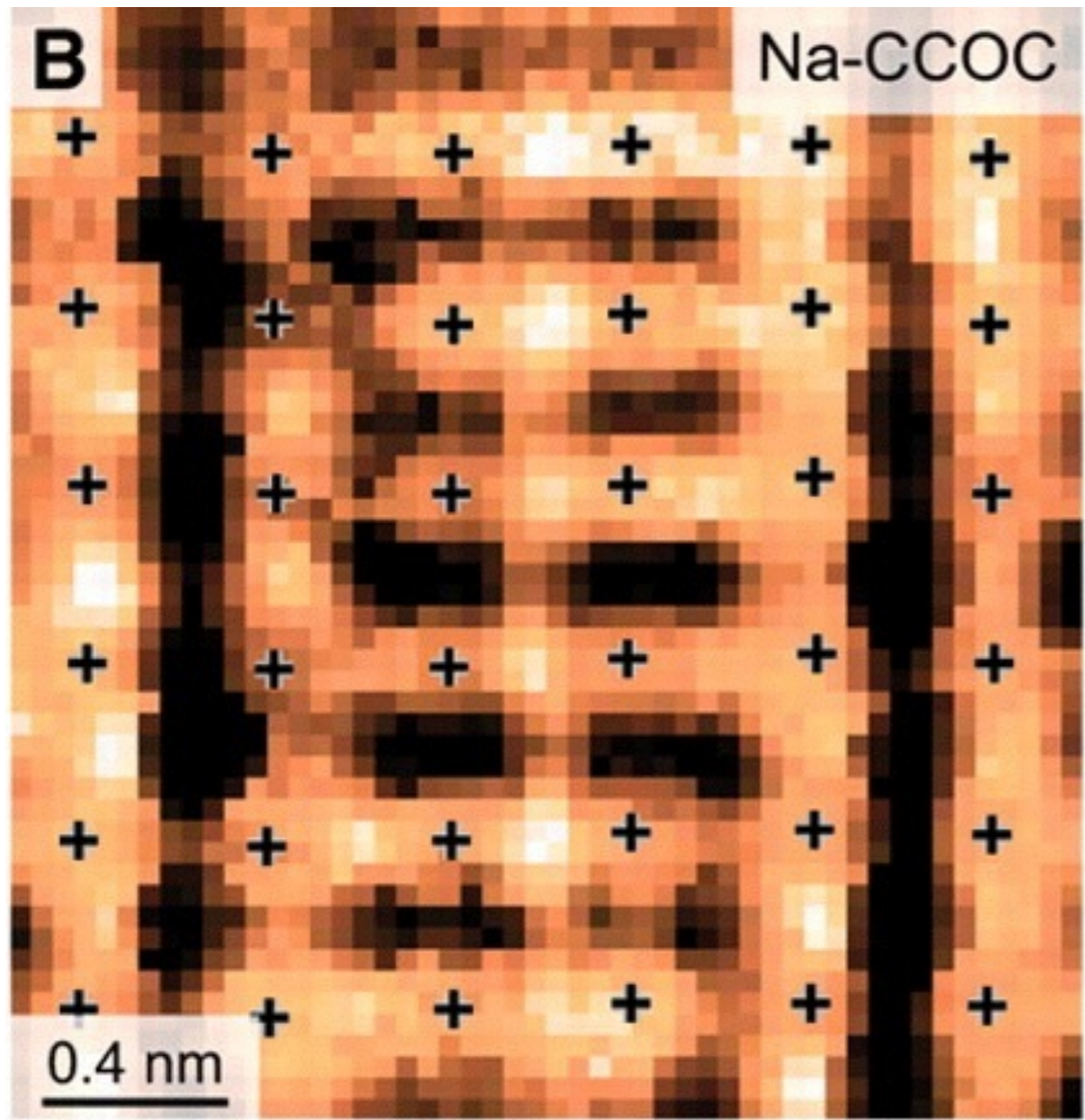
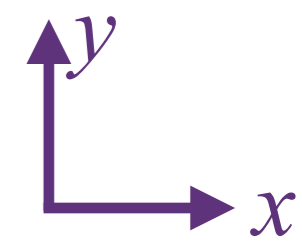


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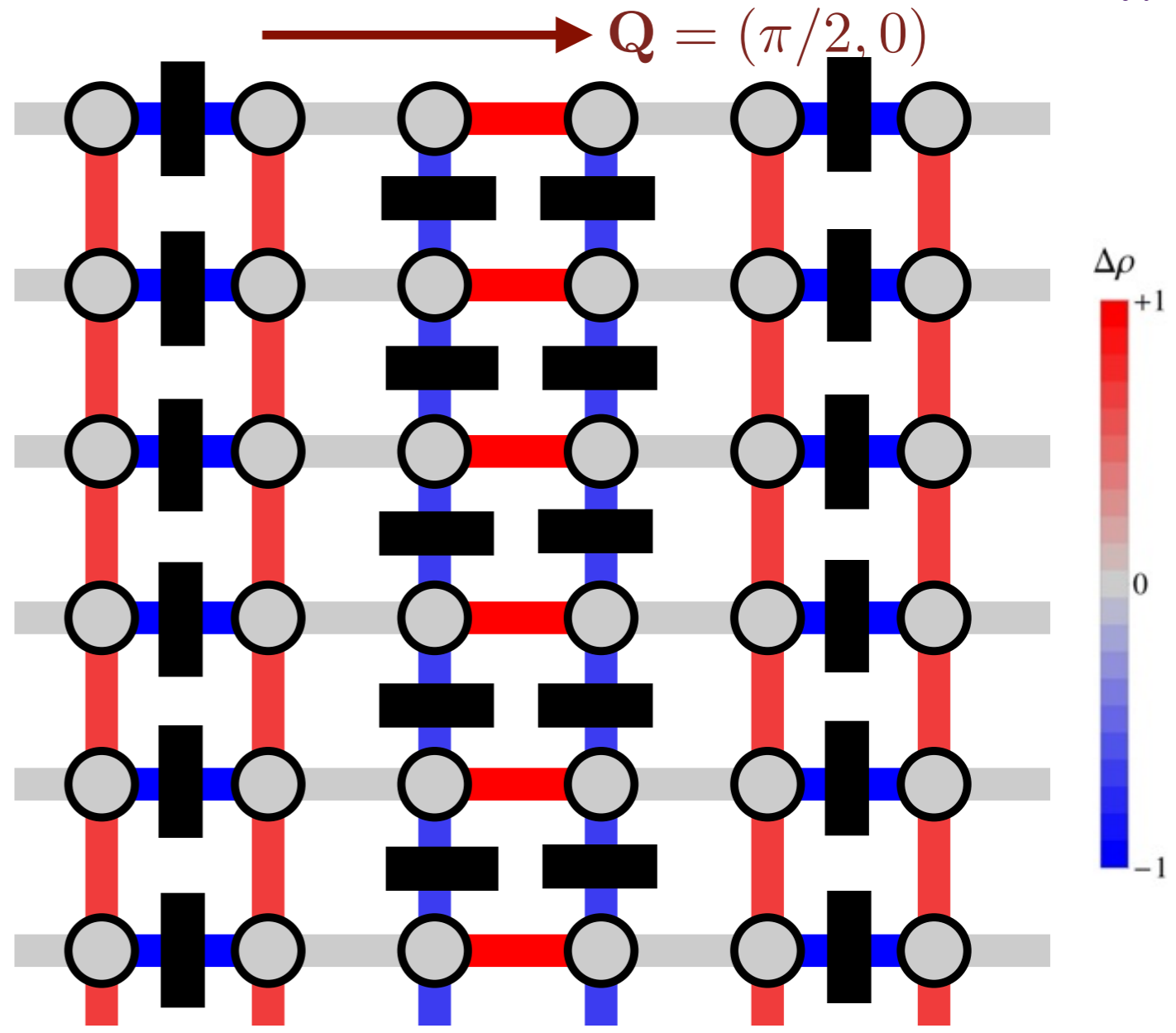


d-form factor density wave order

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d-form factor density wave order

d form factor is compatible with STM measurements on BSCCO, Na-CCOC !

Direct phase-sensitive identification of a d -form factor density wave in underdoped cuprates

Kazuhiro Fujita^{a,b,c,1}, Mohammad H. Hamidian^{a,b,1}, Stephen D. Edkins^{b,d}, Chung Koo Kim^a, Yuhki Kohsaka^e, Masaki Azuma^f, Mikio Takano^g, Hidenori Takagi^{c,h,i}, Hiroshi Eisaki^j, Shin-ichi Uchida^c, Andrea Allais^k, Michael J. Lawler^{b,l}, Eun-Ah Kim^b, Subir Sachdev^{k,m}, and J. C. Séamus Davis^{a,b,d,2}

Proceedings of the National Academy of Sciences **111**, E3026 (2014)



Kazuhiro Fujita
Cornell/ BNL

See talk by
Kazuhiro Fujita on Friday:

1. Measurement of π phase shift between horizontal and vertical bonds, and predominant d -form factor
2. Intimate connection of d -form factor to pseudogap

Outline

1. Density waves in the underdoped cuprates
STM observation of d-form factor density wave
2. RPA theory of density waves
3. Fractionalized Fermi liquids (FL*)
on the Kondo lattice
4. Fractionalized Fermi liquids (FL*) in doped
square lattice antiferromagnets
d-form factor density waves with the correct wavevector

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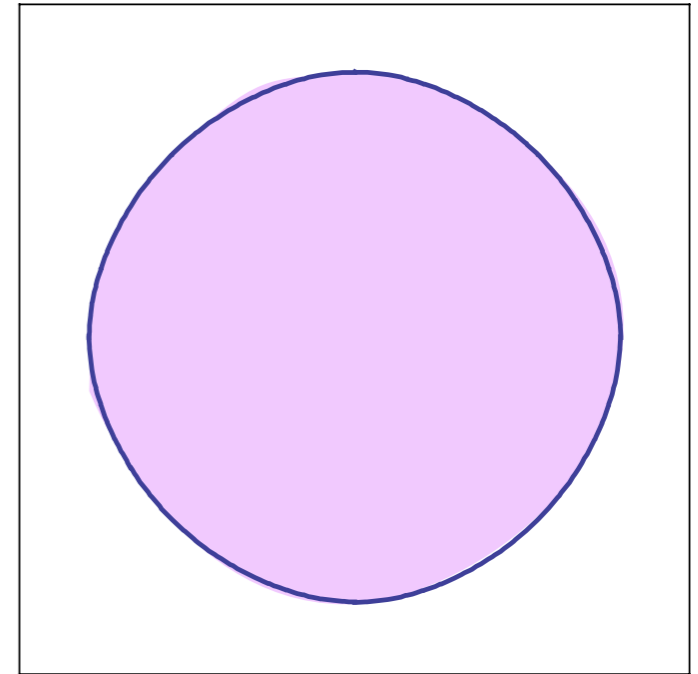
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d-form factor density waves with the correct wavevector

Fermi surface+antiferromagnetism

Metal with “large”
Fermi surface

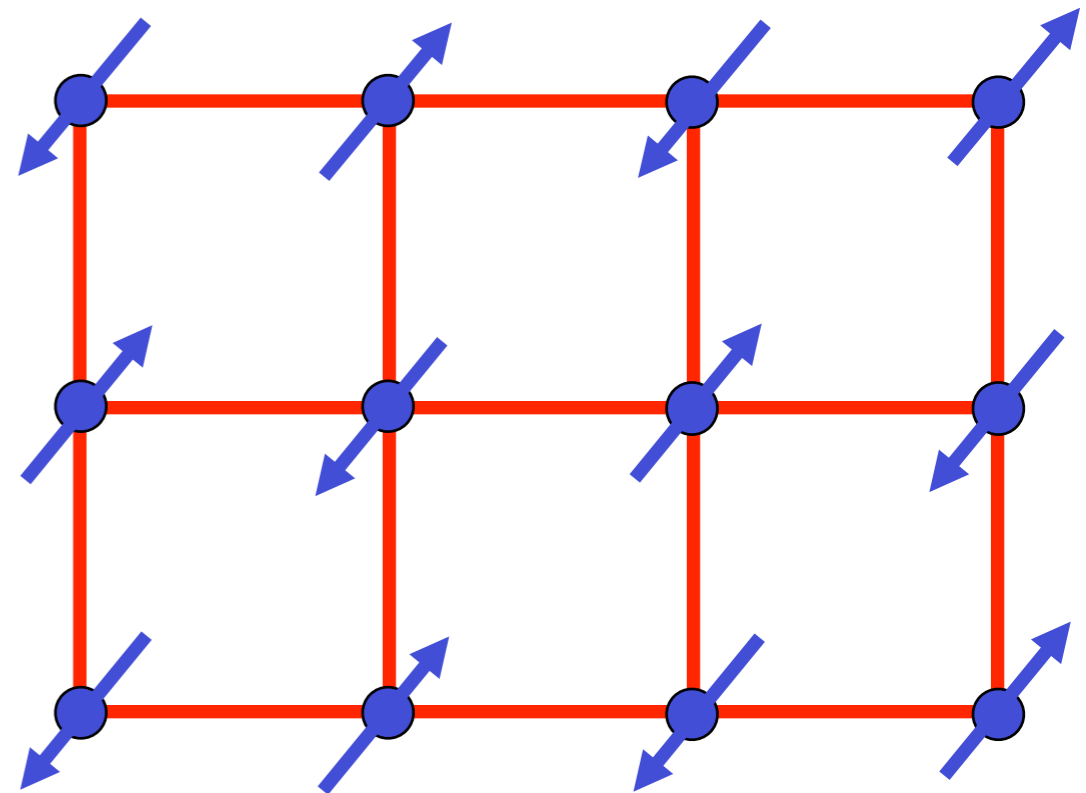


+

The electron spin polarization obeys

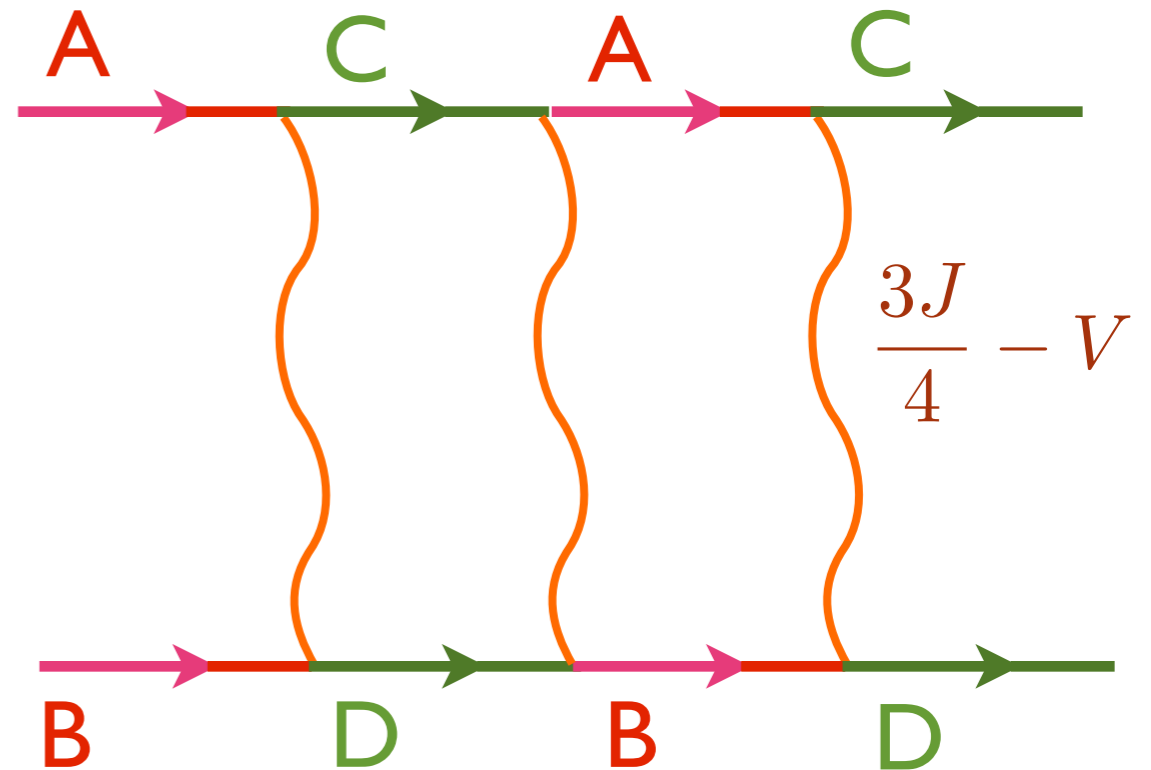
$$\langle \vec{S}(\mathbf{r}, \tau) \rangle = \vec{\varphi}(\mathbf{r}, \tau) e^{i\mathbf{K} \cdot \mathbf{r}}$$

where $\mathbf{K} = (\pi, \pi)$ is the ordering
wavevector.

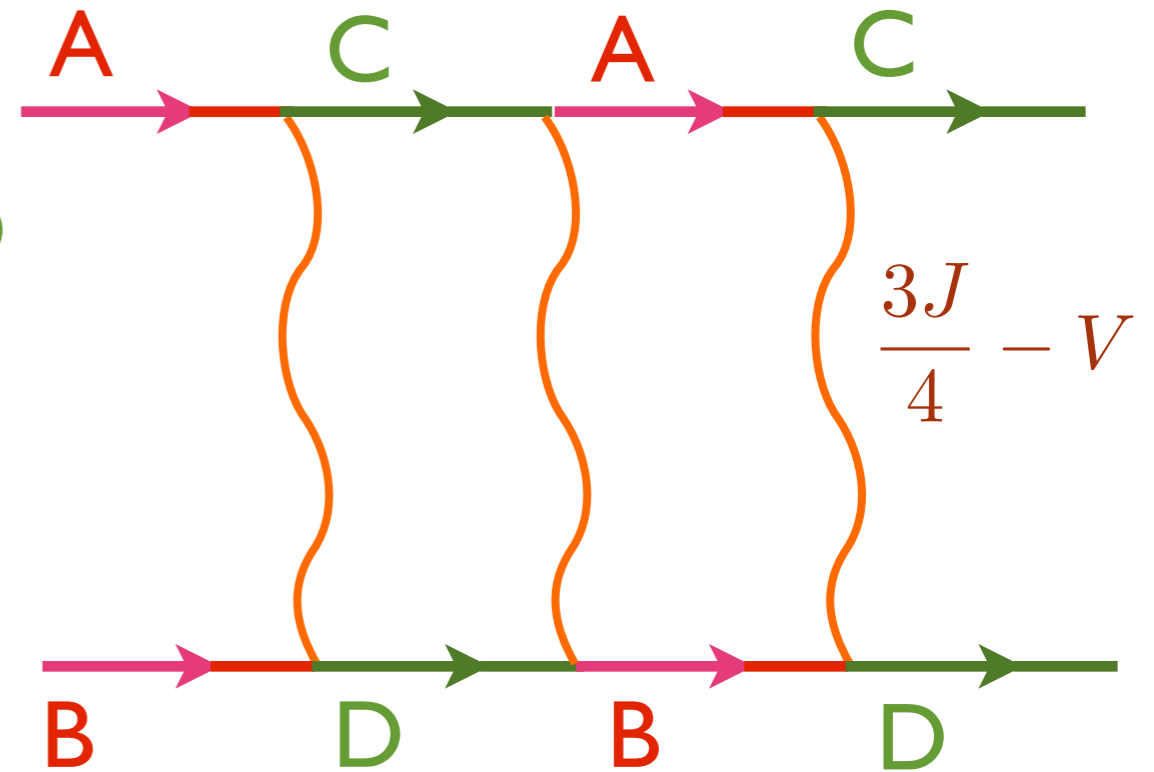
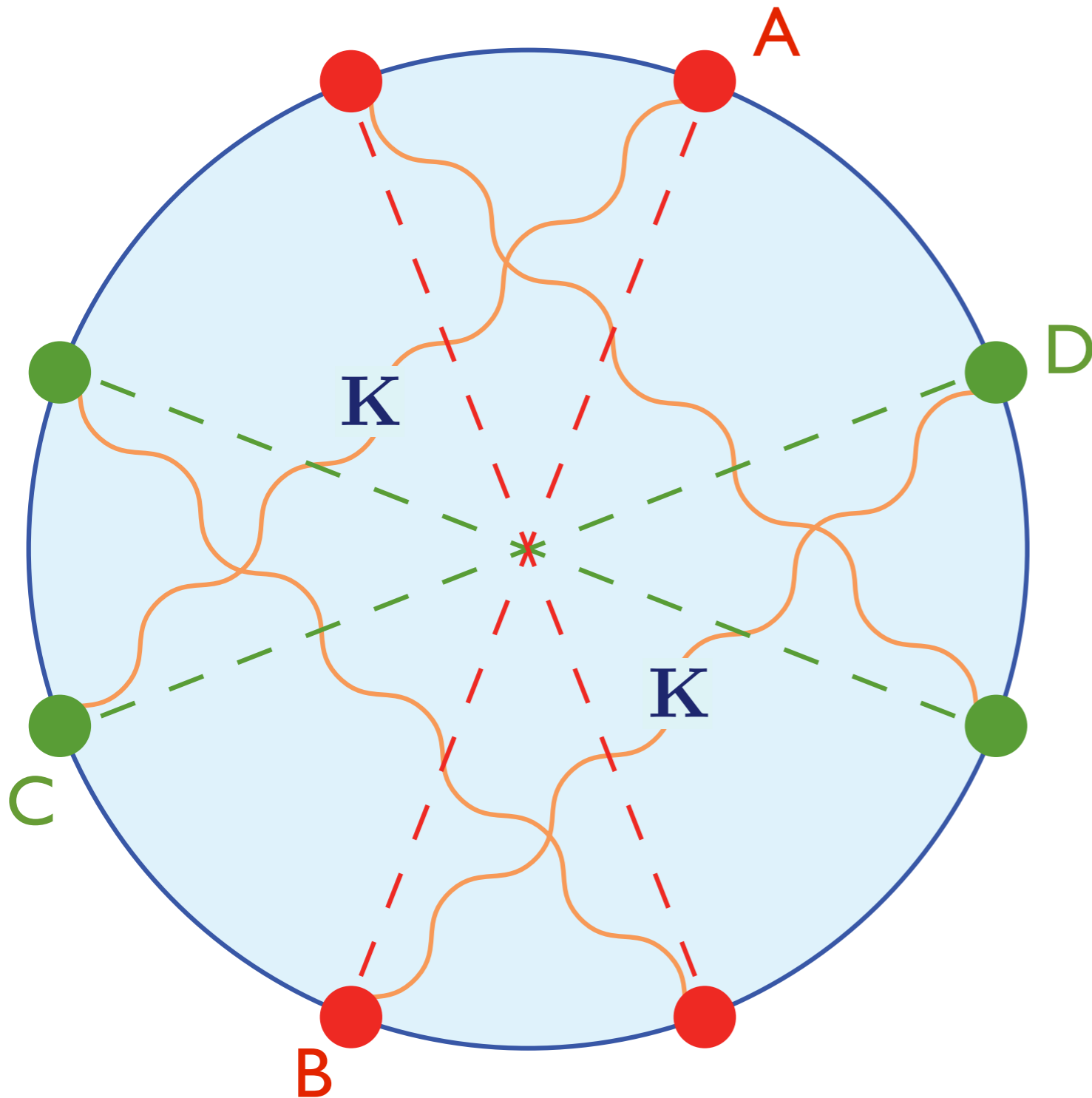


