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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Mohammad Hamidian
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Stephen Edkins
Cornell / St Andrews

Michael Lawler

J. C. Seamus Davis

Eun-Ah Kim

Cornell

Kazuhiro Fujita
Cornell/ BNL

See talk by
Kazuhiro Fujita
on Friday

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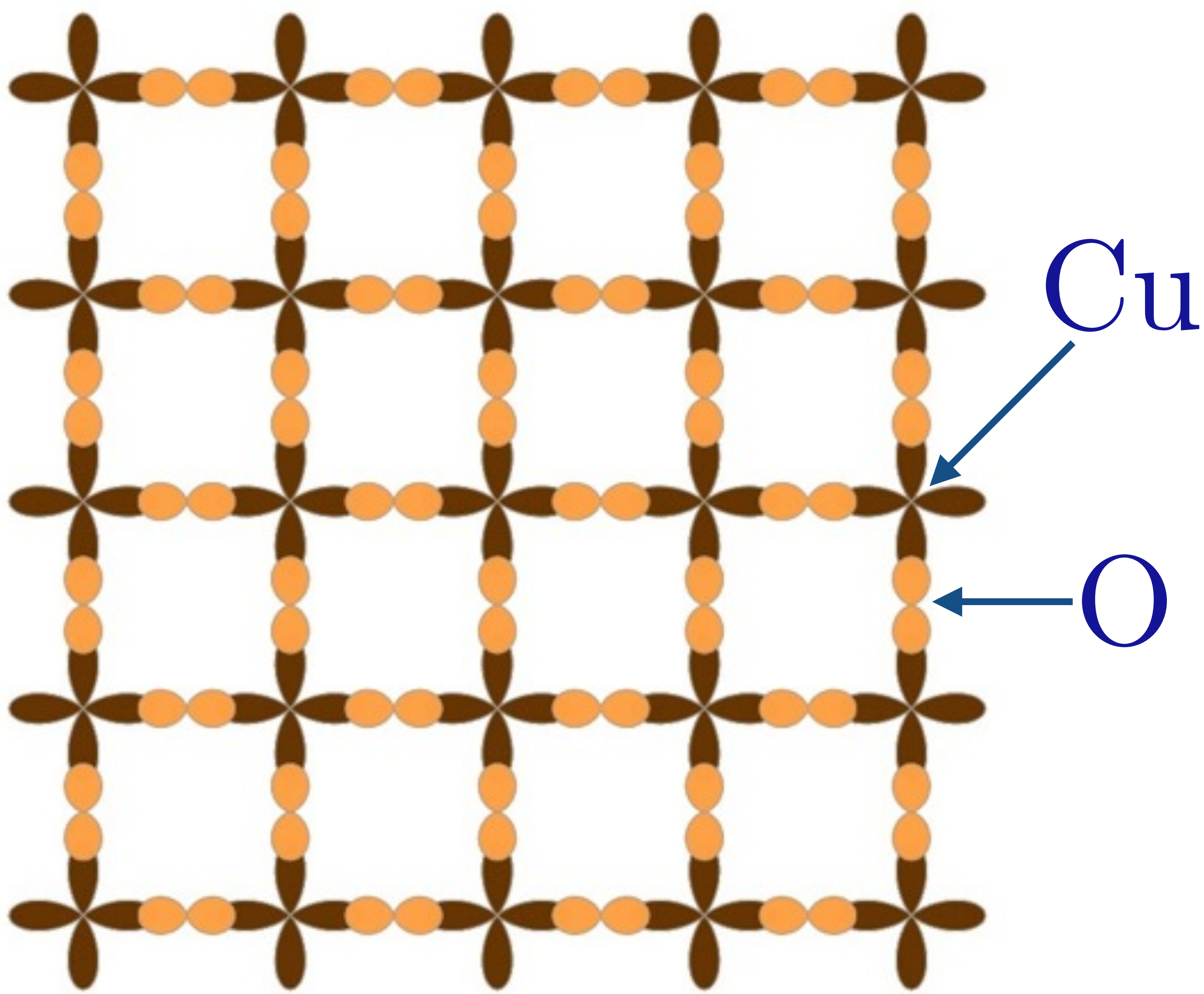
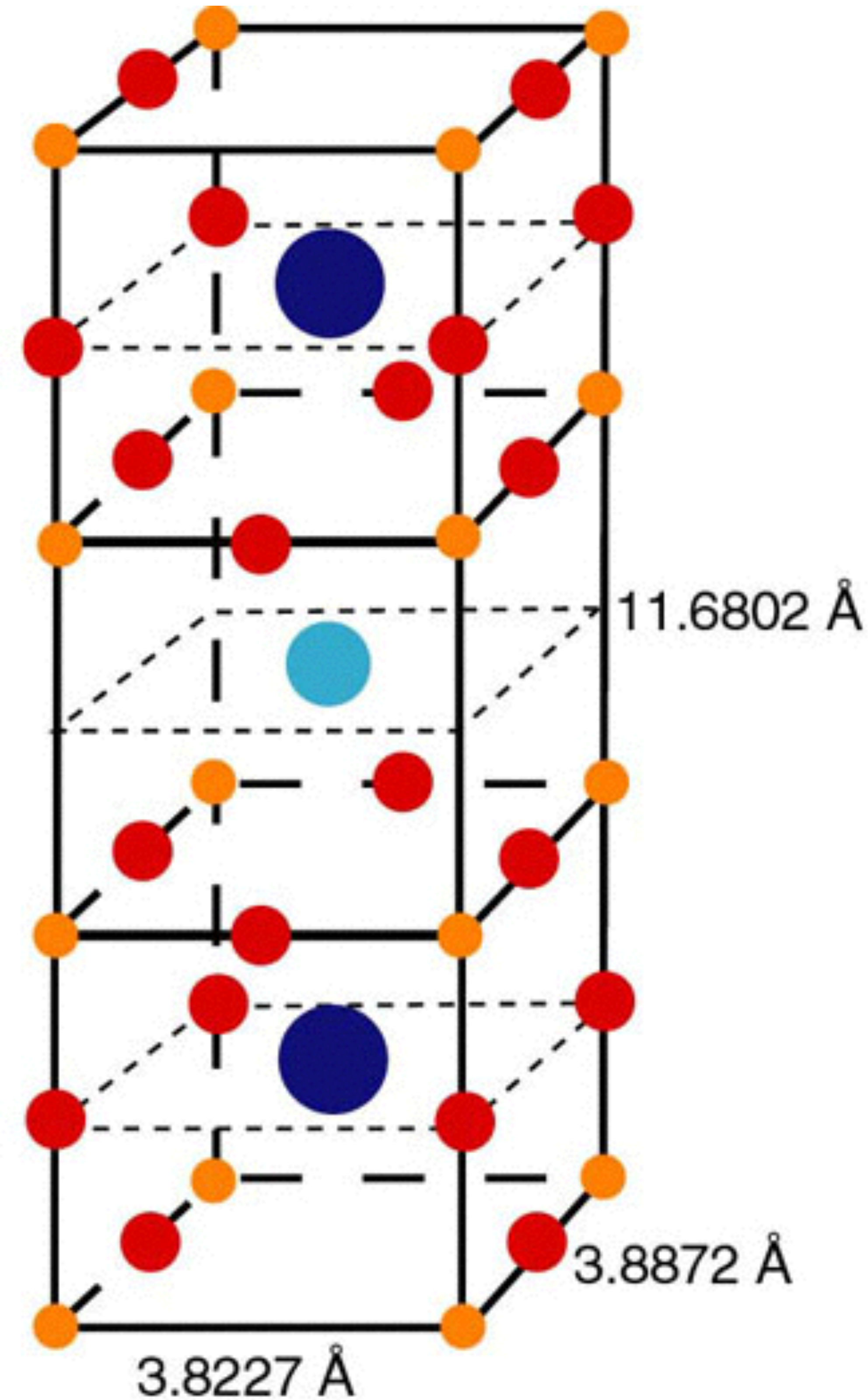
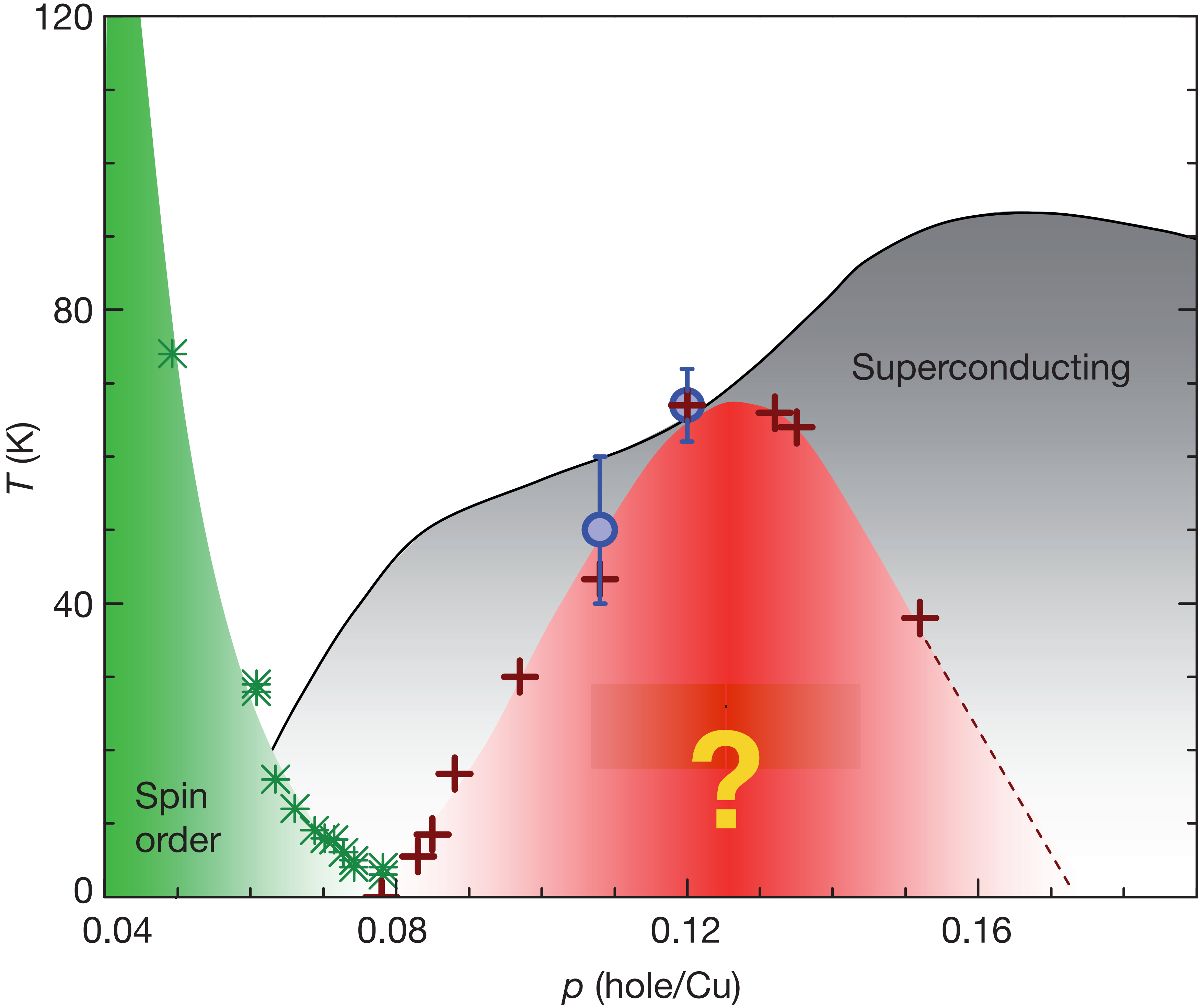
High temperature superconductors

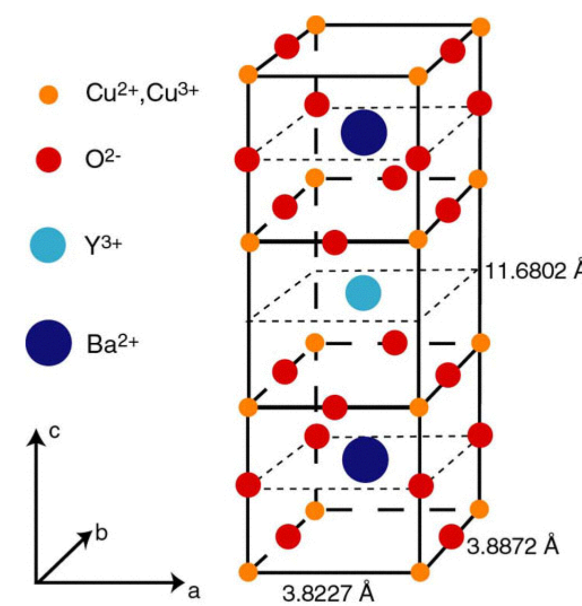


CuO_2 plane

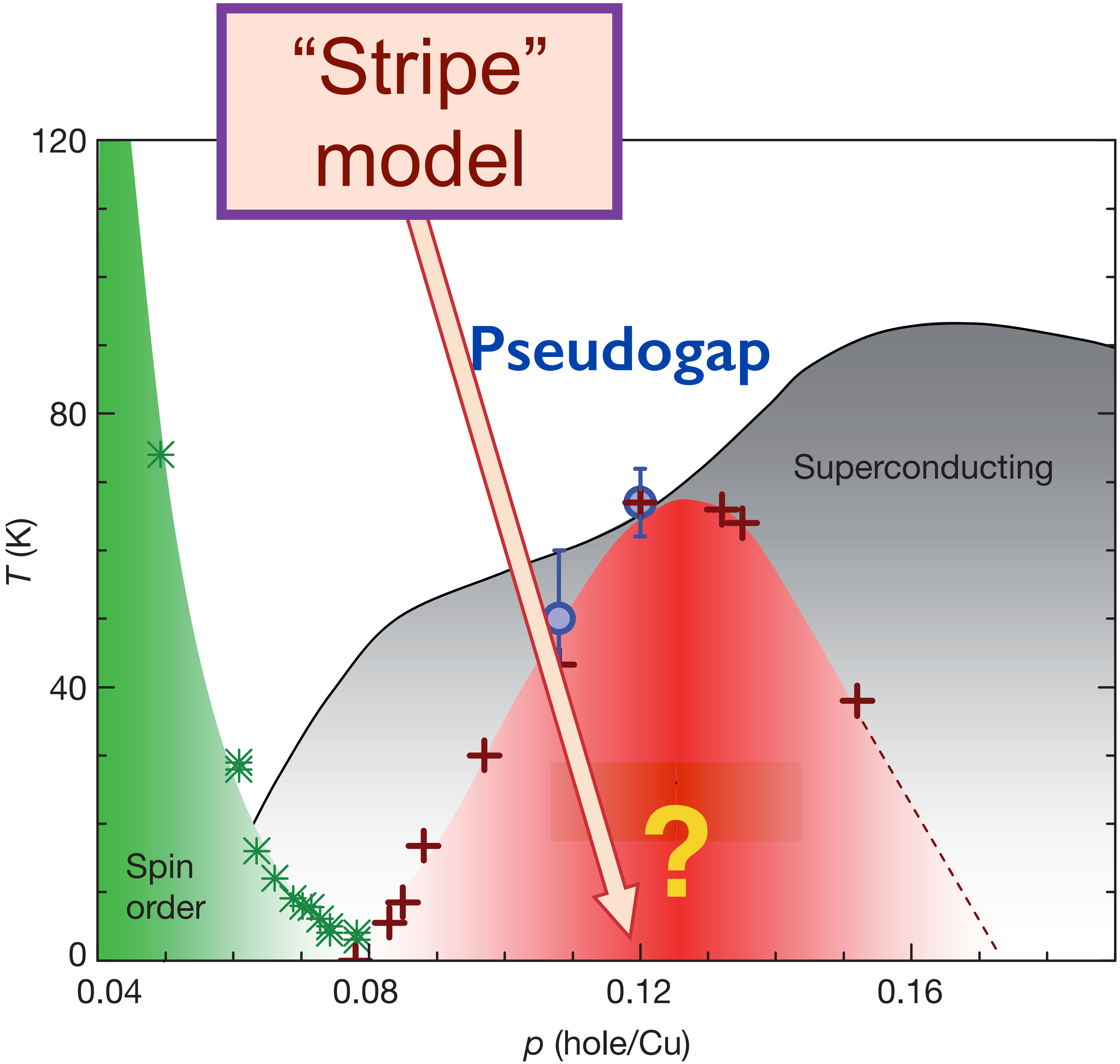


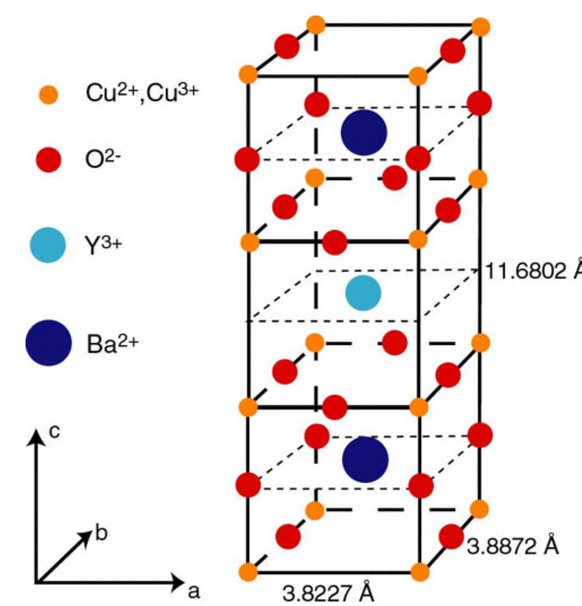
$YBa_2Cu_3O_{6+x}$