Pairing “glue” from antiferromagnetic fluctuations

$$\begin{aligned}
 H = & - \sum_{i,j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} \\
 & + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \\
 & + V \sum_{\langle ij \rangle} n_i n_j + \dots
 \end{aligned}$$

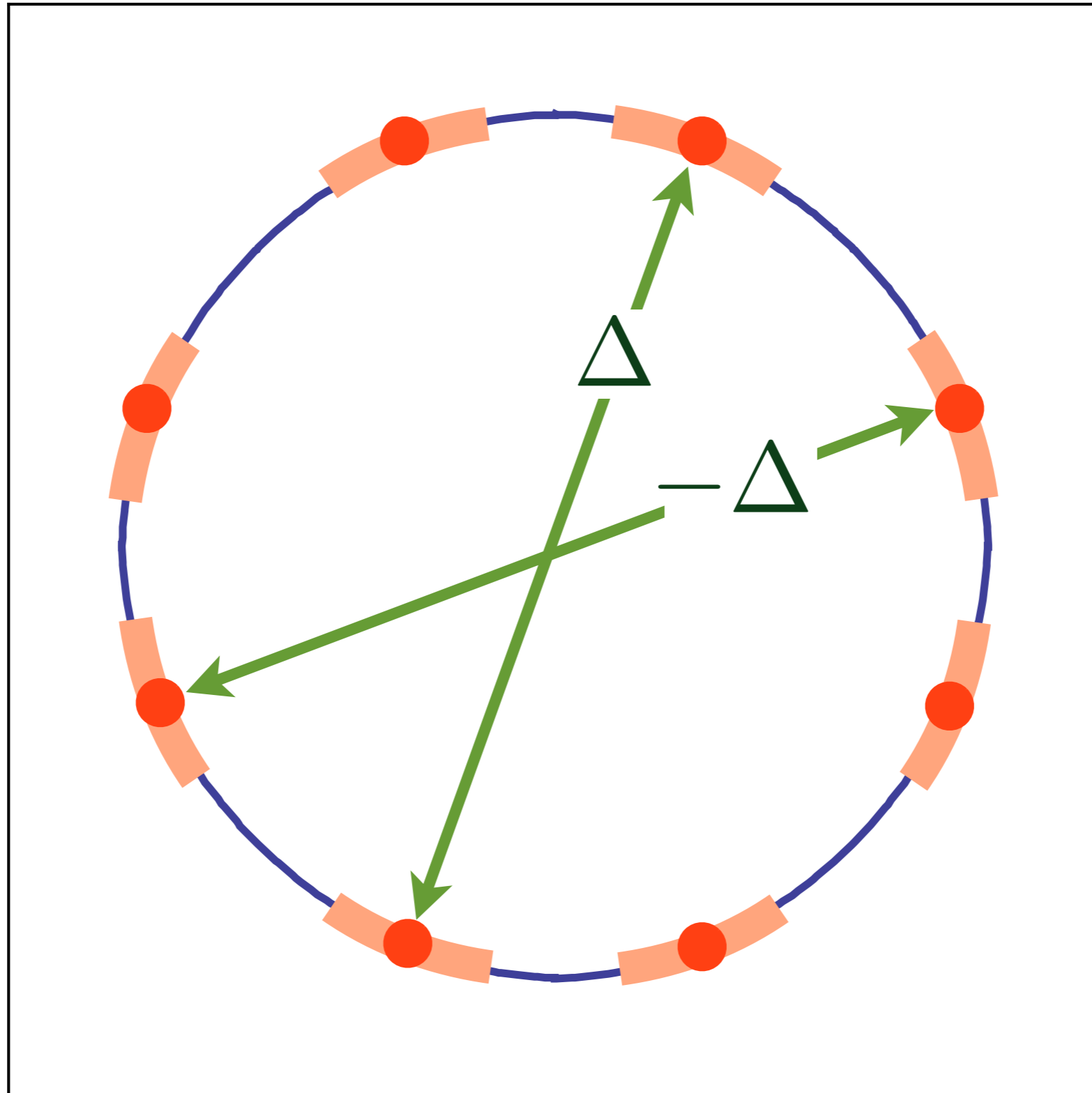


Pairing “glue” from antiferromagnetic fluctuations



V.J. Emery, *J. Phys. (Paris) Colloq.* 44, C3-977 (1983)
D.J. Scalapino, E. Loh, and J.E. Hirsch, *Phys. Rev. B* 34, 8190 (1986)
K. Miyake, S. Schmitt-Rink, and C. M. Varma, *Phys. Rev. B* 34, 6554 (1986)

$$\langle c_{\mathbf{k}\alpha}^\dagger c_{-\mathbf{k}\beta}^\dagger \rangle = \varepsilon_{\alpha\beta} \Delta (\cos k_x - \cos k_y)$$



Unconventional pairing at and near hot spots

Pseudospin symmetry of the exchange interaction

$$H_J = \sum_{i < j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

with $\vec{S}_i = \frac{1}{2} c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\beta}$ is the antiferromagnetic exchange interaction. Introduce the Nambu spinor

$$\Psi_{i\uparrow} = \begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow}^\dagger \end{pmatrix}, \quad \Psi_{i\downarrow} = \begin{pmatrix} c_{i\downarrow} \\ -c_{i\uparrow}^\dagger \end{pmatrix}$$

Then we can write

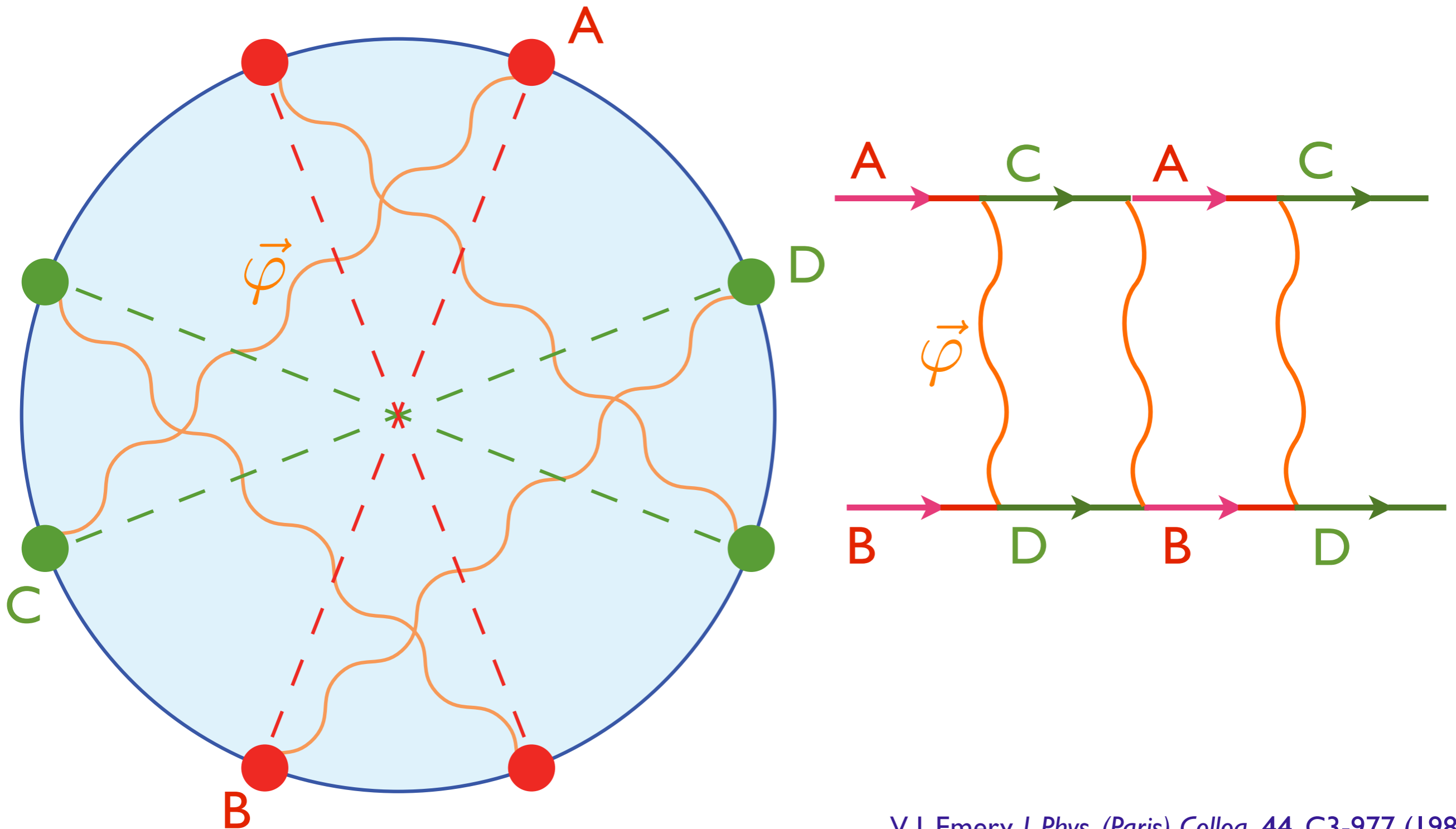
$$H_J = \frac{1}{8} \sum_{i < j} J_{ij} \left(\Psi_{i\alpha a}^\dagger \vec{\sigma}_{\alpha\beta} \Psi_{i\beta a} \right) \cdot \left(\Psi_{j\gamma b}^\dagger \vec{\sigma}_{\gamma\delta} \Psi_{j\delta b} \right)$$

where a, b are the Nambu indices. This form makes explicit the symmetry under *independent* SU(2) pseudospin transformations on each site

$$\Psi_{i\alpha a} \rightarrow U_{i,ab} \Psi_{i\alpha b}$$

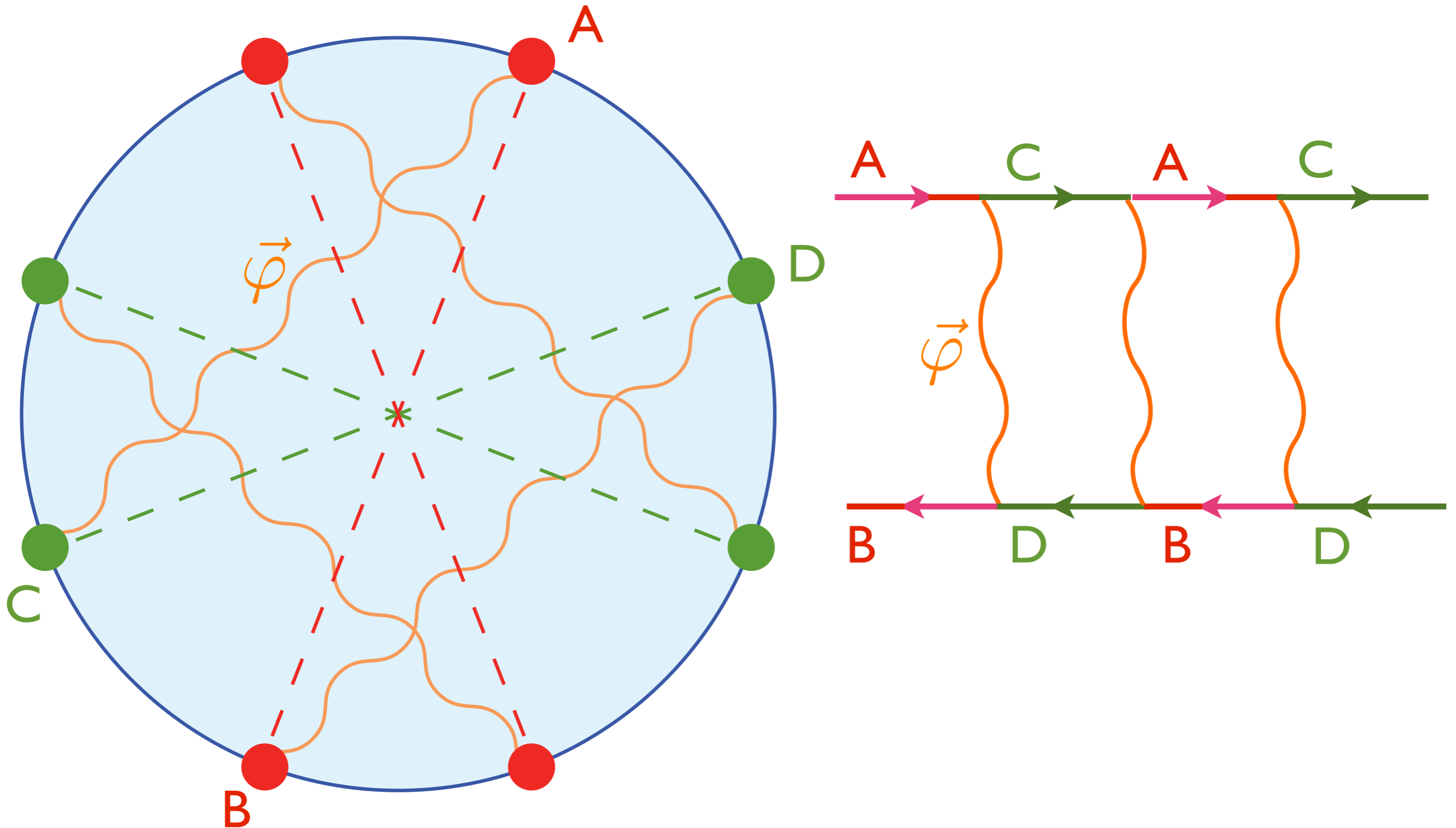
- I. Affleck, Z. Zou, T. Hsu, and P. W. Anderson, Phys. Rev. B **38**, 745 (1988)
- E. Dagotto, E. Fradkin, and A. Moreo, Phys. Rev. B **38**, 2926 (1988)
- P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. **78**, 17 (2006)

Pairing “glue” from antiferromagnetic fluctuations

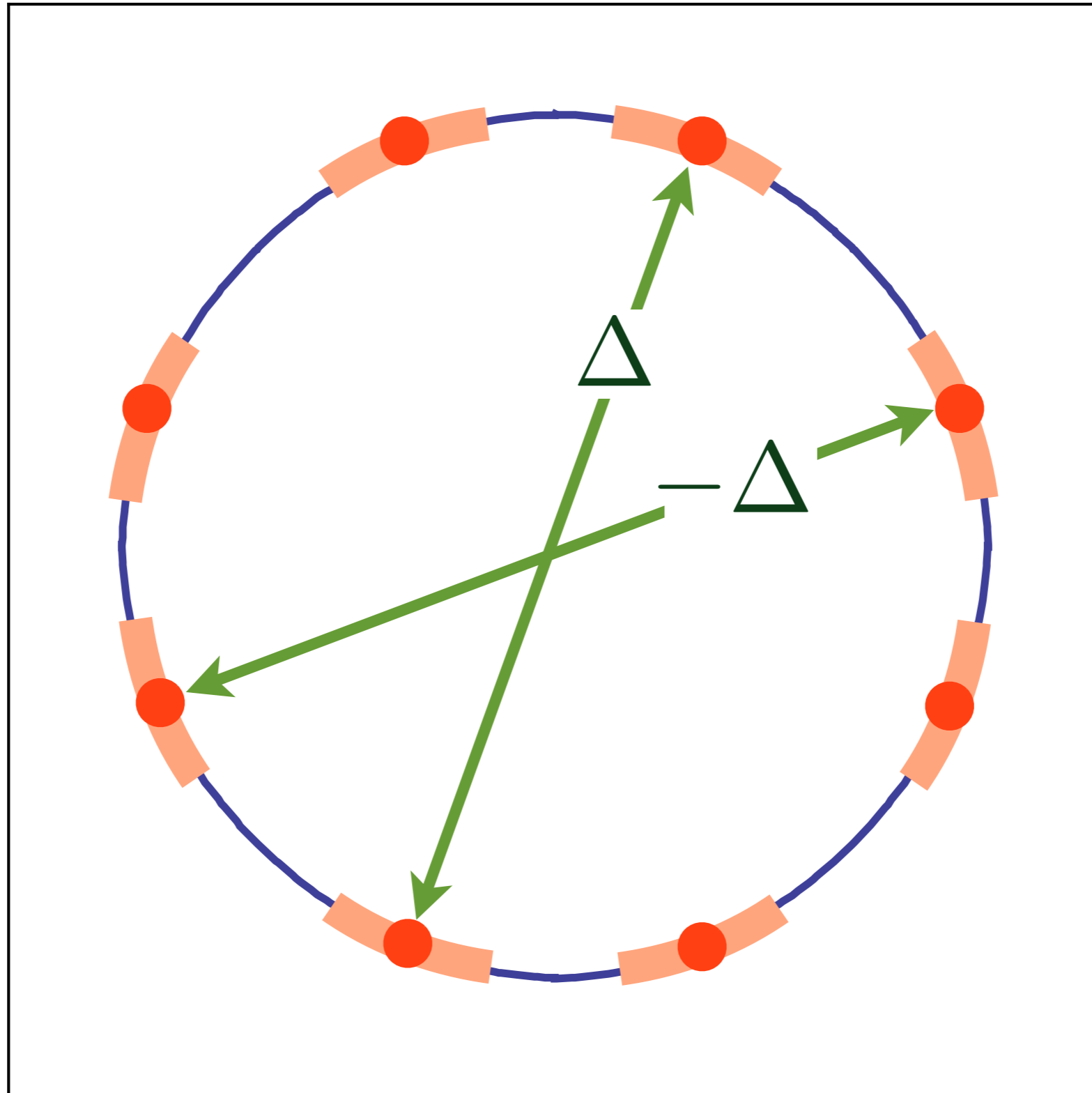


V. J. Emery, *J. Phys. (Paris) Colloq.* 44, C3-977 (1983)
D. J. Scalapino, E. Loh, and J. E. Hirsch, *Phys. Rev. B* 34, 8190 (1986)
K. Miyake, S. Schmitt-Rink, and C. M. Varma, *Phys. Rev. B* 34, 6554 (1986)
S. Raghu, S. A. Kivelson, and D. J. Scalapino, *Phys. Rev. B* 81, 224505 (2010)

Perform pseudospin rotation on **B** and **D** electrons, but not on **A** and **C** electrons: Same “glue” leads to particle-hole pairing



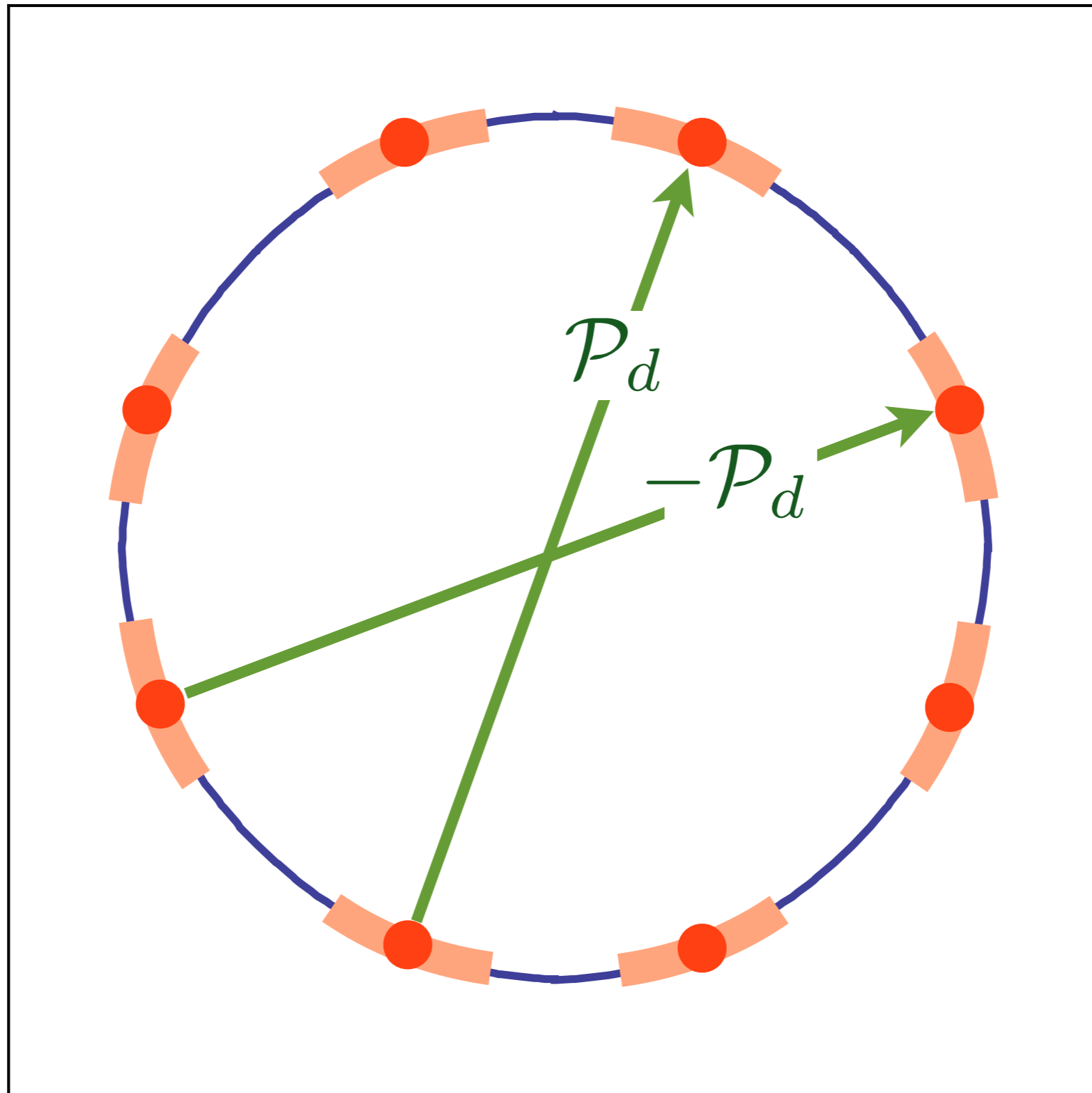
$$\langle c_{\mathbf{k}\alpha}^\dagger c_{-\mathbf{k}\beta}^\dagger \rangle = \varepsilon_{\alpha\beta} \Delta (\cos k_x - \cos k_y)$$



Unconventional pairing at and near hot spots

$$\left\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \right\rangle = \mathcal{P}_d (\cos k_x - \cos k_y)$$

After pseudospin
rotation on *half*
the hot-spots



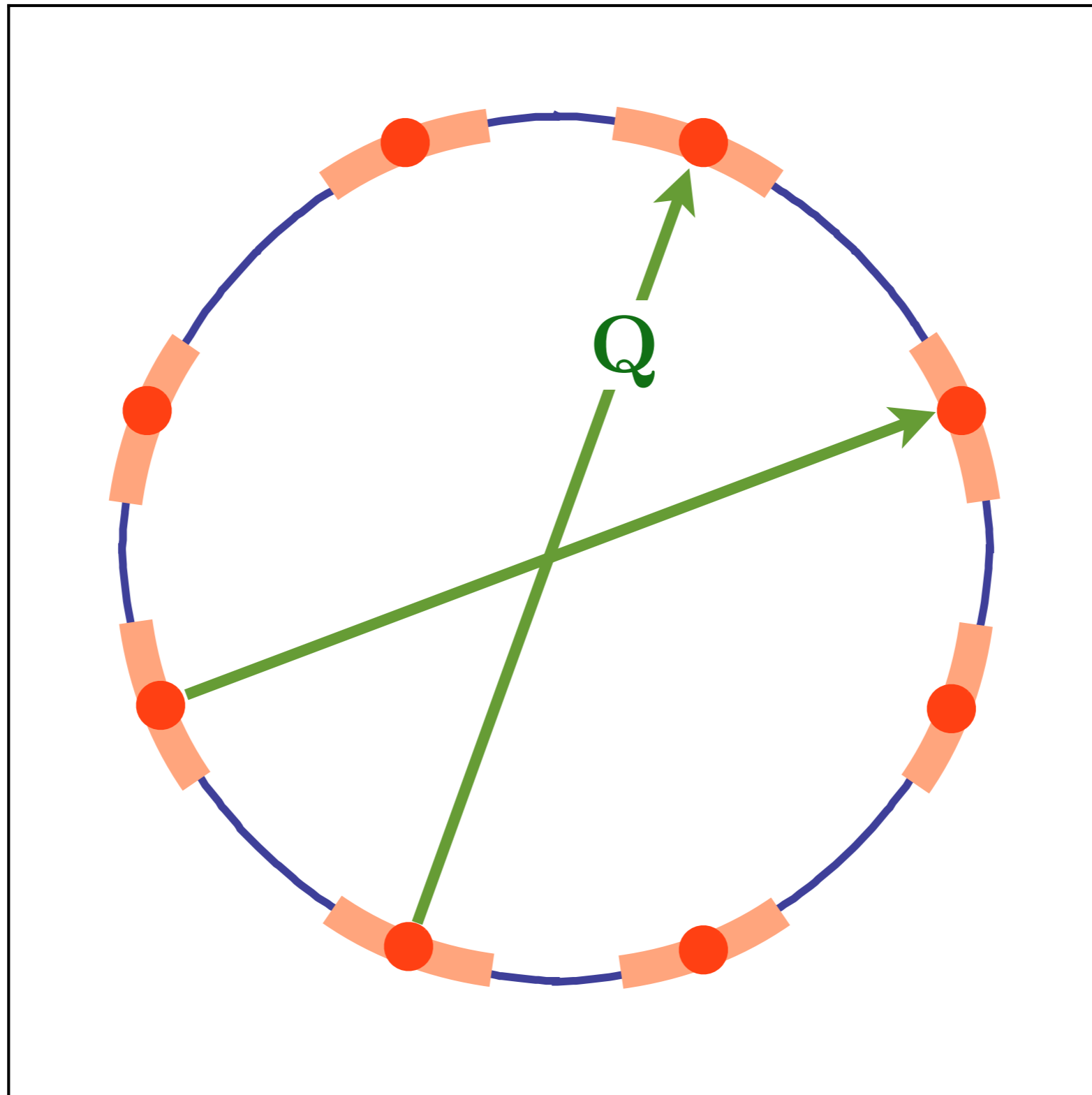
M.A. Metlitski and
S. Sachdev,
Phys. Rev. B **85**,
075127 (2010)

“*d*-form factor” density wave

$$\left\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \right\rangle = \mathcal{P}_d(\cos k_x - \cos k_y)$$

\mathbf{Q} is ' $2k_F$ '
wavevector

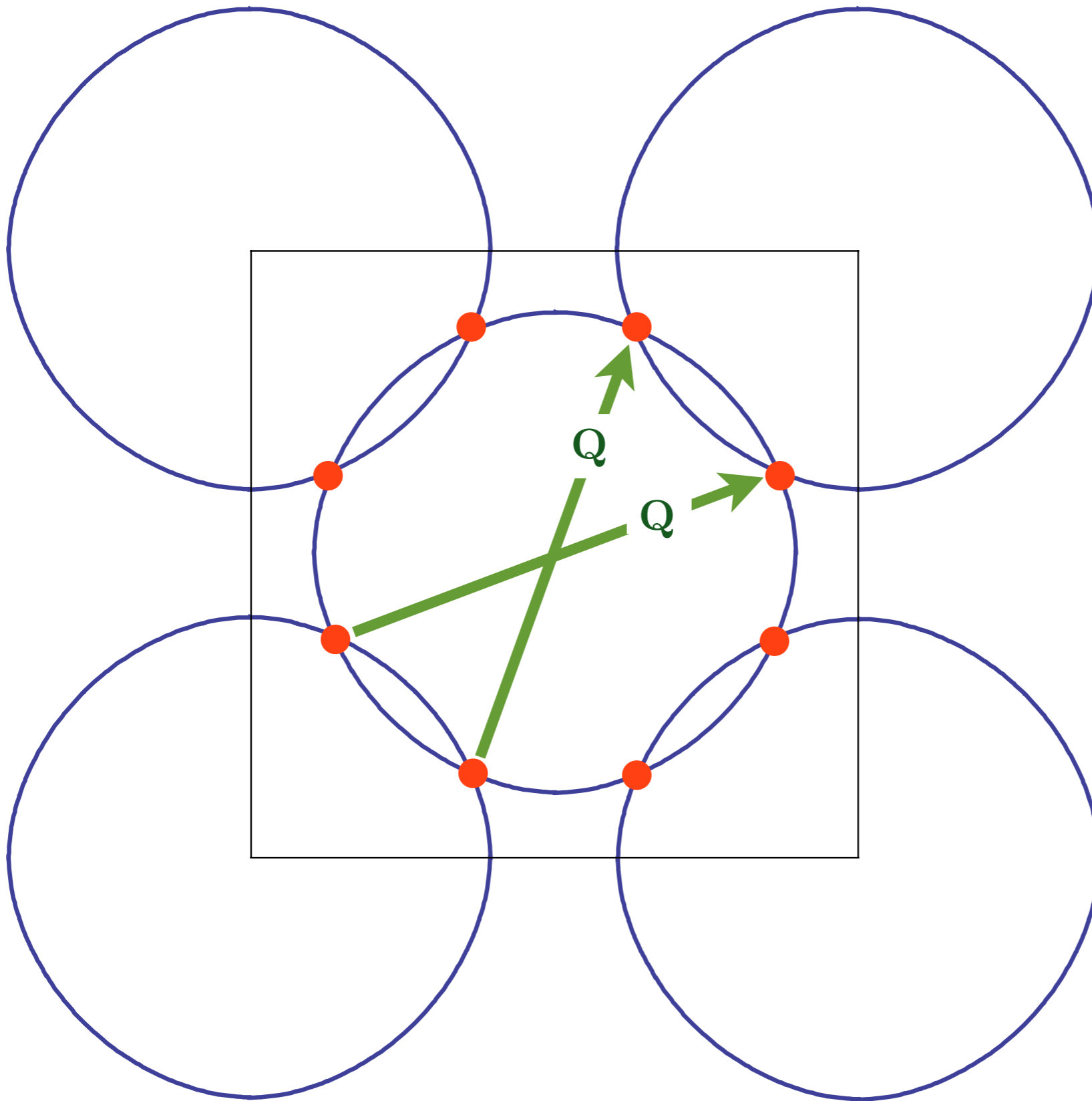
After pseudospin
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the hot-spots



M.A. Metlitski and
S. Sachdev,
Phys. Rev. B **85**,
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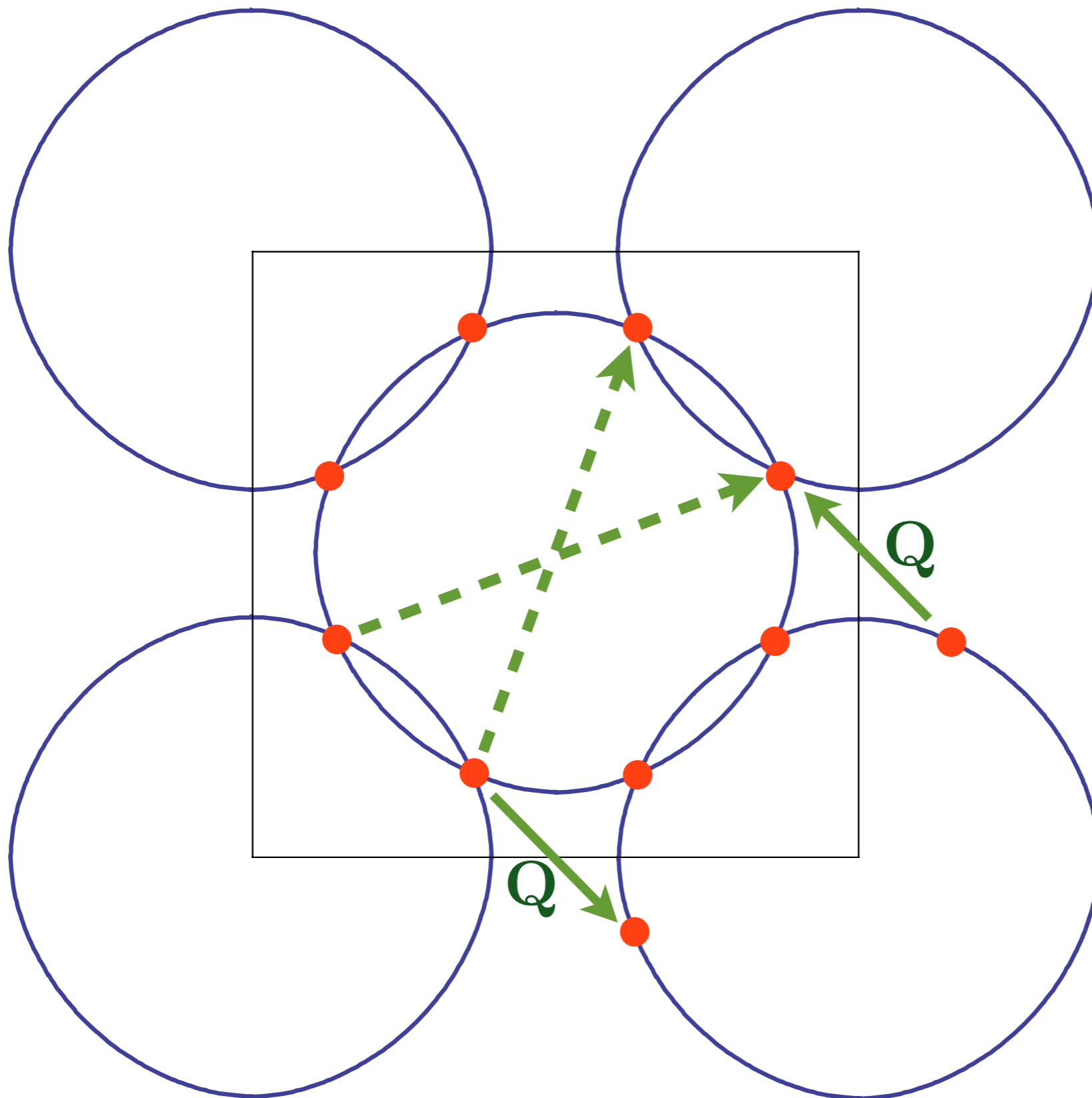
“*d*-form factor” density wave

d -form factor density wave

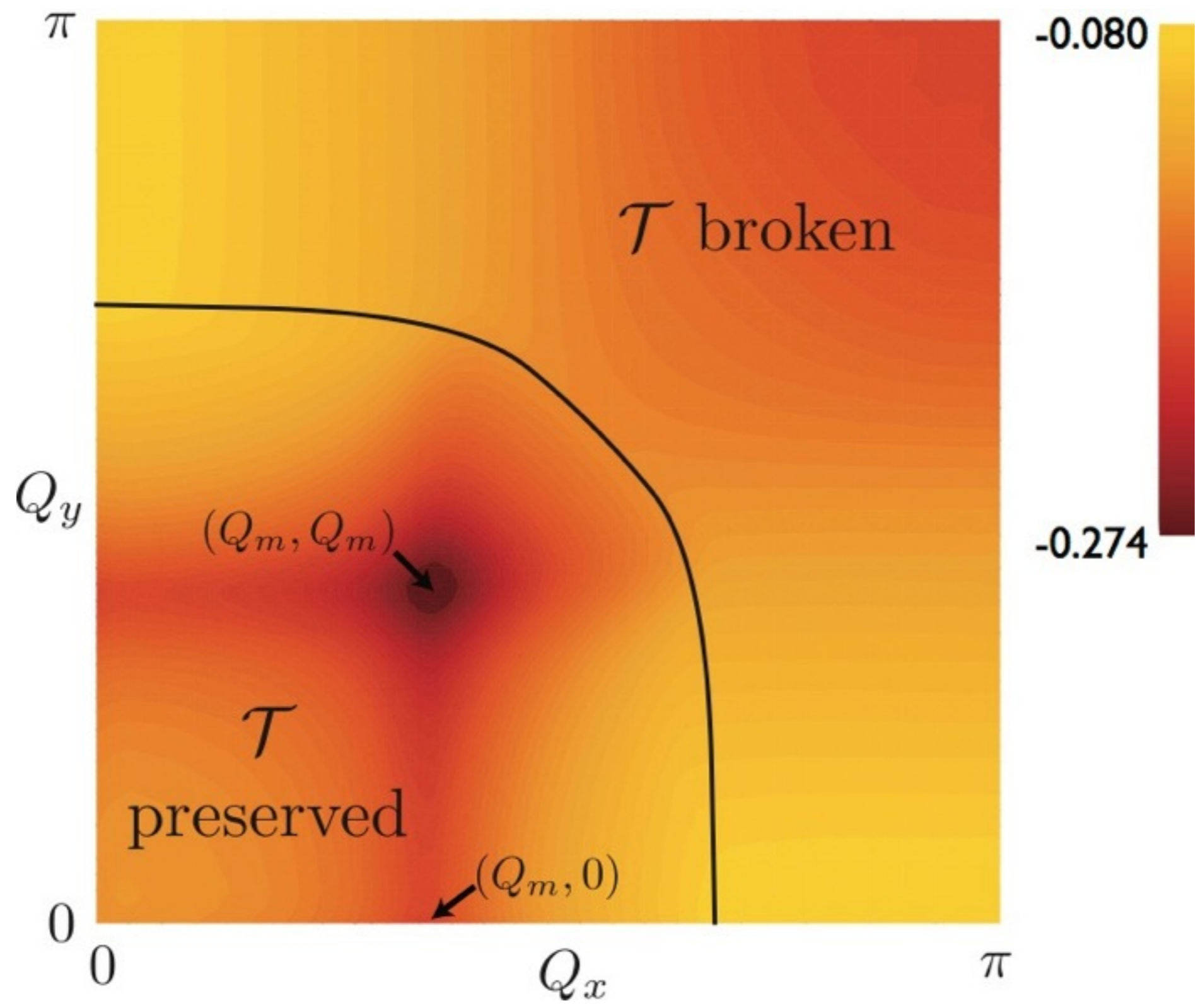


$$\left\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \right\rangle = \mathcal{P}_d(\cos k_x - \cos k_y)$$