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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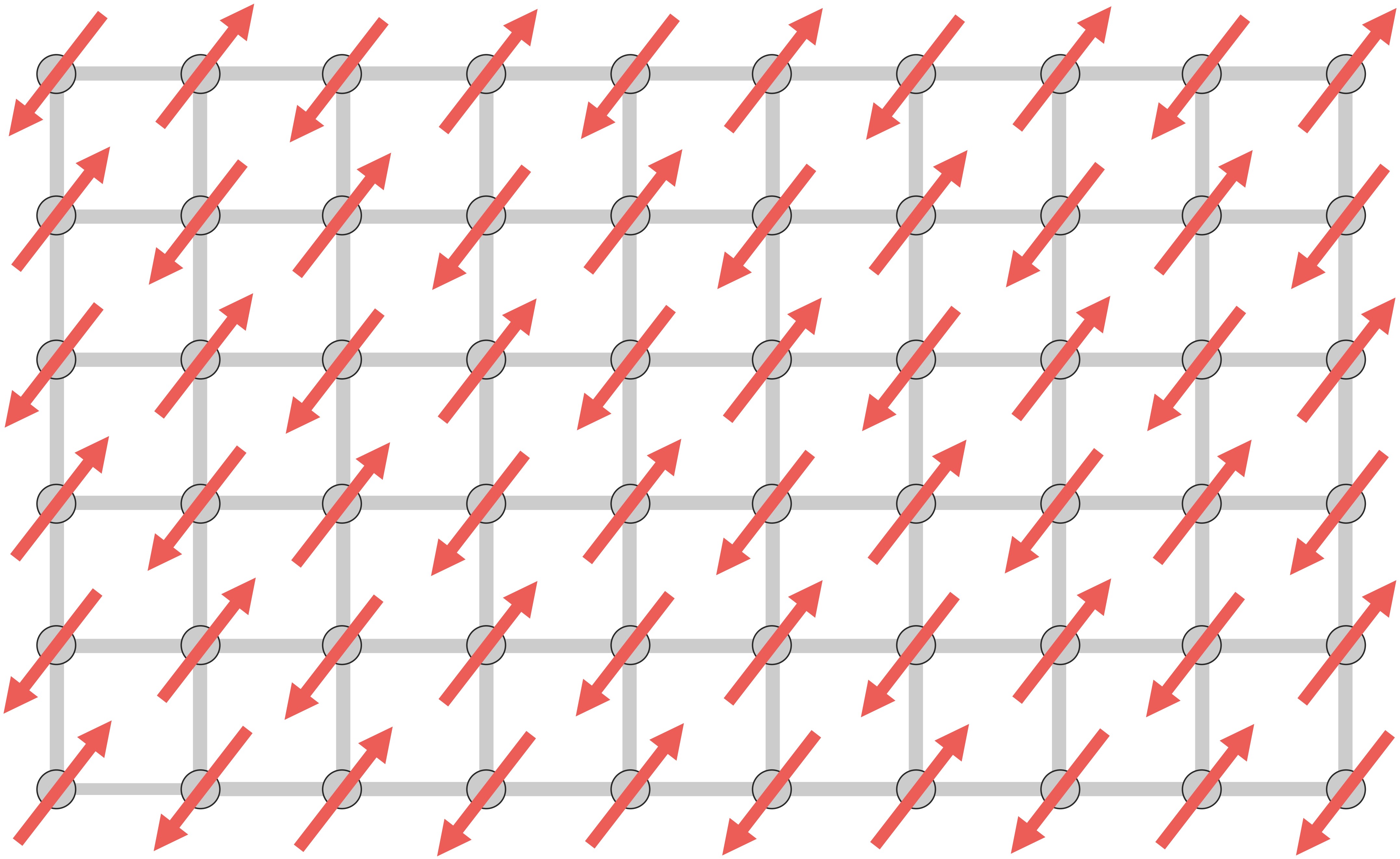
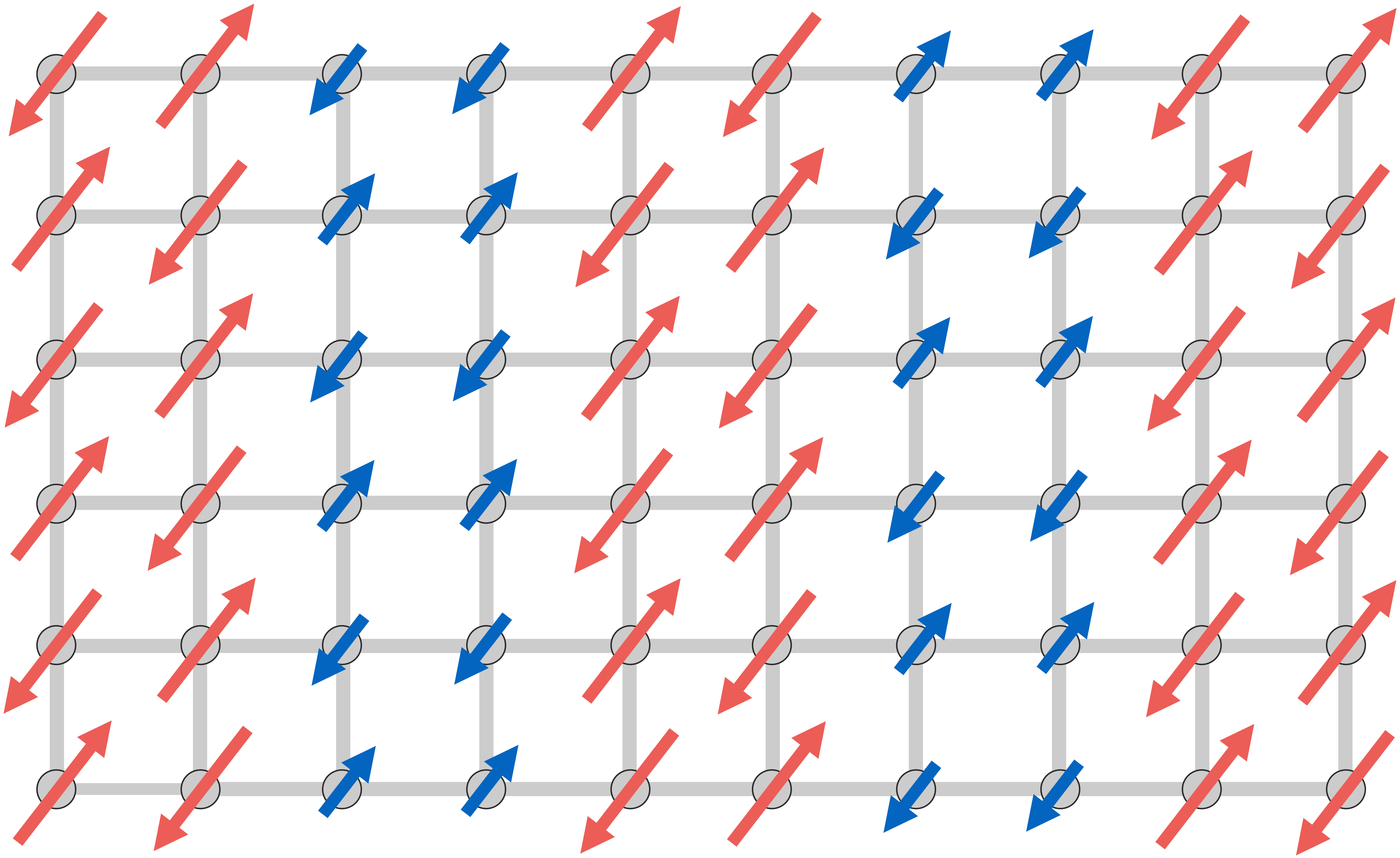
"Stripe" model



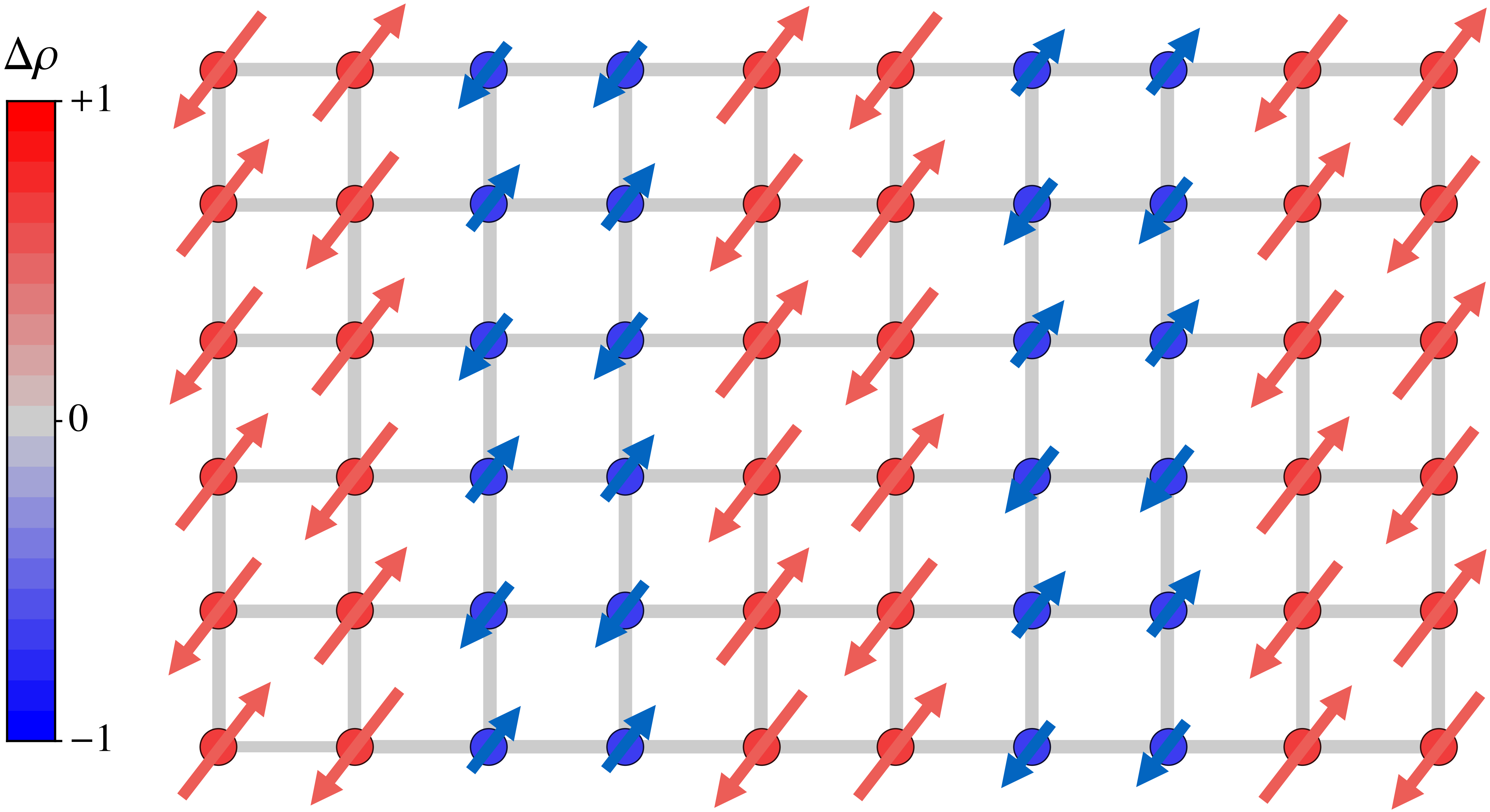
Start with an antiferromagnet

"Stripe" model



Domain walls 4 lattice spacings apart

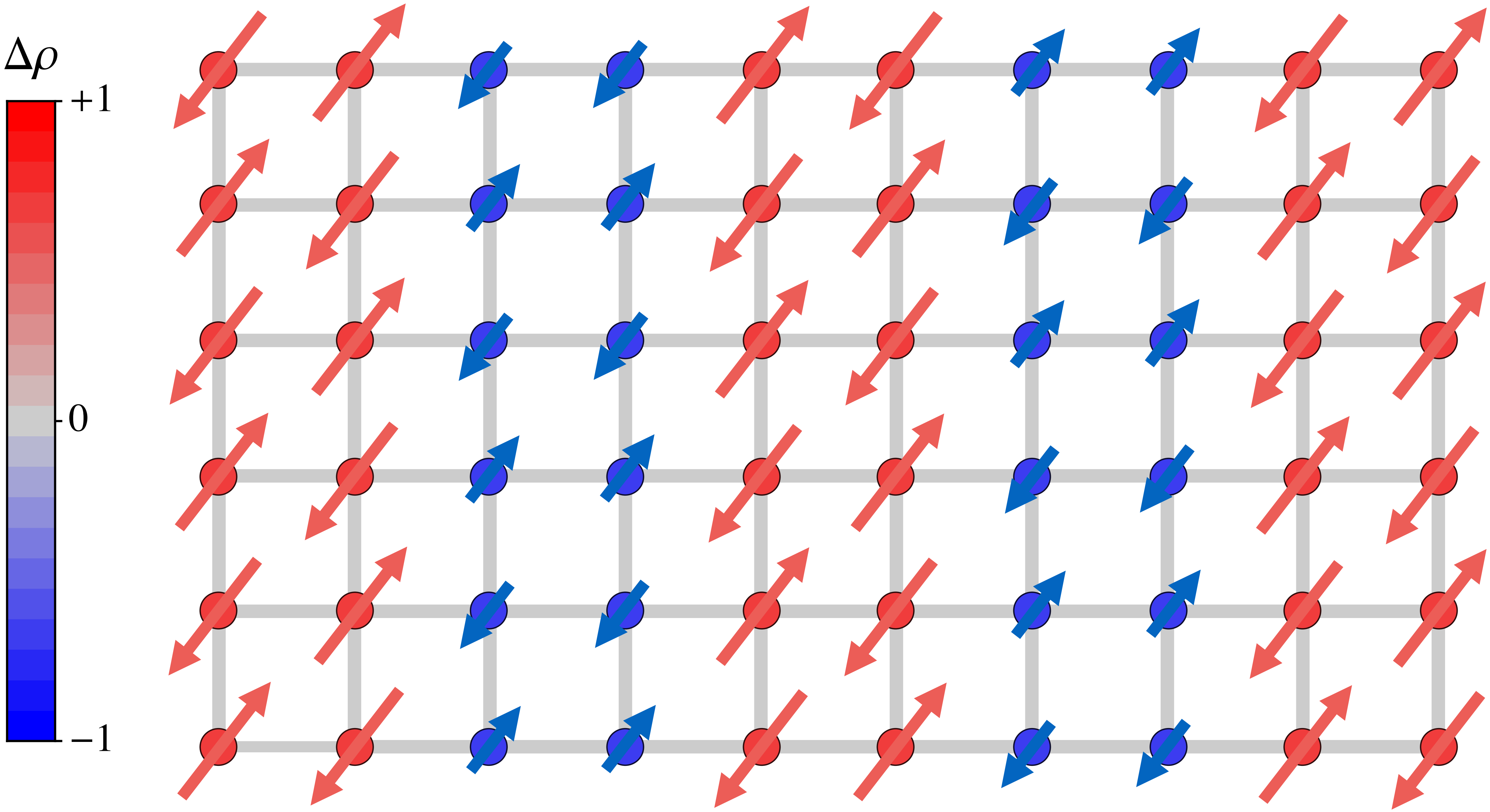
“Stripe” model



Put the holes in the domain walls

Observed in La-based compounds (Tranquada..)