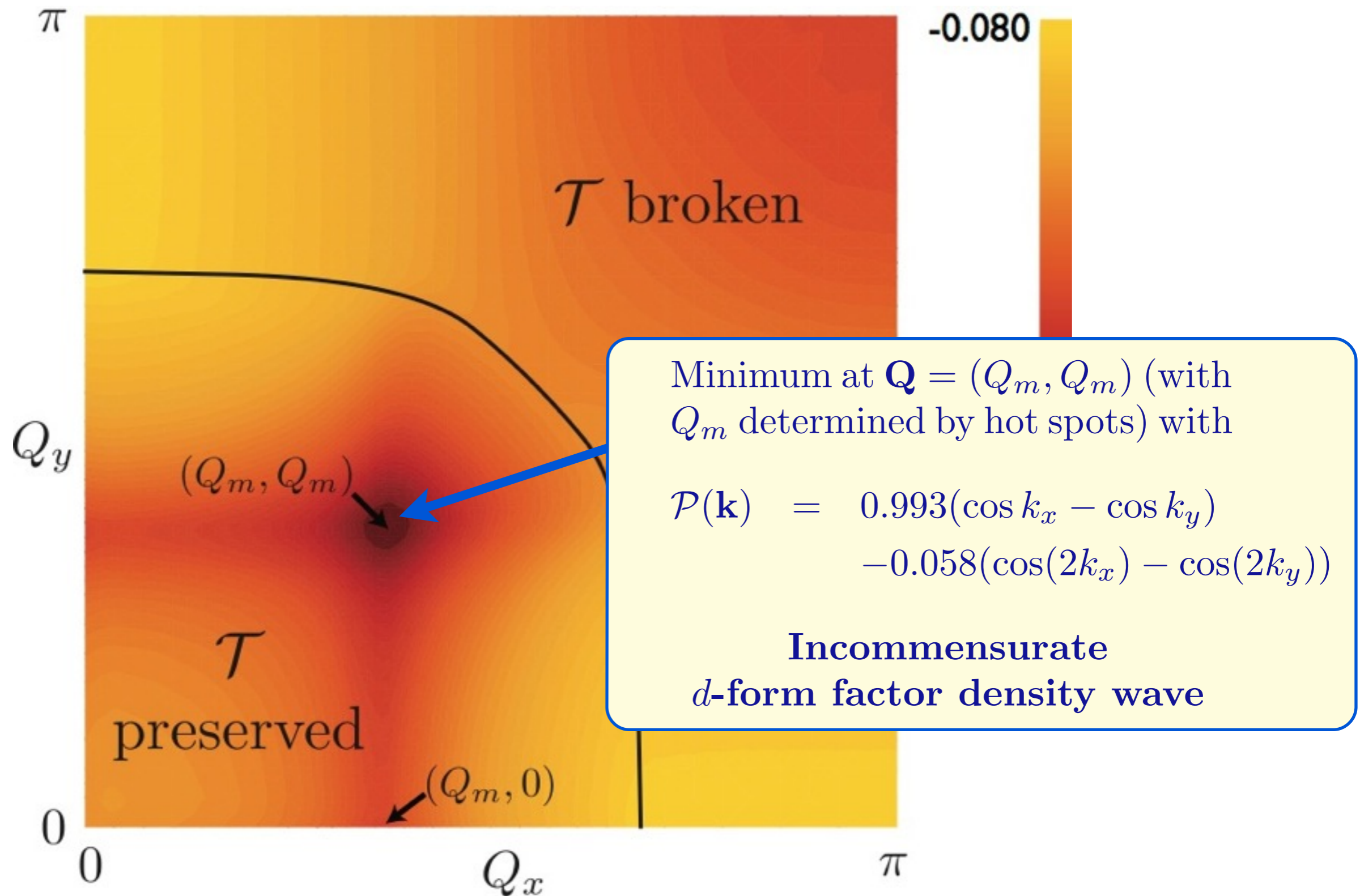
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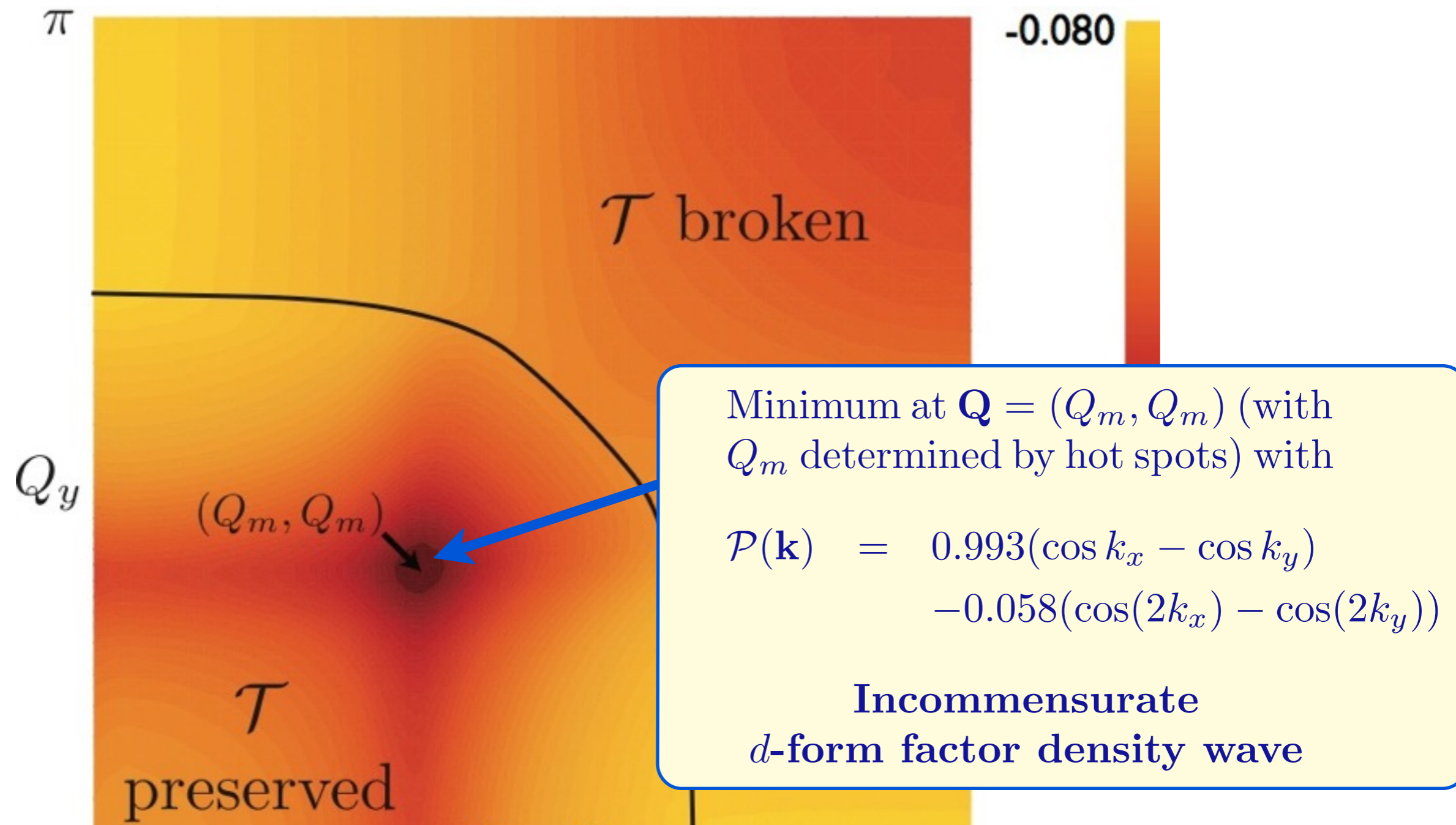


Eigenvalues, $\lambda(\mathbf{Q})$, of the spin-singlet, particle-hole propagator. The corresponding eigenvector is $\mathcal{P}(\mathbf{k})$ and this leads to the order $\langle c_{i\alpha}^\dagger c_{j\alpha} \rangle = [\int_{\mathbf{k}} \mathcal{P}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)}] e^{i\mathbf{Q}\cdot(\mathbf{r}_i + \mathbf{r}_j)/2}$

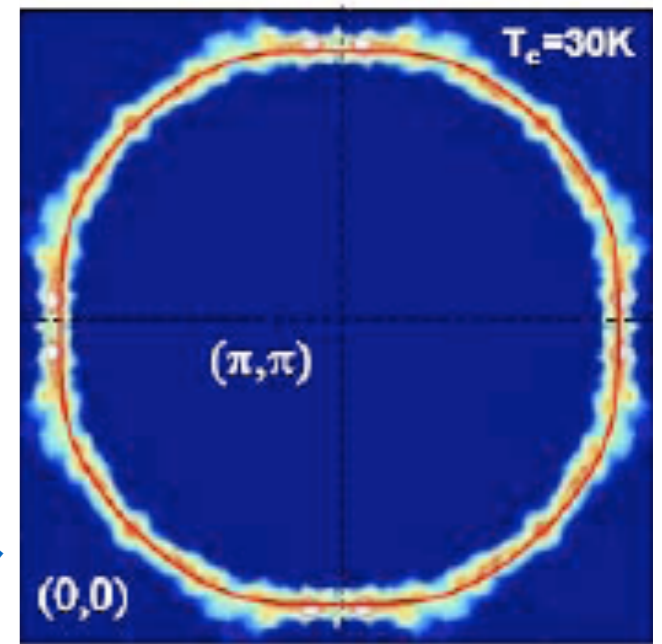
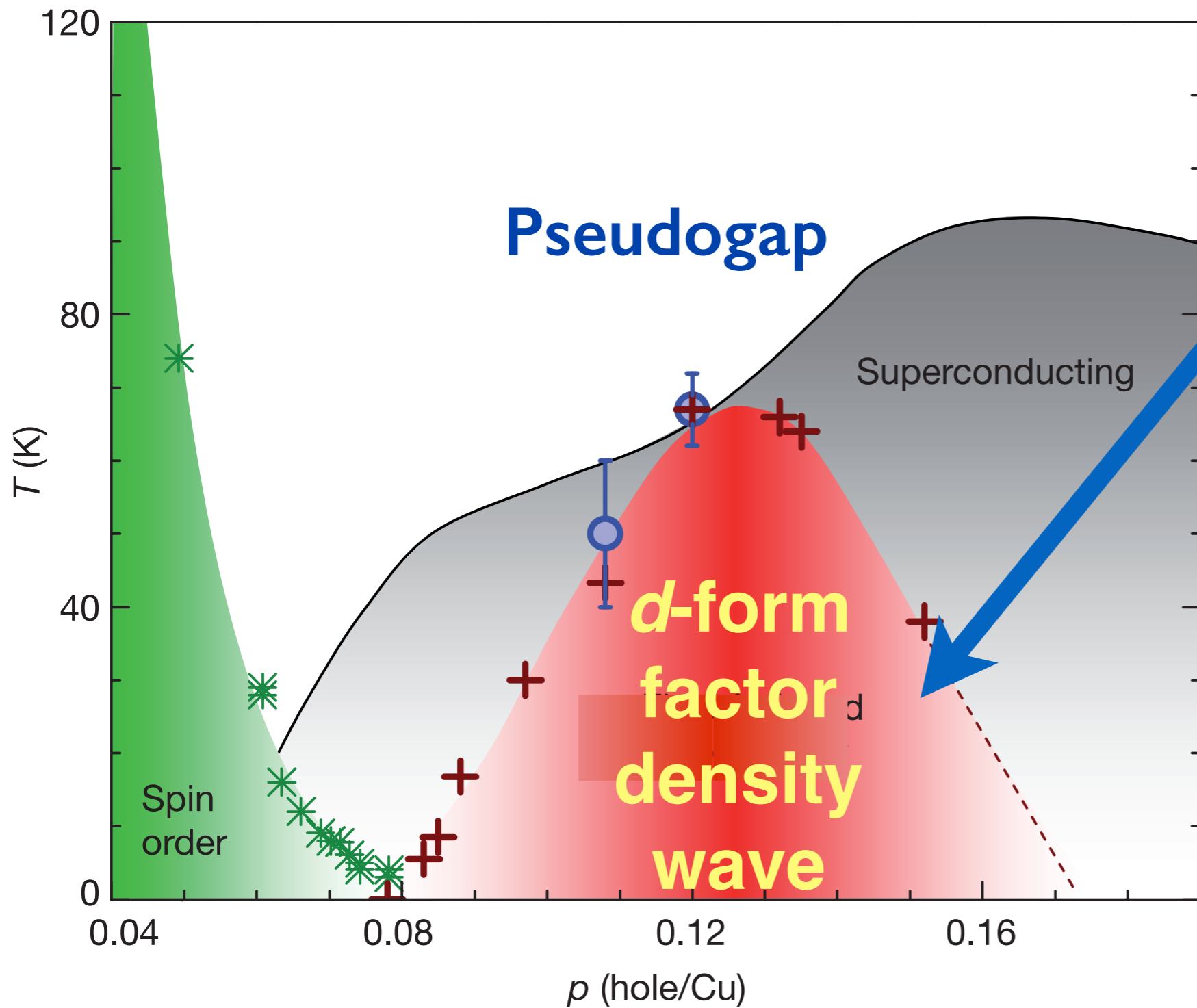


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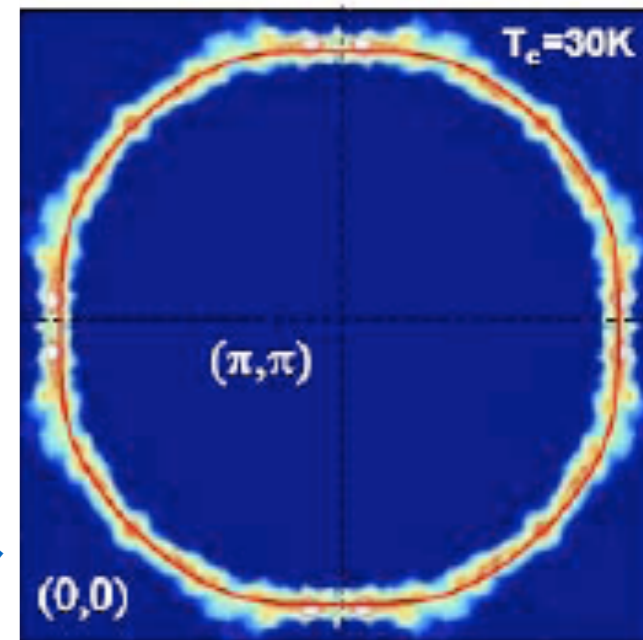
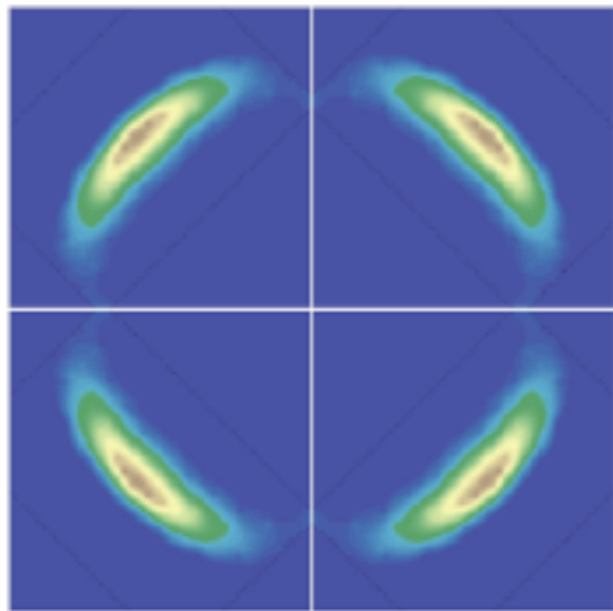
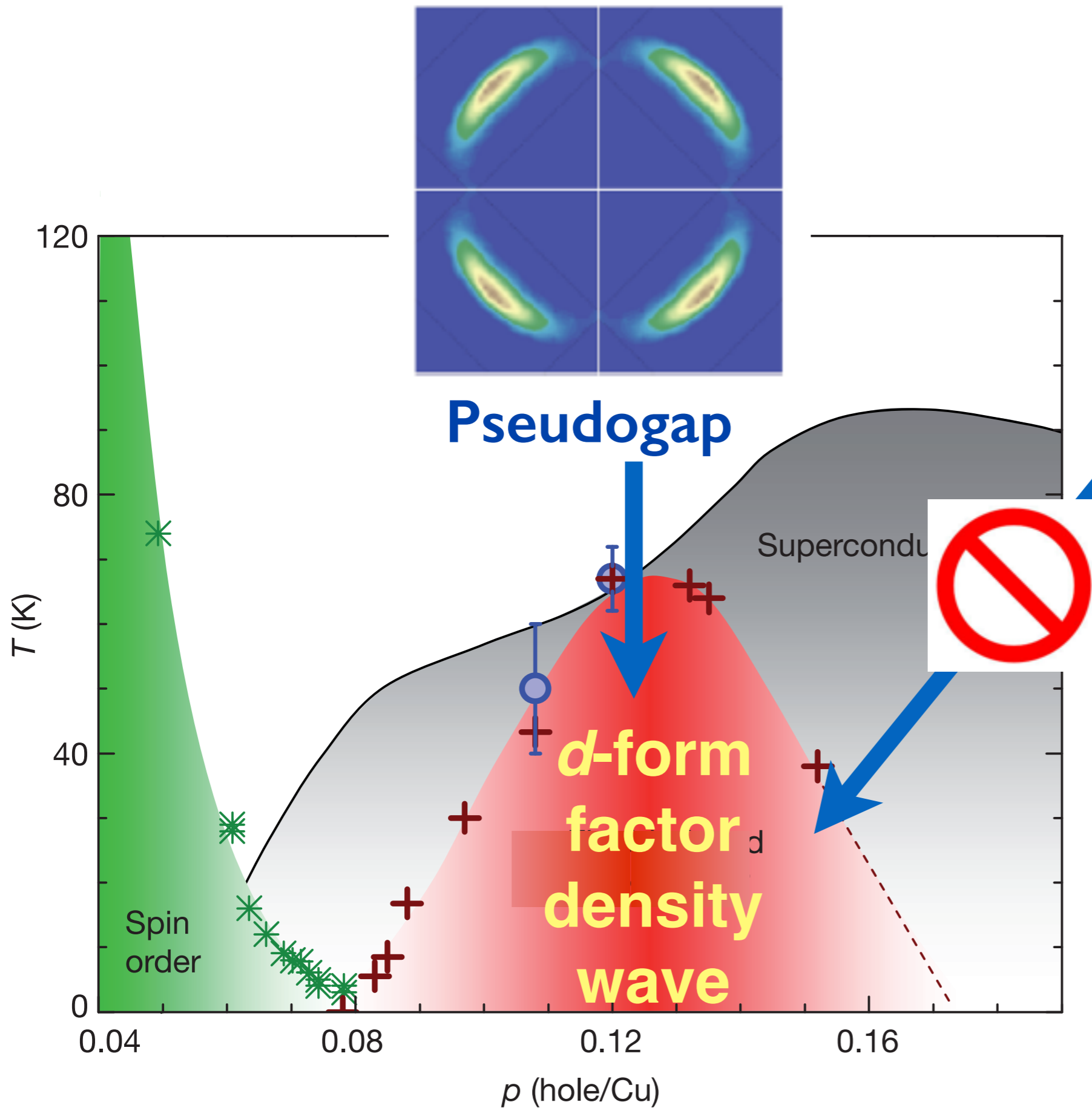
$$\langle c_{i\alpha}^\dagger c_{j\alpha} \rangle = \left[\int_{\mathbf{k}} \mathcal{P}(\mathbf{k}) e^{i\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right] e^{i\mathbf{Q} \cdot (\mathbf{r}_i + \mathbf{r}_j)/2}$$



This theory yields the correct form factor, but the incorrect \mathbf{Q} . We have found the same features in all theories (one- and three-band) with a large Fermi surface



Have examined density wave instabilities of large Fermi surface, not the “Fermi arc” state found at low doping.