"Stripe" model



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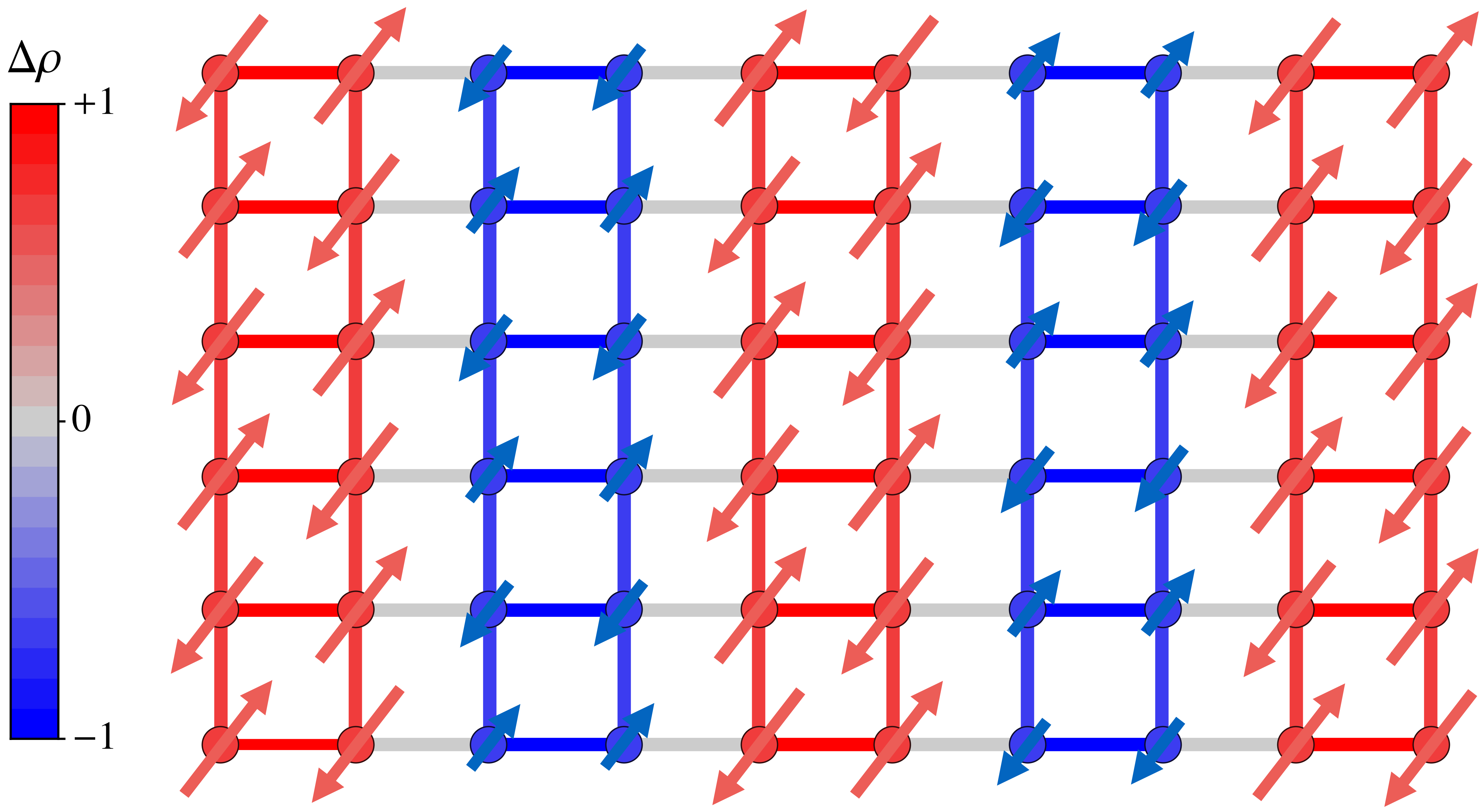