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1. Density waves in the underdoped cuprates
STM observation of d-form factor density wave
2. RPA theory of density waves
3. Fractionalized Fermi liquids (FL*)
on the Kondo lattice
4. Fractionalized Fermi liquids (FL*) in doped
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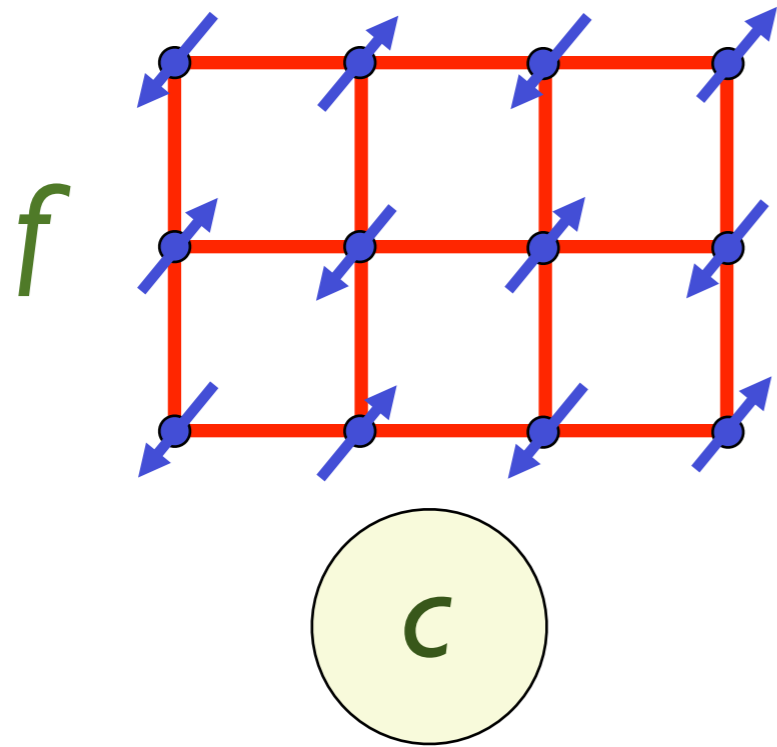
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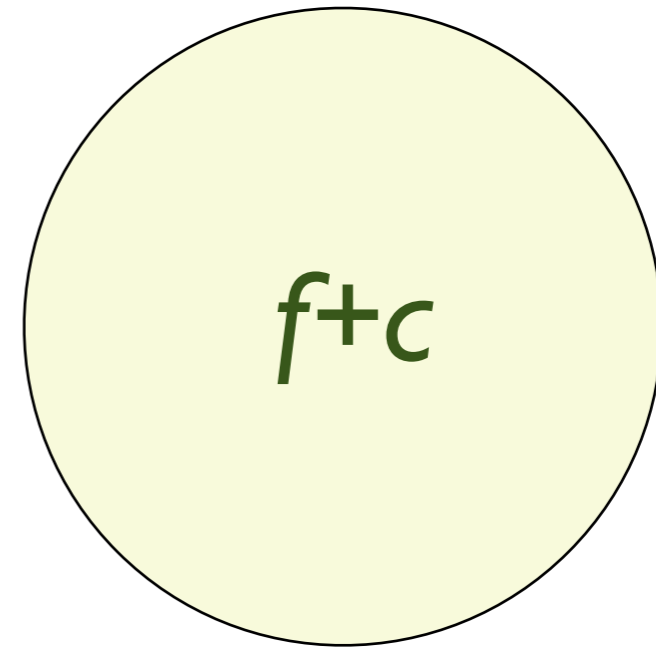
d-form factor density waves with the correct wavevector

Magnetic order and the heavy Fermi liquid in the Kondo lattice



$$\langle \vec{\varphi} \rangle \neq 0$$

Magnetic Metal:
f-electron moments
and
c-conduction electron
Fermi surface

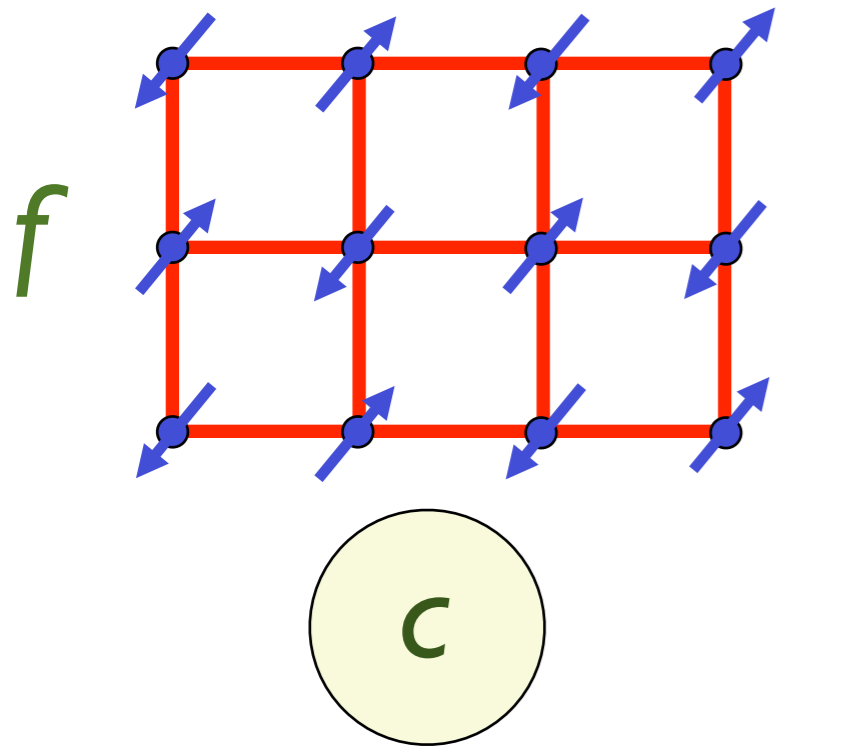


$$\langle \vec{\varphi} \rangle = 0$$

Heavy Fermi liquid
with “large” Fermi
surface of
hybridized f and
c-conduction
electrons

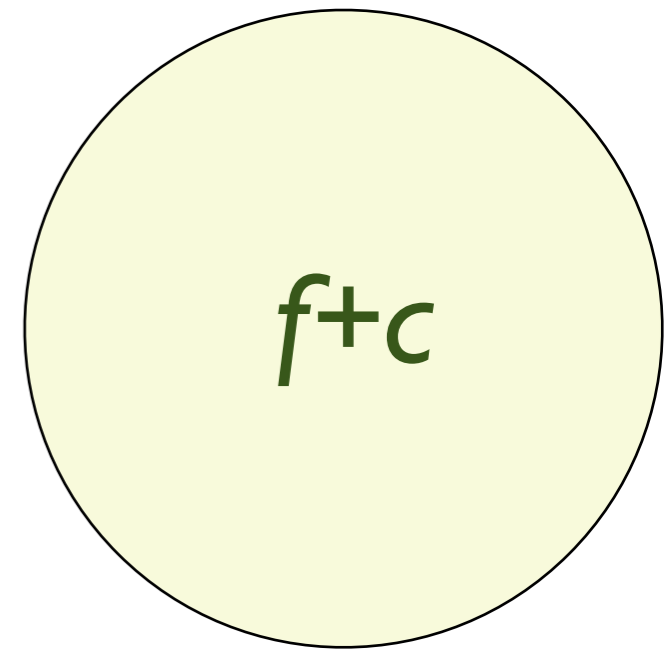


Separating onset of SDW order and the heavy Fermi liquid in the Kondo lattice



$$\langle \vec{\varphi} \rangle \neq 0$$

Magnetic Metal:
f-electron moments
and
c-conduction electron
Fermi surface

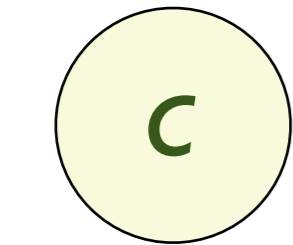
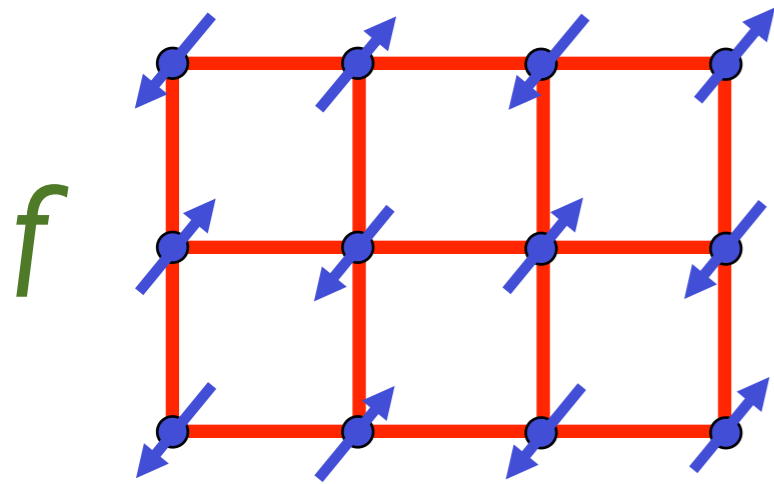


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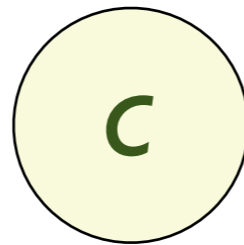
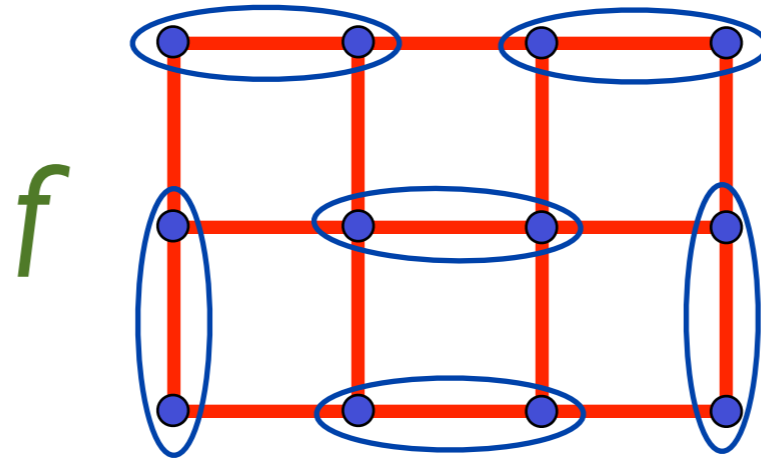


Separating onset of SDW order and the heavy Fermi liquid in the Kondo lattice



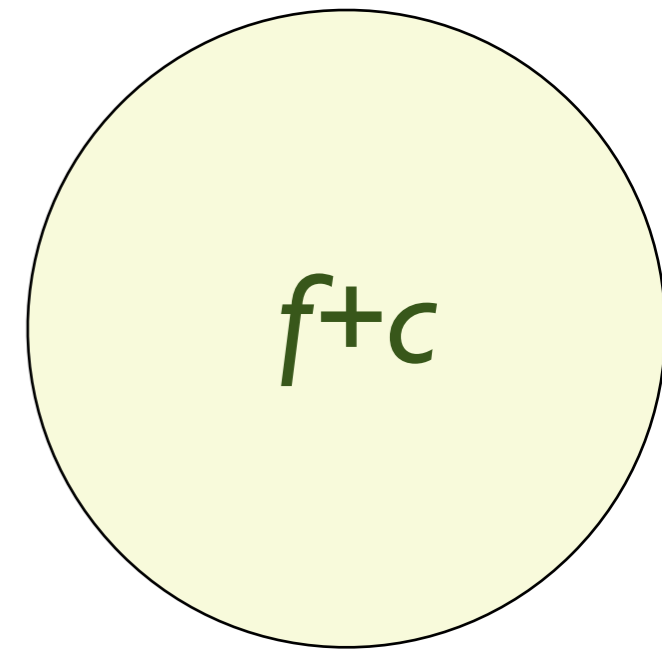
$$\langle \vec{\varphi} \rangle \neq 0$$

Magnetic Metal:
f-electron moments
and
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Fermi surface



$$\langle \vec{\varphi} \rangle = 0$$

Conduction electron
Fermi surface
and
spin-liquid of
f-electrons

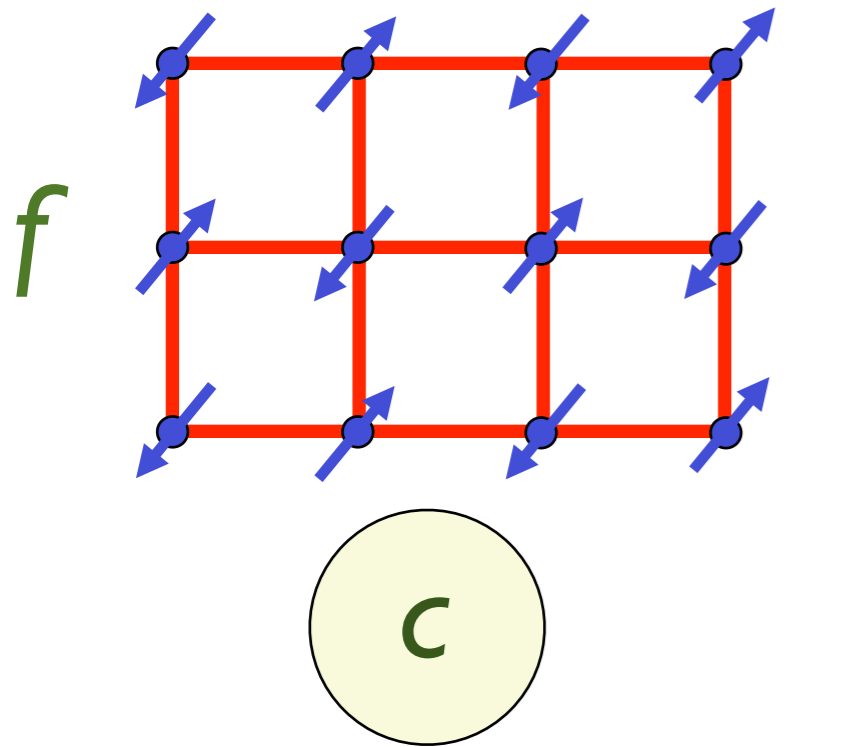


$$\langle \vec{\varphi} \rangle = 0$$

Heavy Fermi liquid
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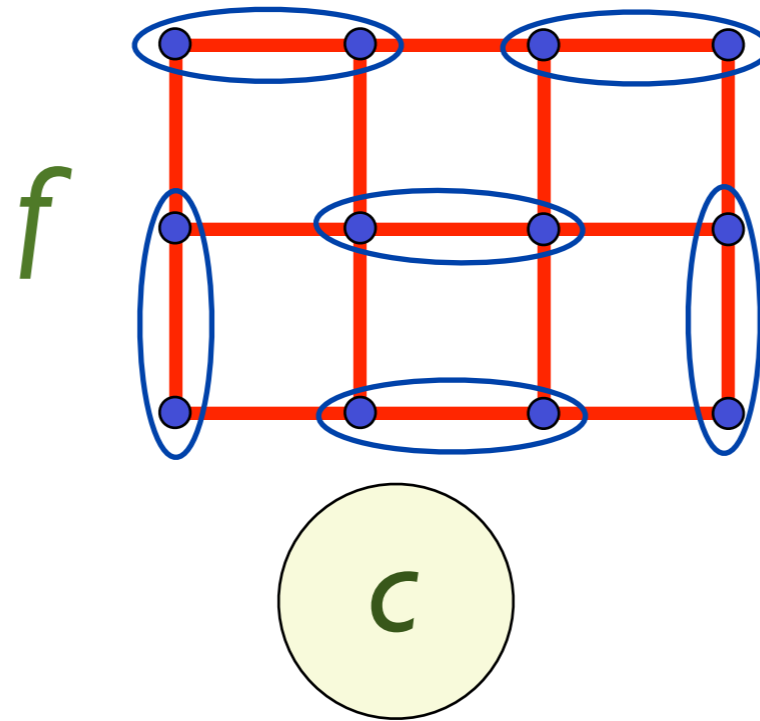


Separating onset of SDW order and the heavy Fermi liquid in the Kondo lattice



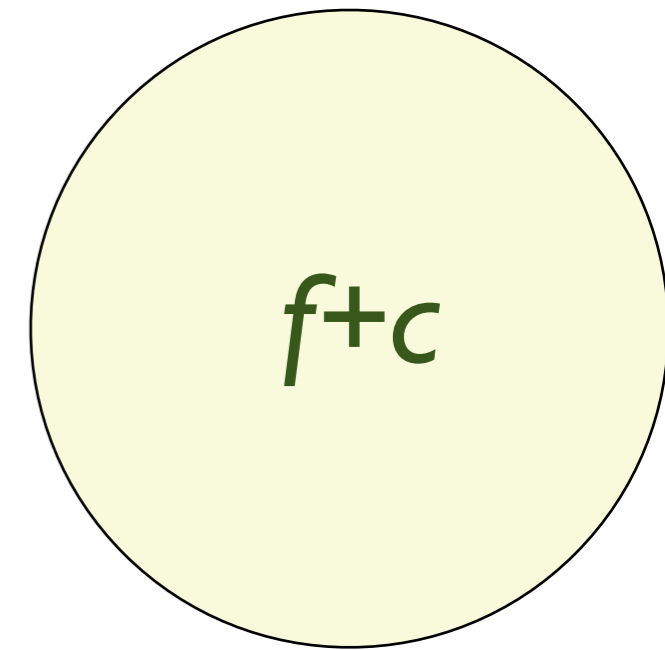
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Magnetic Metal:
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$$\langle \vec{\varphi} \rangle = 0$$

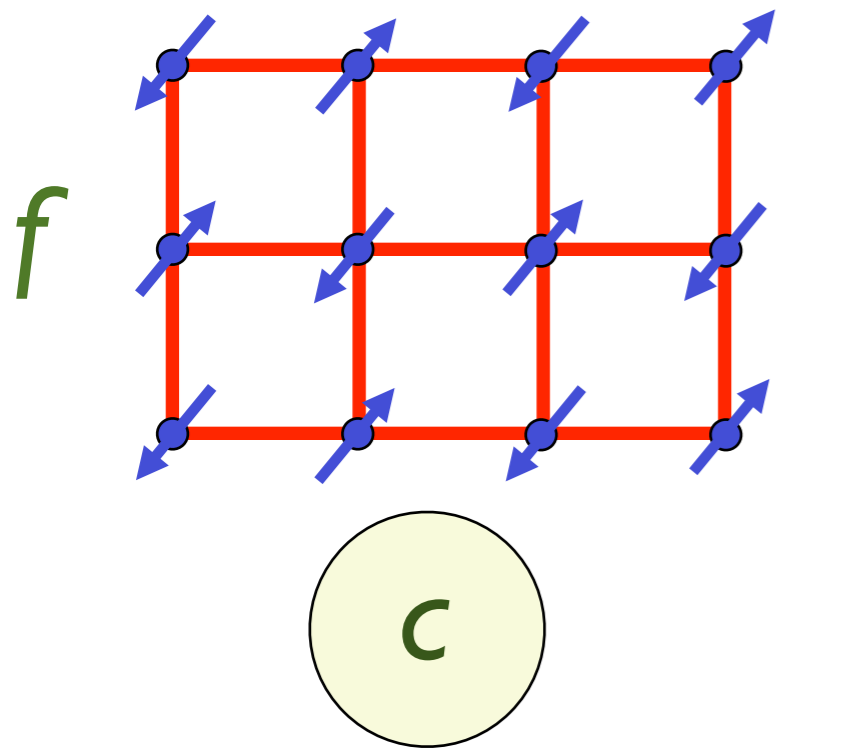
Fractionalized Fermi
liquid (FL*) phase
with no symmetry
breaking and “small”
Fermi surface



$$\langle \vec{\varphi} \rangle = 0$$

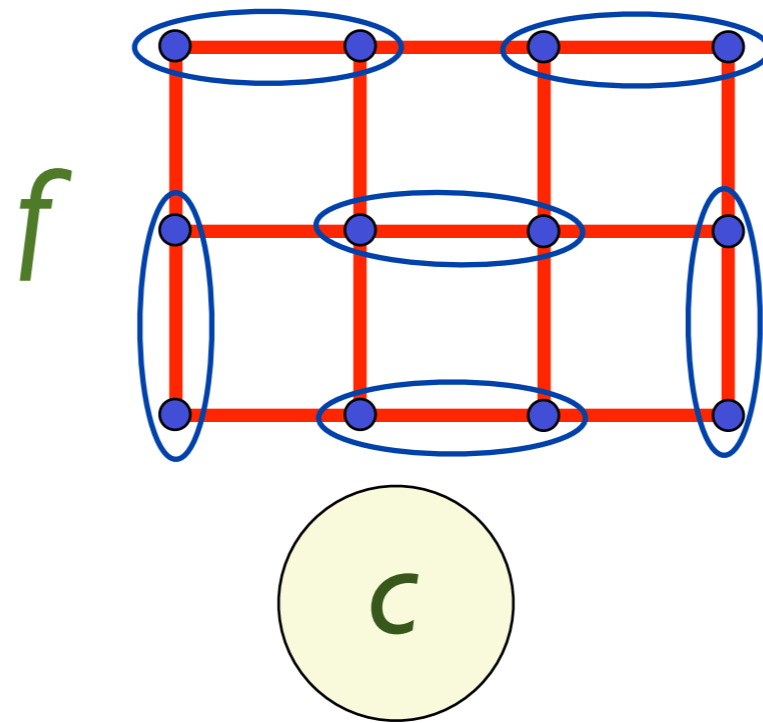
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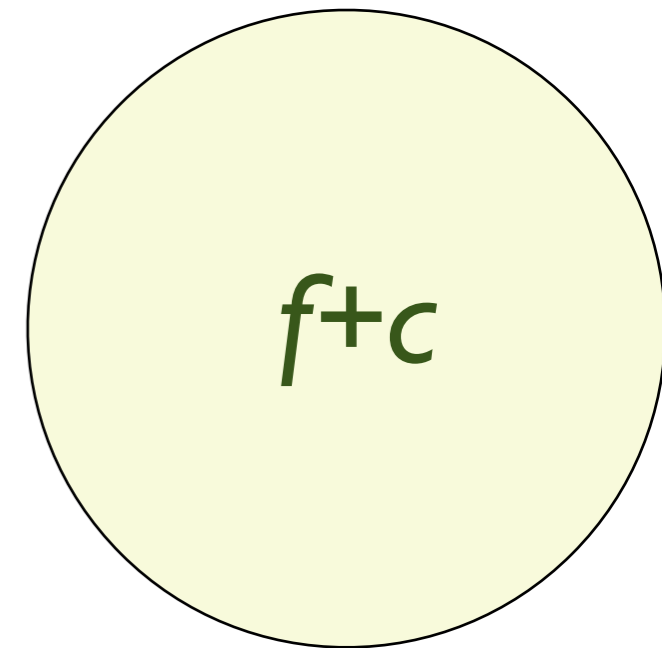


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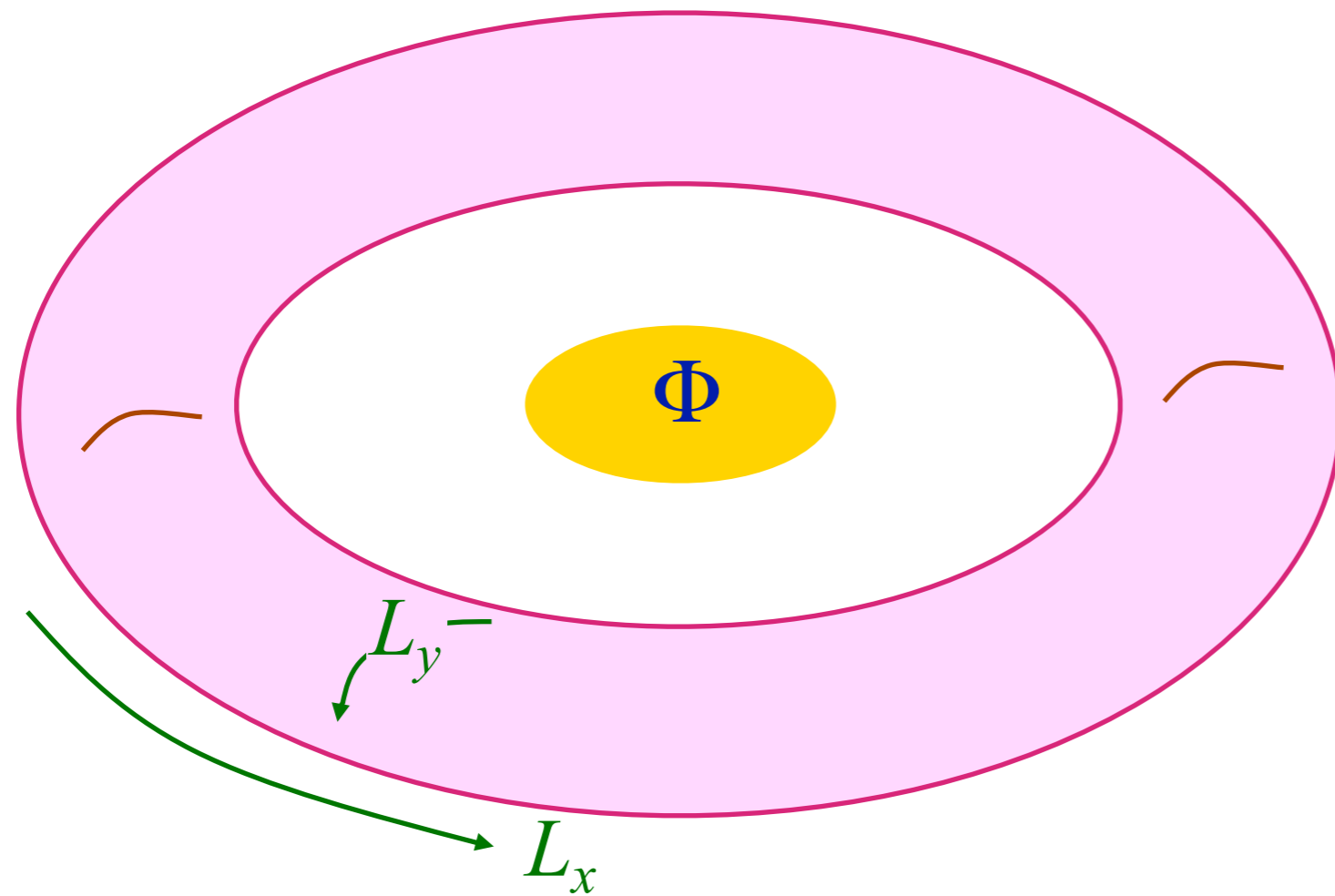
$$\langle \vec{\varphi} \rangle = 0$$

A “topological”
phase transition
with no
conventional
order parameter

Characteristics of FL* phase

- Fermi surface volume does not count all electrons.
- Such a phase *must* have low energy collective gauge excitations (“topological” order).
- These low energy gauge excitations are needed to account for the deficit in the Fermi surface volume, in M. Oshikawa’s proof of the Luttinger theorem.

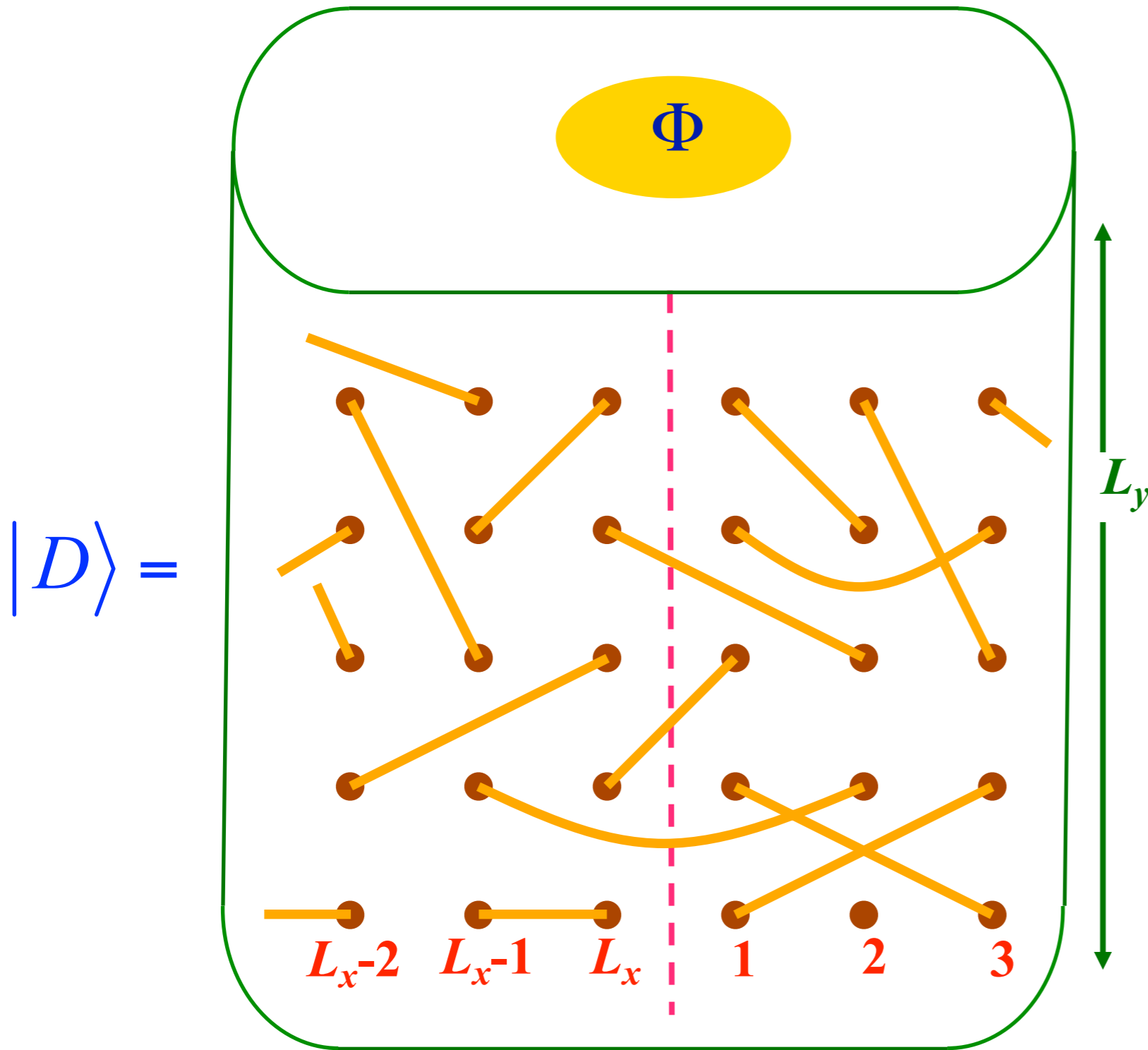
Lieb-Schultz-Mattis-Laughlin-Bonesteel-Affleck-Yamanaka-Oshikawa flux-piercing arguments



Unit cell a_x, a_y .
 $L_x/a_x, L_y/a_y$
coprime integers

Compute change in momentum due to inserting a single flux quantum. Equating this to the momentum acquired by the quasiparticles, we obtain the Luttinger theorem for the volume of the Fermi surface of a Fermi liquid.

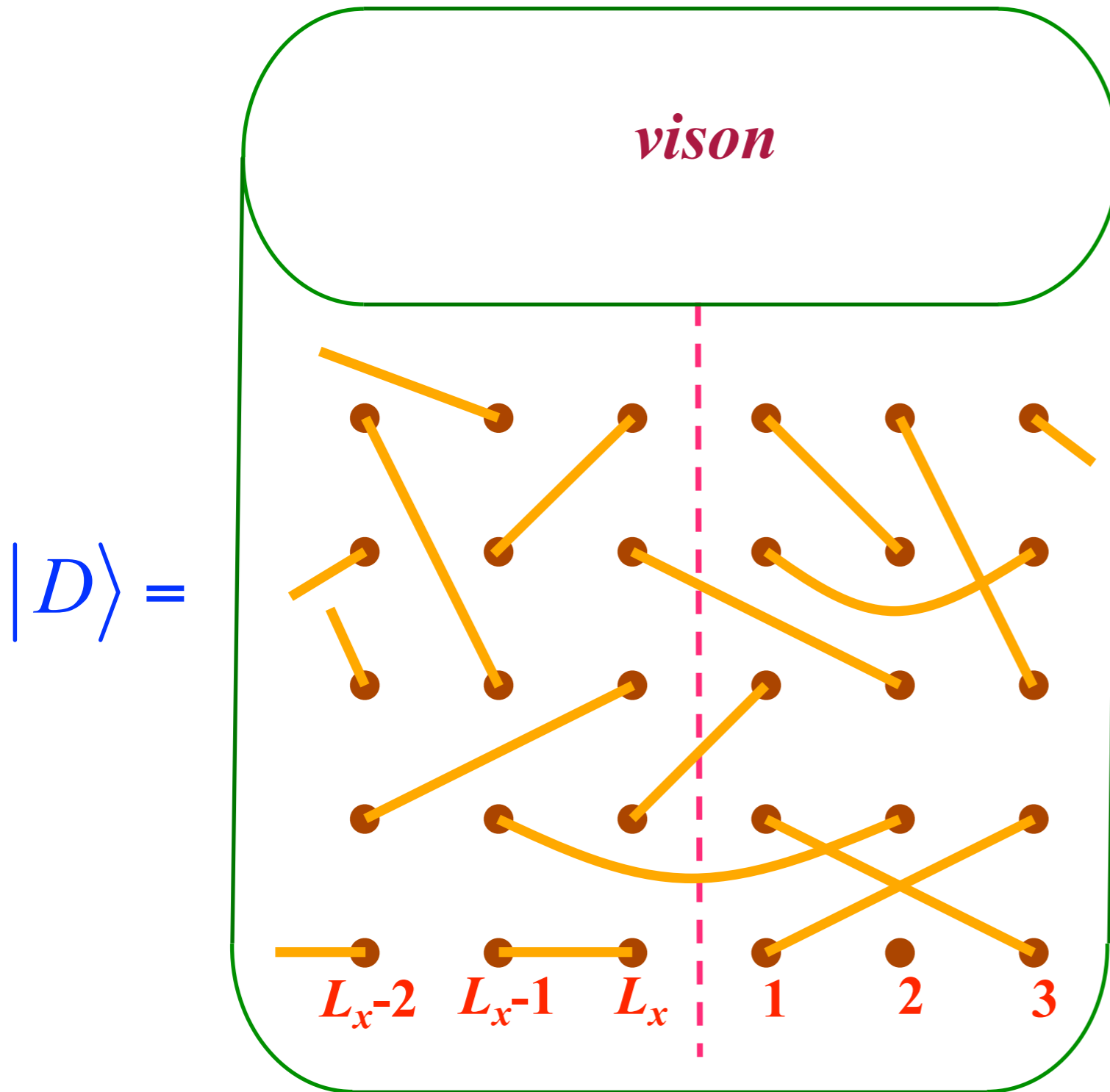
Effect of flux-piercing on a spin liquid



N. E. Bonesteel,
Phys. Rev. B **40**, 8954 (1989).
G. Misguich, C. Lhuillier,
M. Mambrini, and P. Sindzingre,
Eur. Phys. J. B **26**, 167 (2002).

$$|\Psi\rangle = \sum_D a_D |D\rangle$$

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$$|\Psi\rangle = \sum_D a_D |D\rangle$$

After flux insertion $|D\rangle \Rightarrow$

$$(-1)^{\text{Number of bonds cutting dashed line}} |D\rangle;$$

The vison contributes to the momentum count. A fractionalized Fermi liquid has *both* vison-like topological excitations and electron-like quasiparticles, and so the flux-piercing argument is compatible with a “small” Fermi surface.

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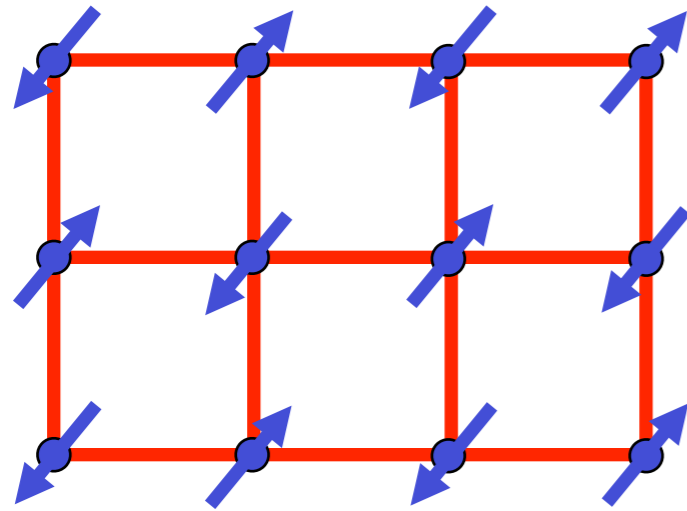
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d-form factor density waves with the correct wavevector

Quantum “disordering” magnetic order



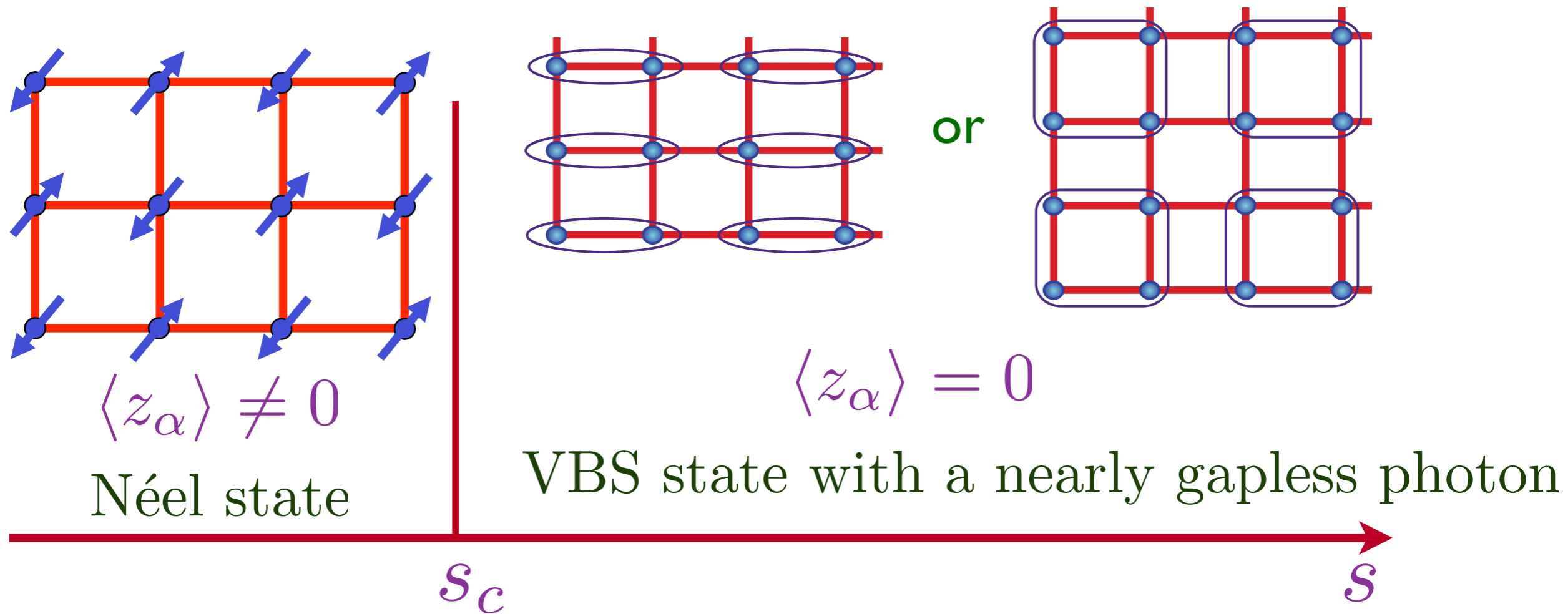
collinear Néel state

Spin liquid with a “**photon**”, which is unstable to the appearance of valence bond solid (VBS) order