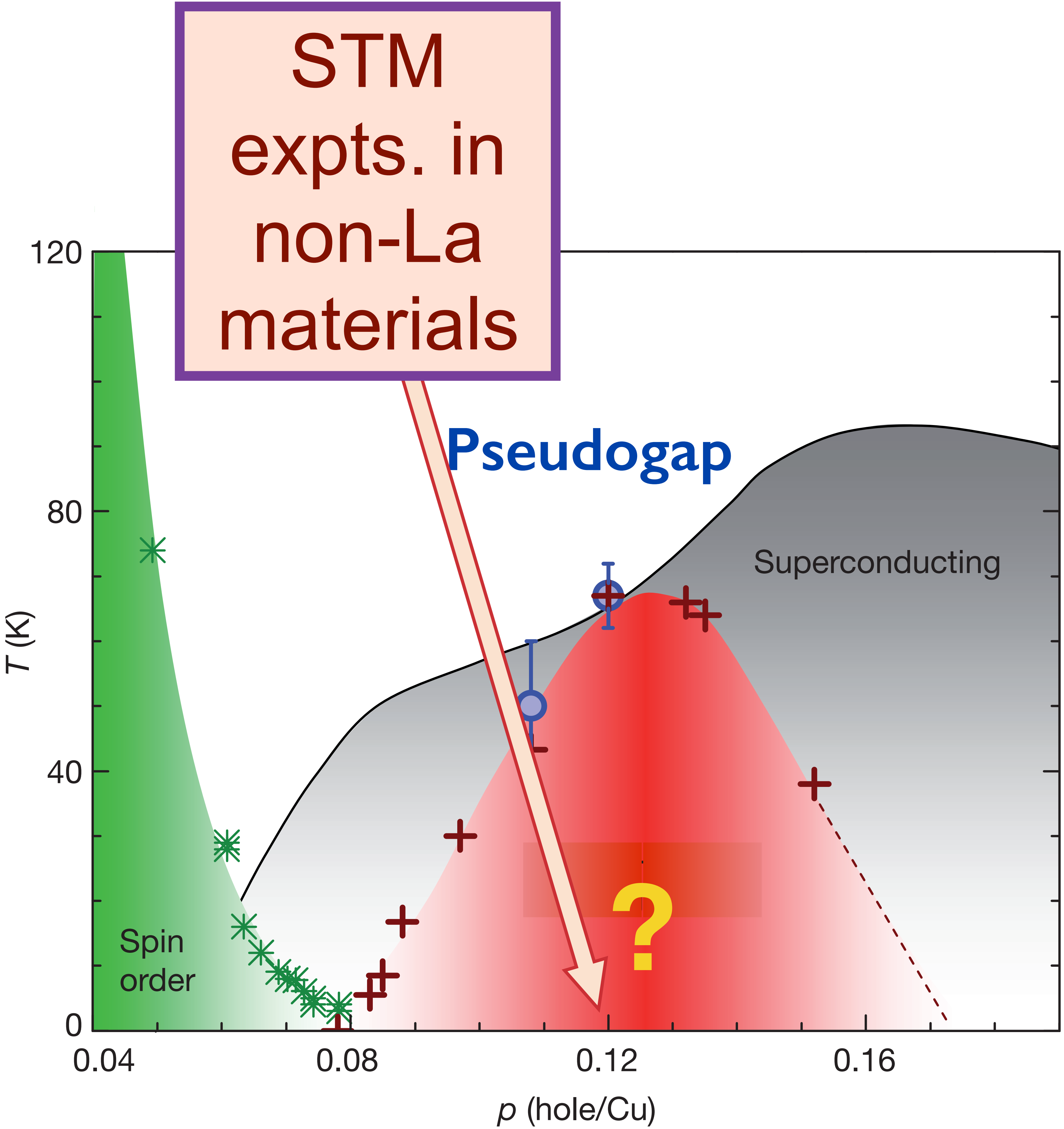
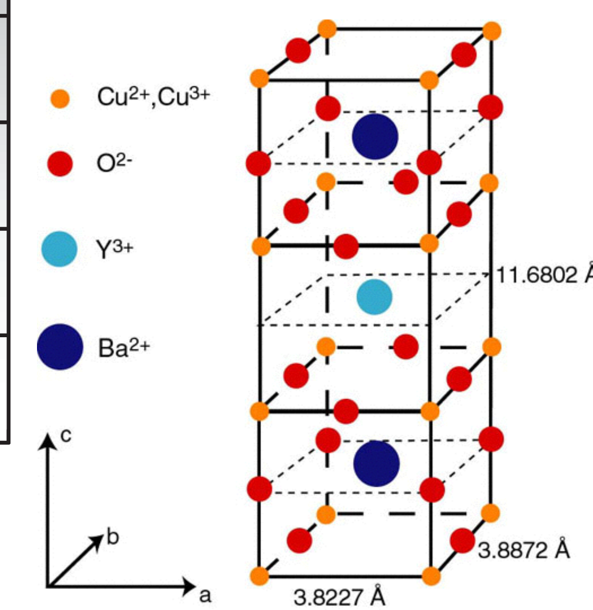