S_c

S

Neel-VBS quantum transition

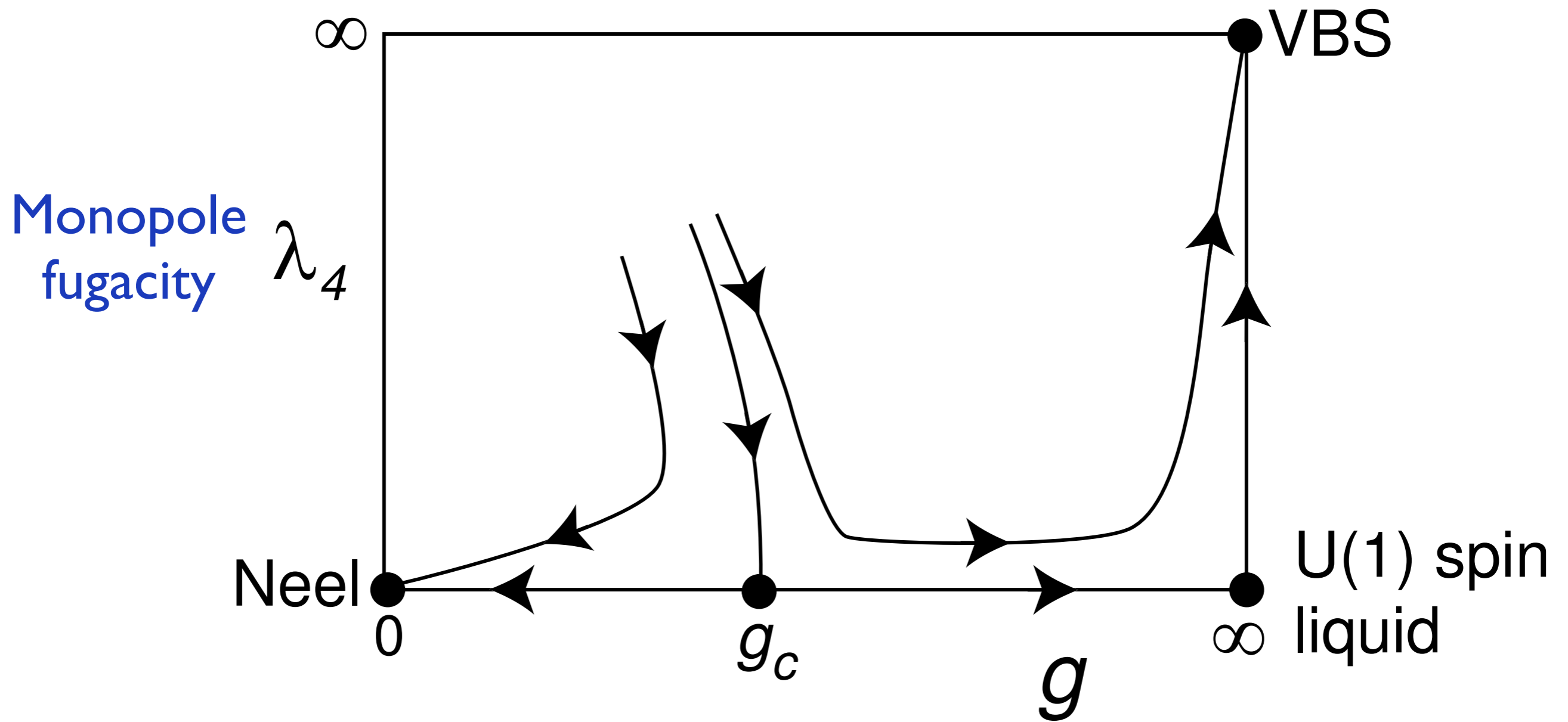


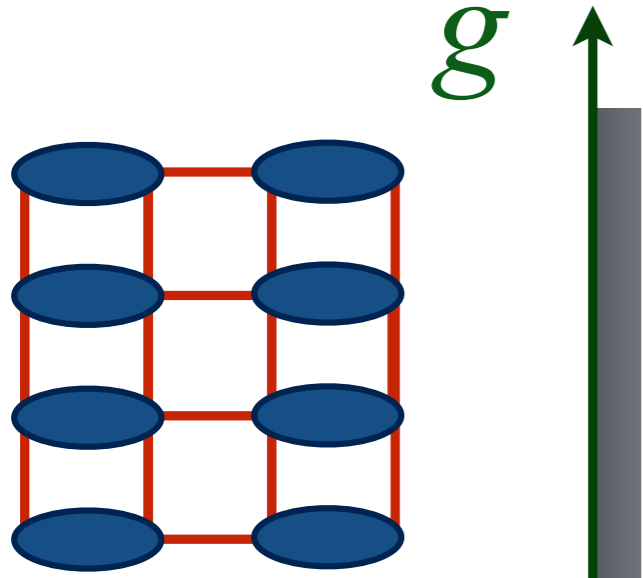
Critical theory for photons and deconfined spinons:

$$\mathcal{S}_z = \int d^2r d\tau \left[|(\partial_\mu - iA_\mu)z_\alpha|^2 + s|z_\alpha|^2 + u(|z_\alpha|^2)^2 + \frac{1}{2e_0^2} (\epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda)^2 \right]$$

O.I. Motrunich and A. Vishwanath, *Phys. Rev. B* **70**, 075104 (2004).

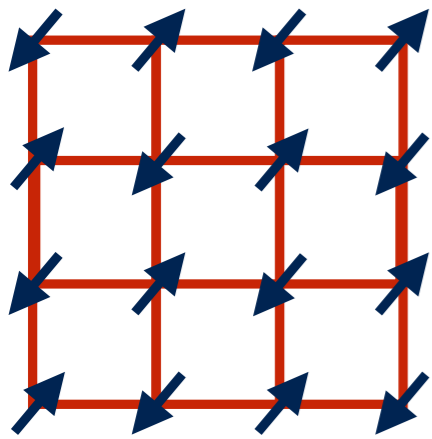
T. Senthil, A. Vishwanath, L. Balents, S. Sachdev and M.P.A. Fisher, *Science* **303**, 1490 (2004).





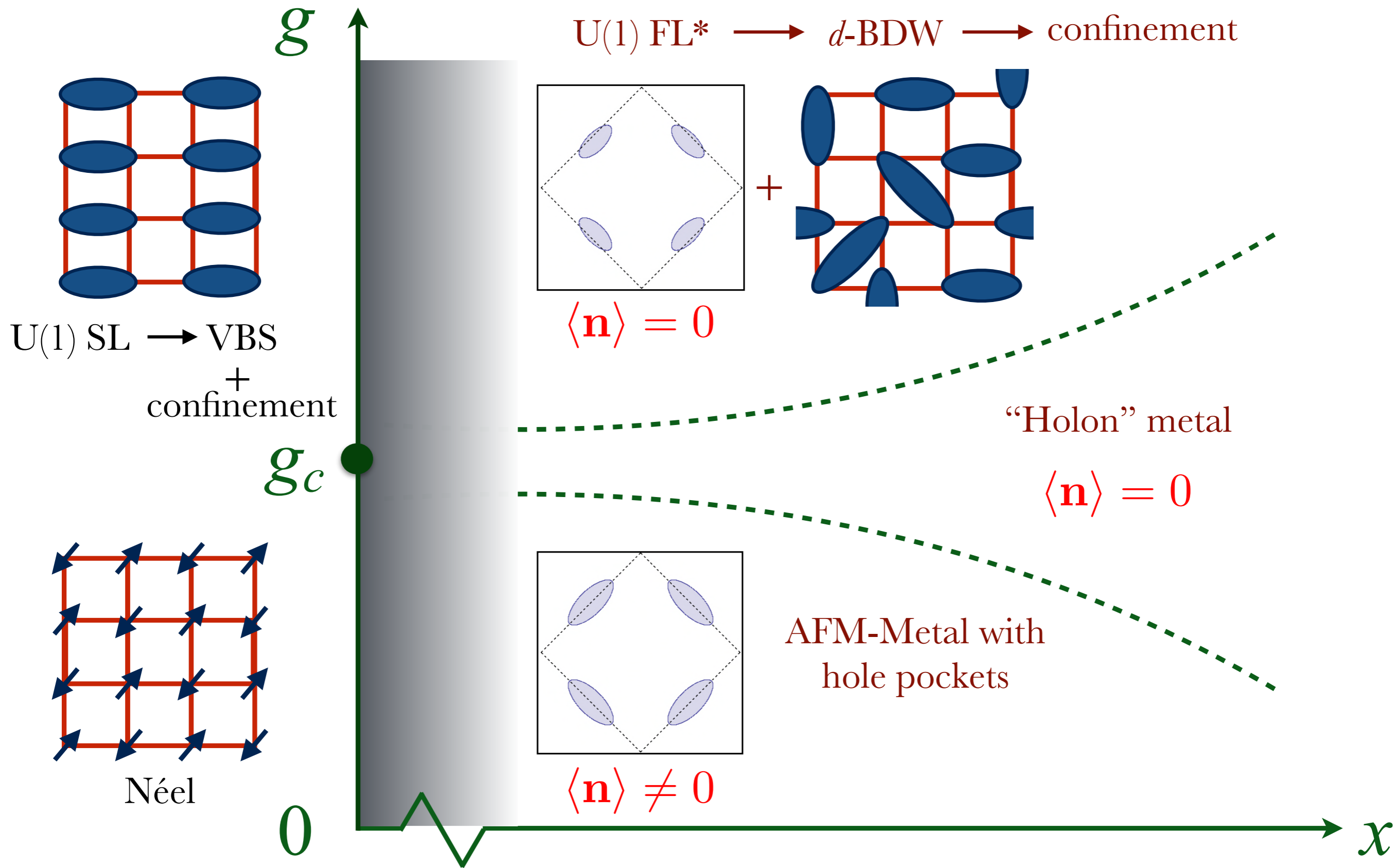
$U(1)$ SL \rightarrow VBS
+ confinement

g_c



Néel

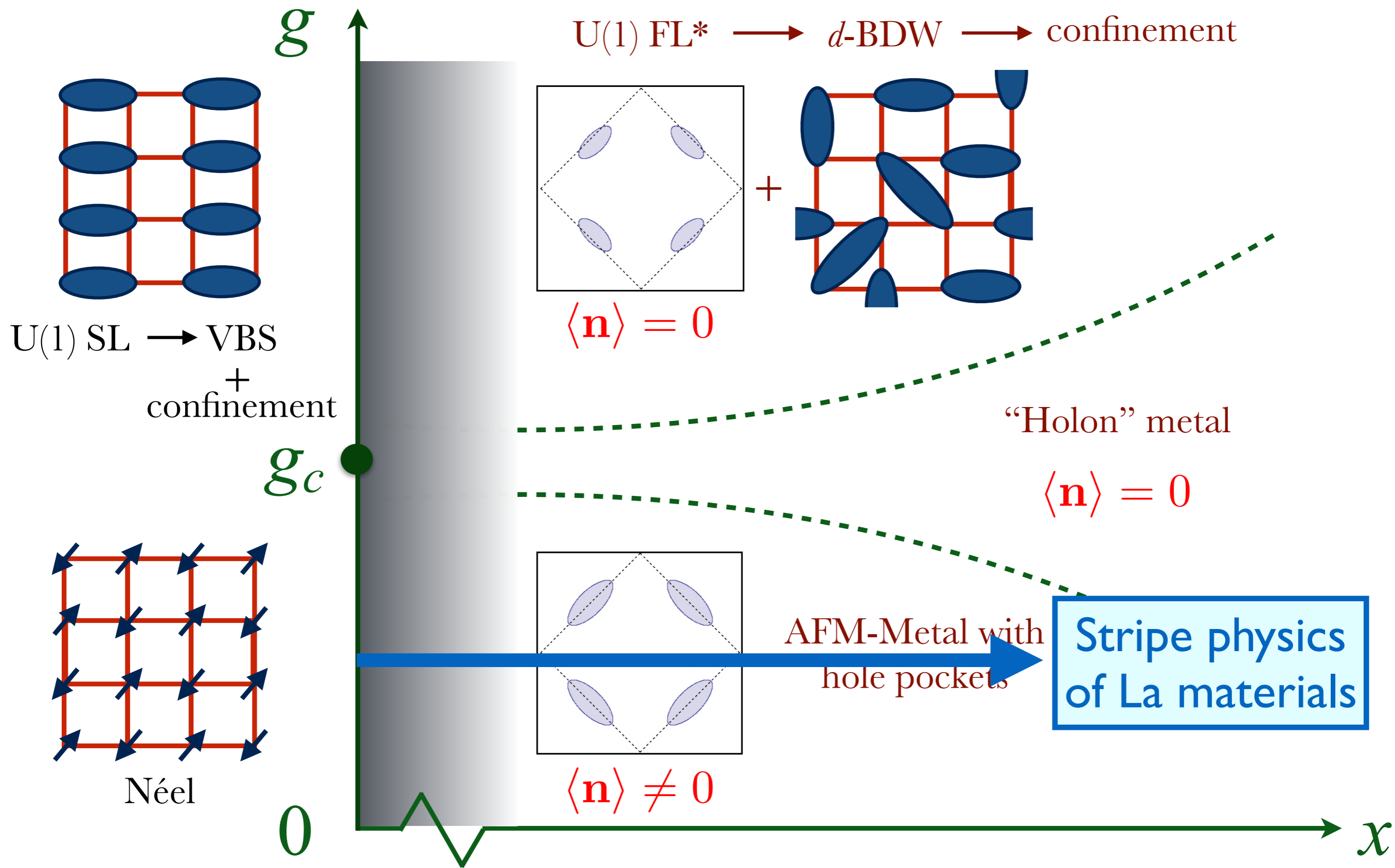
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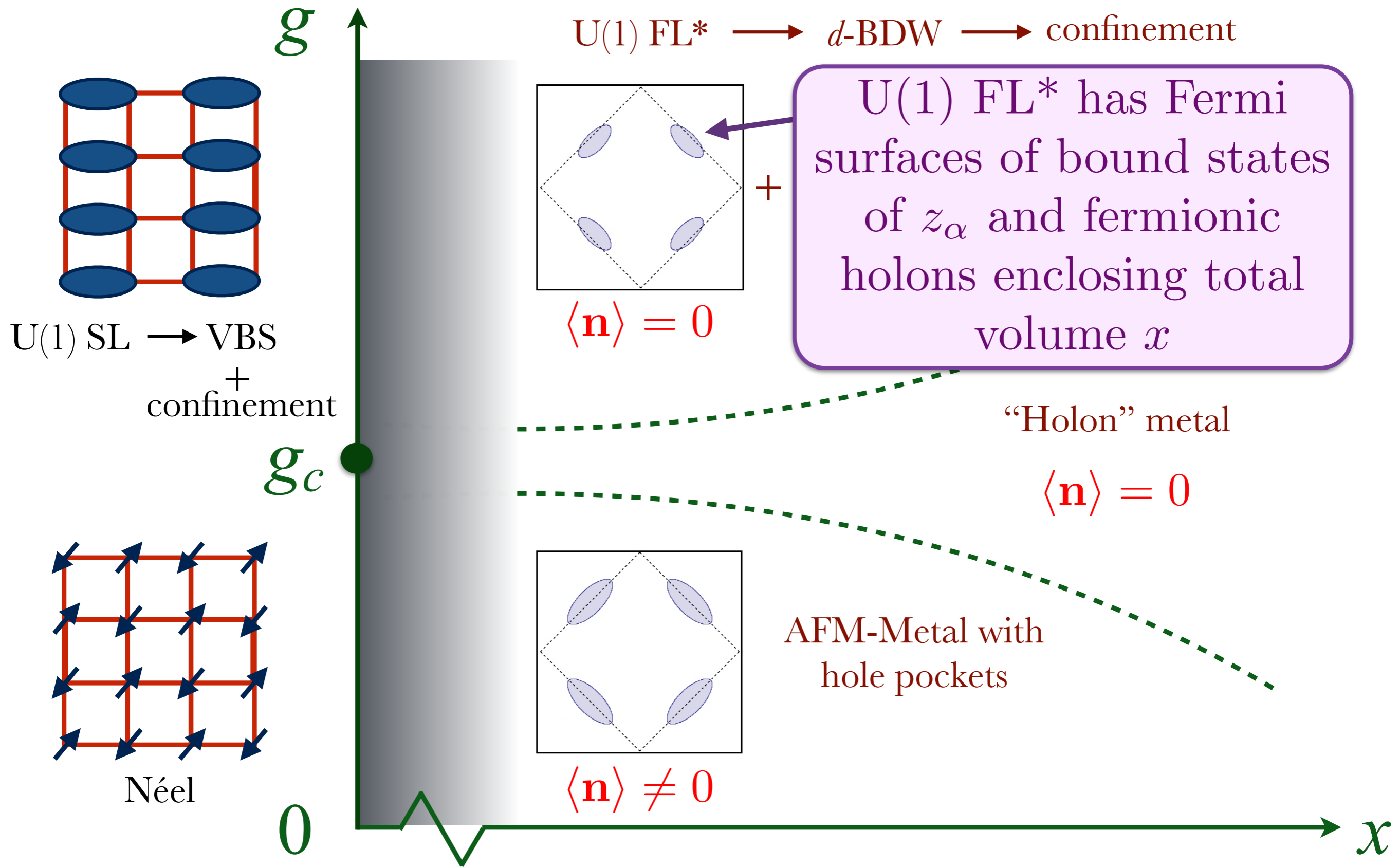


R. K. Kaul, A. Kolezhuk, M. Levin, S. Sachdev, and T. Senthil, Phys. Rev. B **75**, 235122 (2007)

Y. Qi and S. Sachdev, Phys. Rev. B **81**, 115129 (2010)

D. Chowdhury and S. Sachdev, arXiv:1409.5430

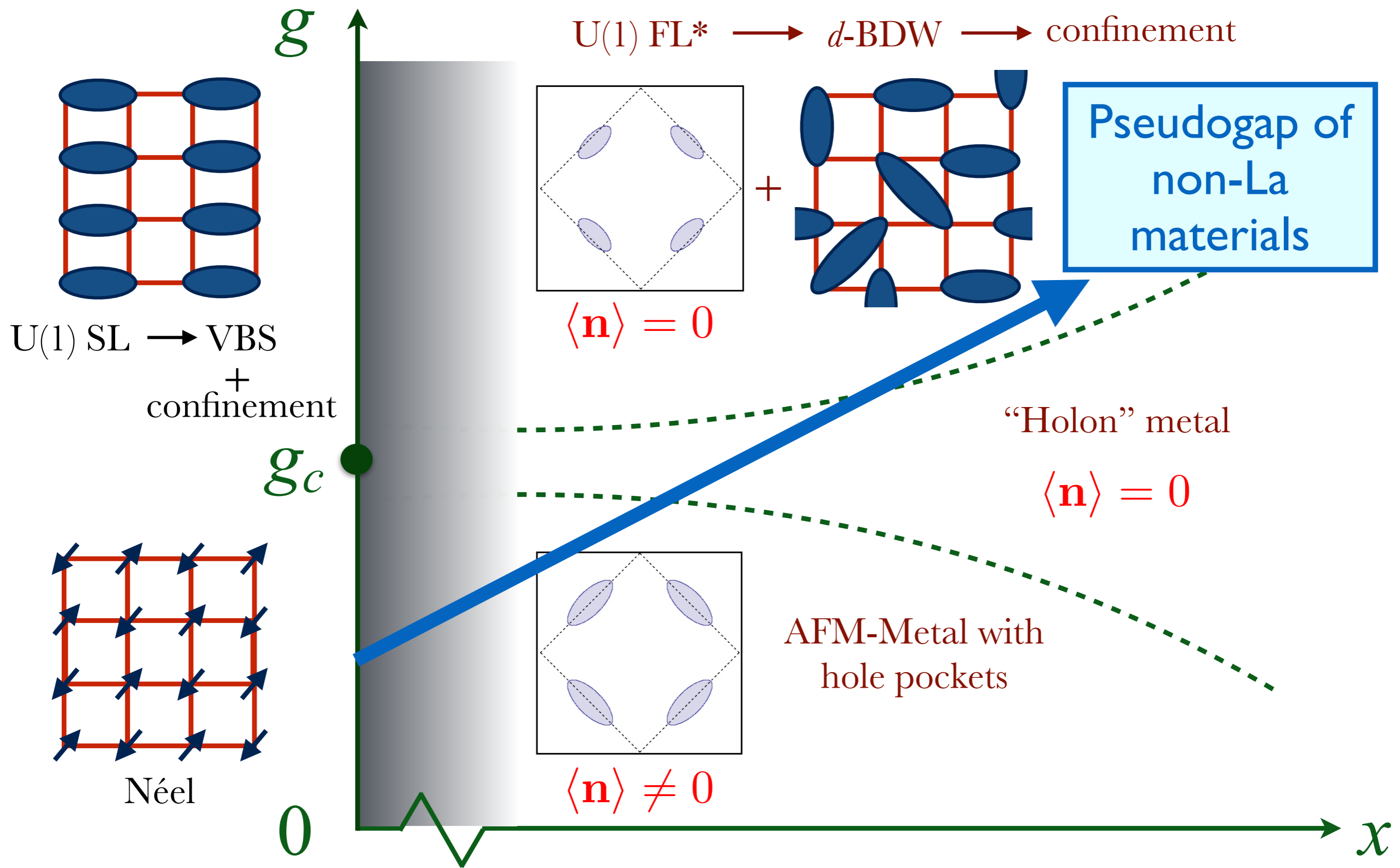


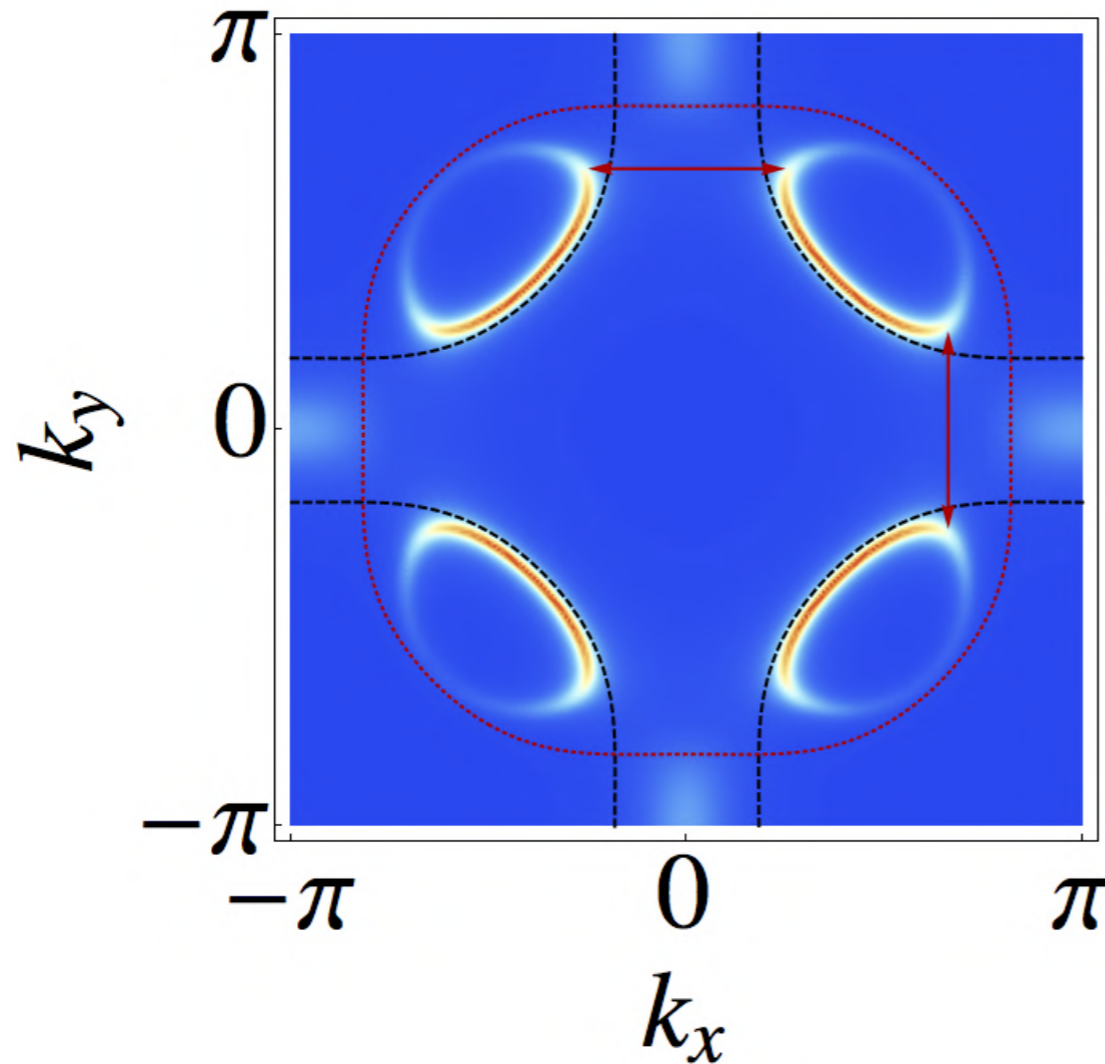


R. K. Kaul, A. Kolezhuk, M. Levin, S. Sachdev, and T. Senthil, Phys. Rev. B **75**, 235122 (2007)

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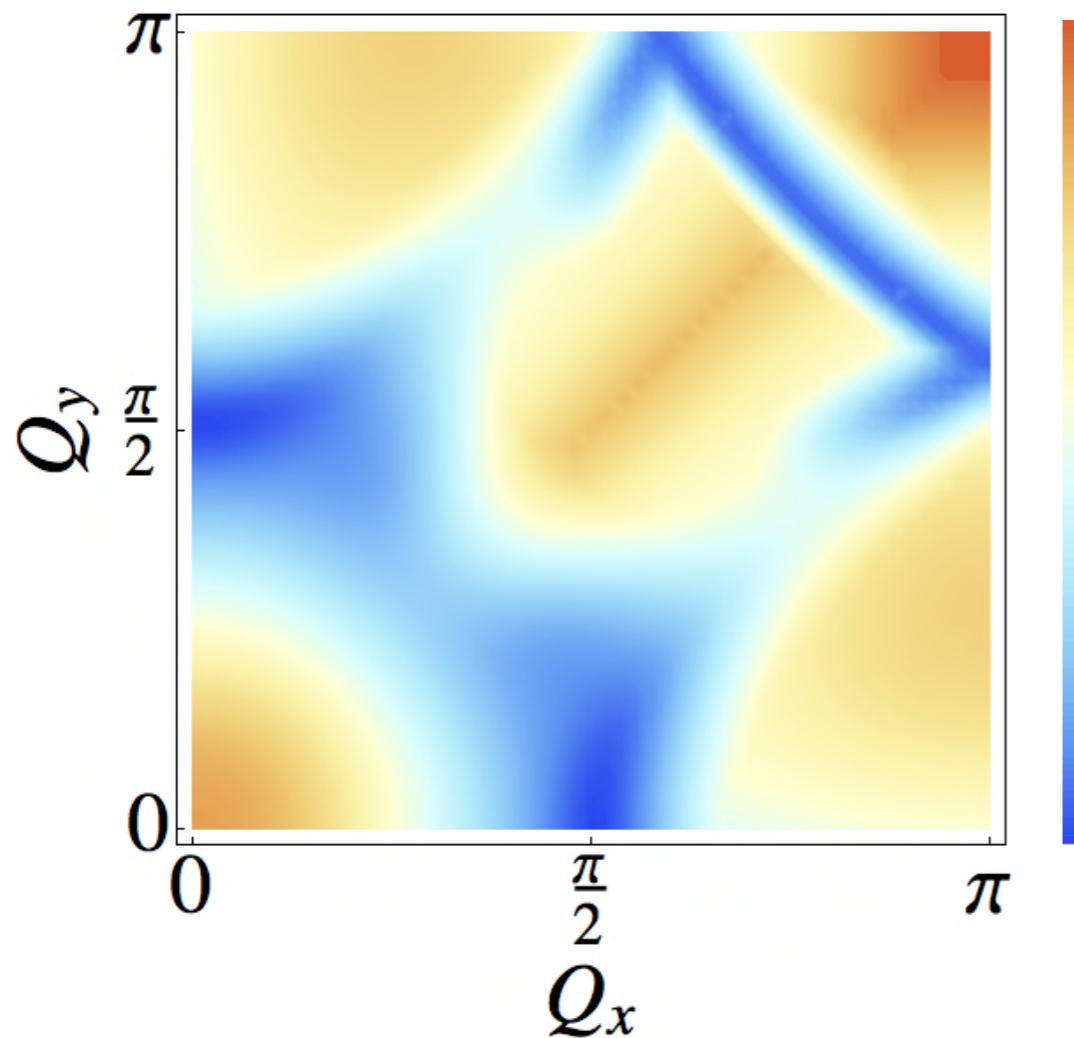
D. Chowdhury and S. Sachdev, arXiv:1409.5430





Electron spectral
function of FL*

The pseudogap is described by the U(1)-FL*: a state with hole pockets on a background of a spin-liquid described by a U(1) gauge theory. Its dominant density wave instability is a predominantly d -form factor density wave with a wavevector \mathbf{Q} along the $(1, 0)$ and $(0, 1)$ square lattice directions, in agreement with observations on the non-La-based cuprates.



Eigenvalues of spin-singlet,
time-reversal-preserving
particle-hole propagator

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Conclusions

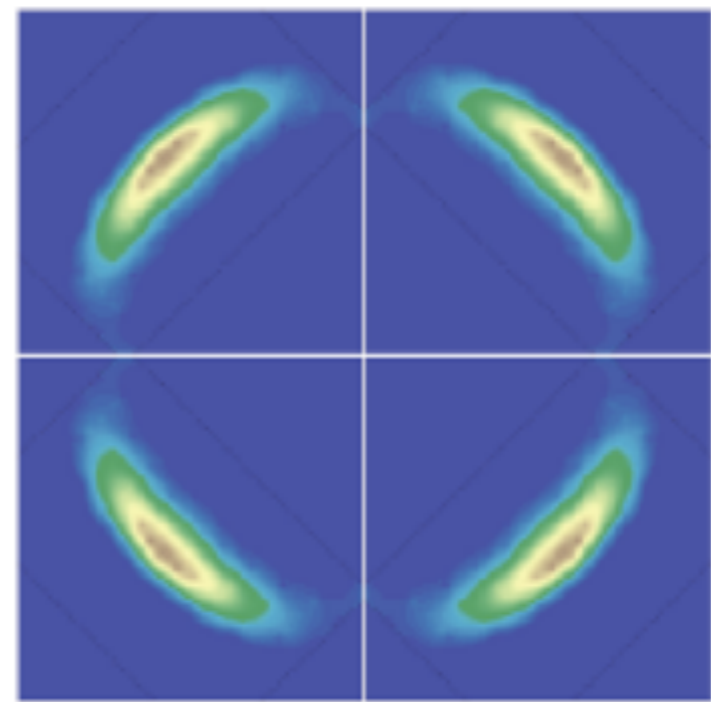
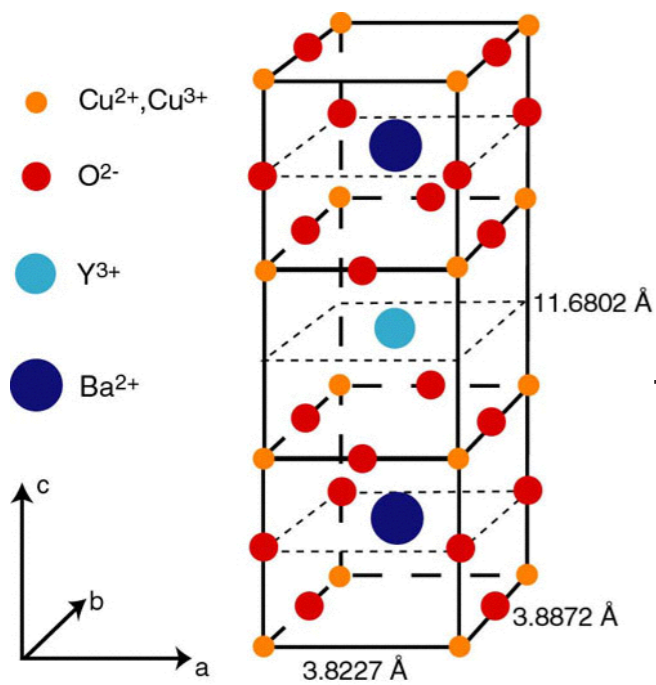
1. d -form factor density wave order observed in the non-La hole-doped cuprate superconductors.

Conclusions

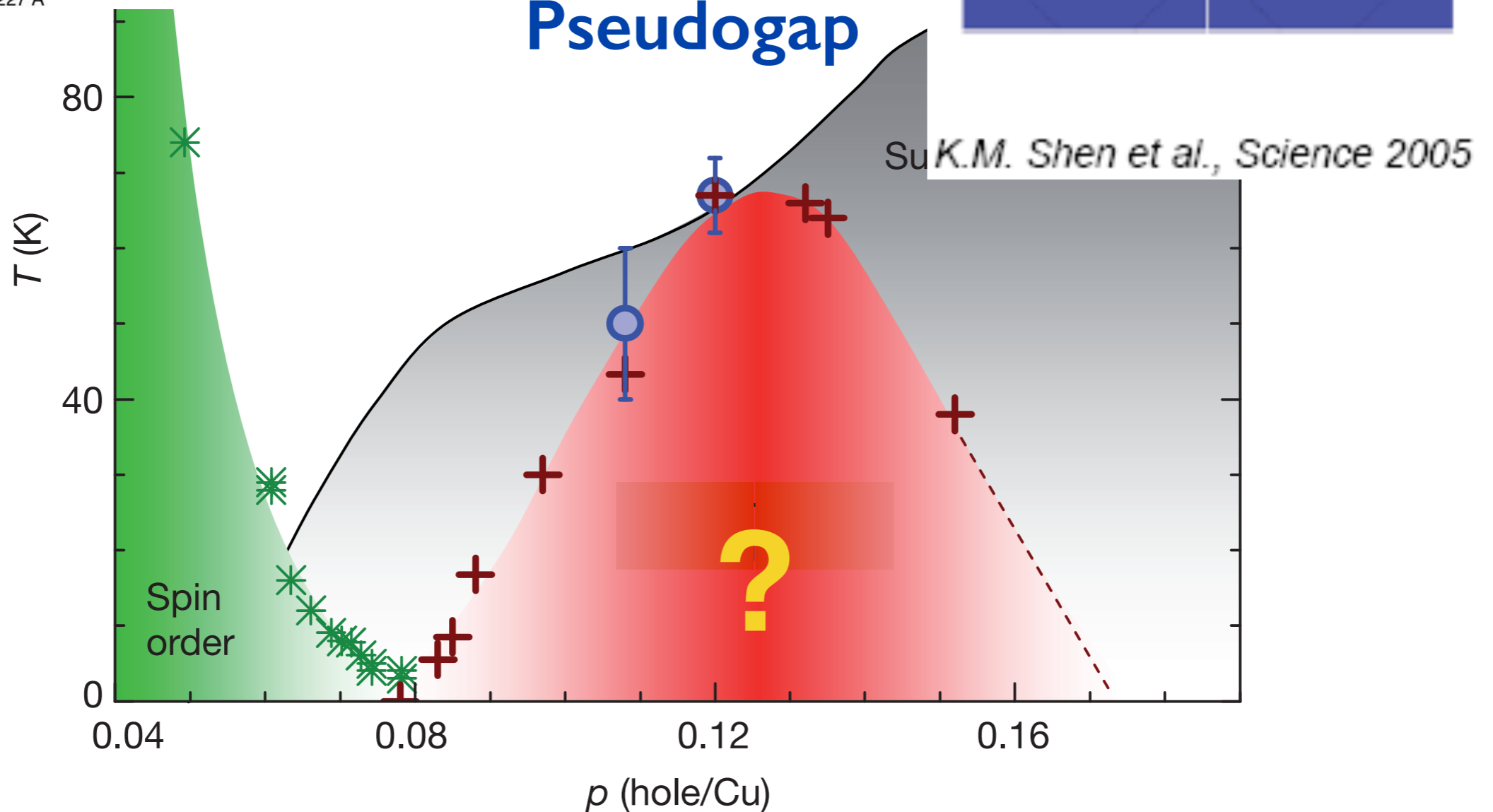
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2. The “stripe” model corresponds to a s' -form factor, and this describes the La-based, lower T_c , hole-doped cuprate superconductors.

Conclusions

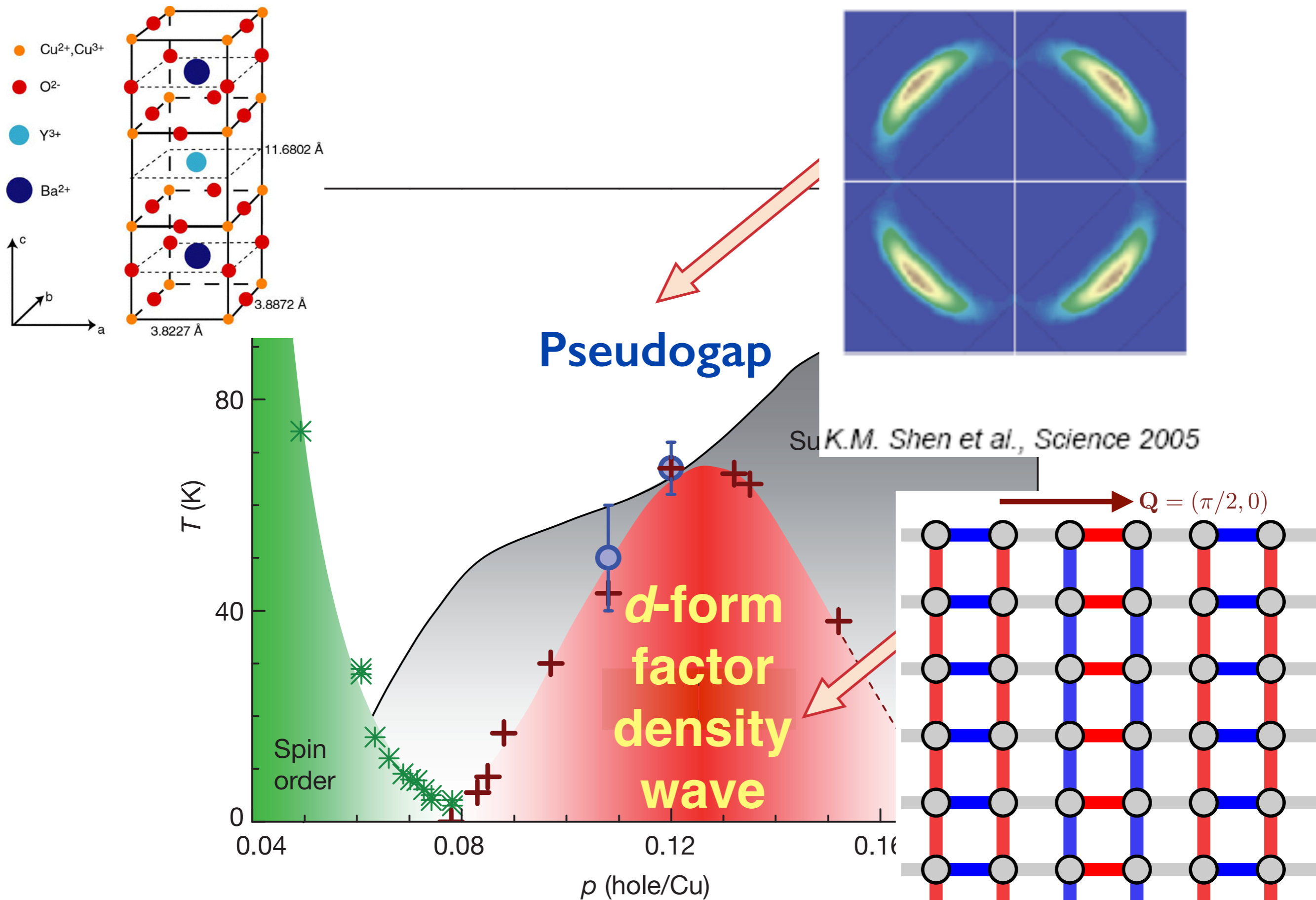
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3. Is the d -form factor an unexpected window into the spin-liquid physics of the pseudogap ?



Pseudogap



T. Wu, H. Mayaffre, S. Kramer, M. Horvatic, C. Berthier, W.N. Hardy, R. Liang, D.A. Bonn, and M.-H. Julien, *Nature* **477**, 191 (2011).



K. Fujita, M. H Hamidian, S. D. Edkins, Chung Koo Kim, Y. Kohsaka, M. Azuma, M. Takano, H. Takagi, H. Eisaki, S. Uchida, A. Allais, M. J. Lawler, E.-A. Kim, S. Sachdev, and J. C. Davis, PNAS 111, E3026 (2014)