Colors on the bonds map the local exchange energy





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

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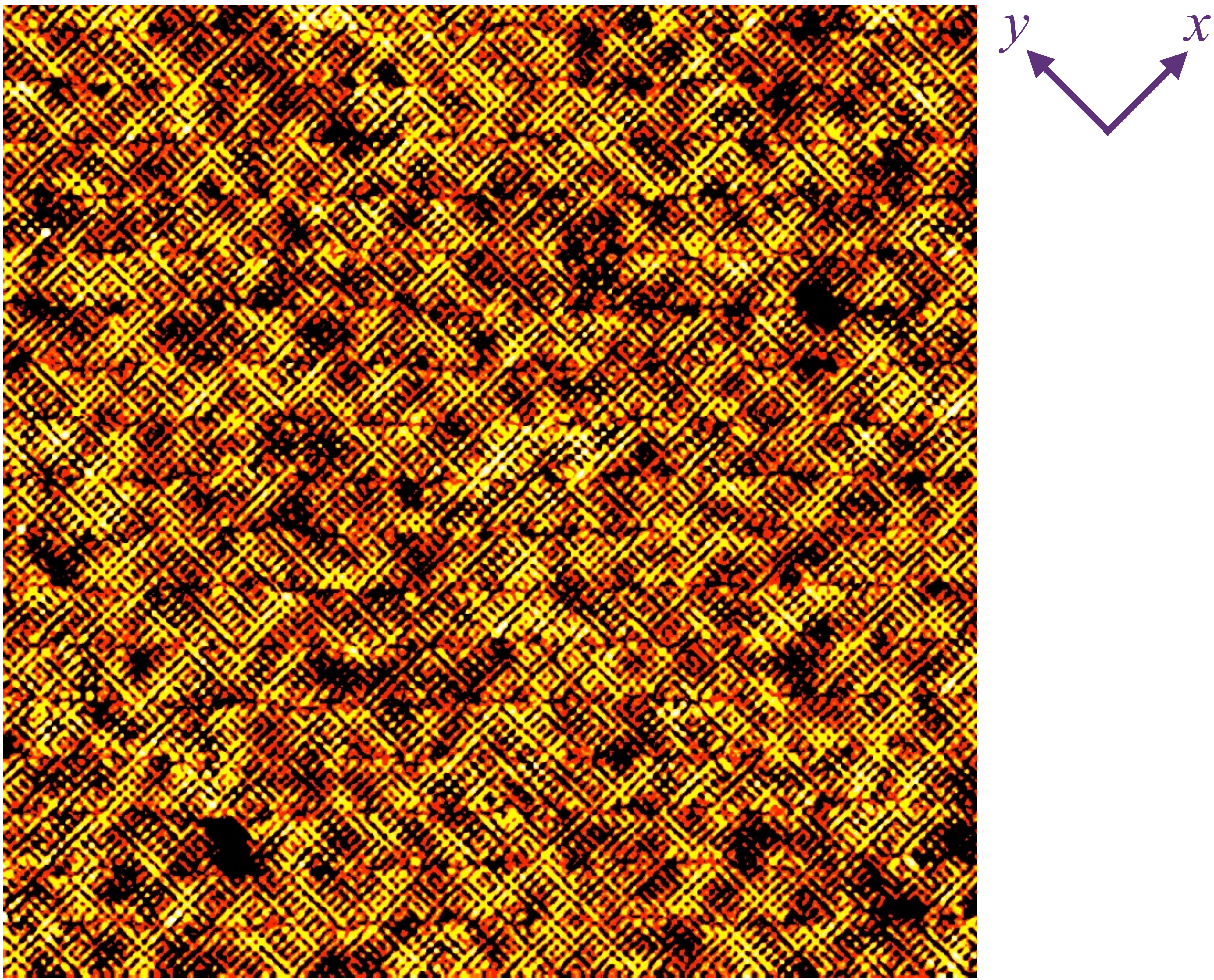

"R-map" of BSCCO in zero magnetic field, similar to those published in Y. Kohsaka, C. Taylor, K. Fujita, A. Schmidt, C. Lupien, T. Hanaguri, M. Azuma, M. Takano, H. Eisaki, H. Takagi, S. Uchida, and J. C. Davis, *Science* **315**, 1380 (2007). Davis group has sub-angstrom resolution capabilities, with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

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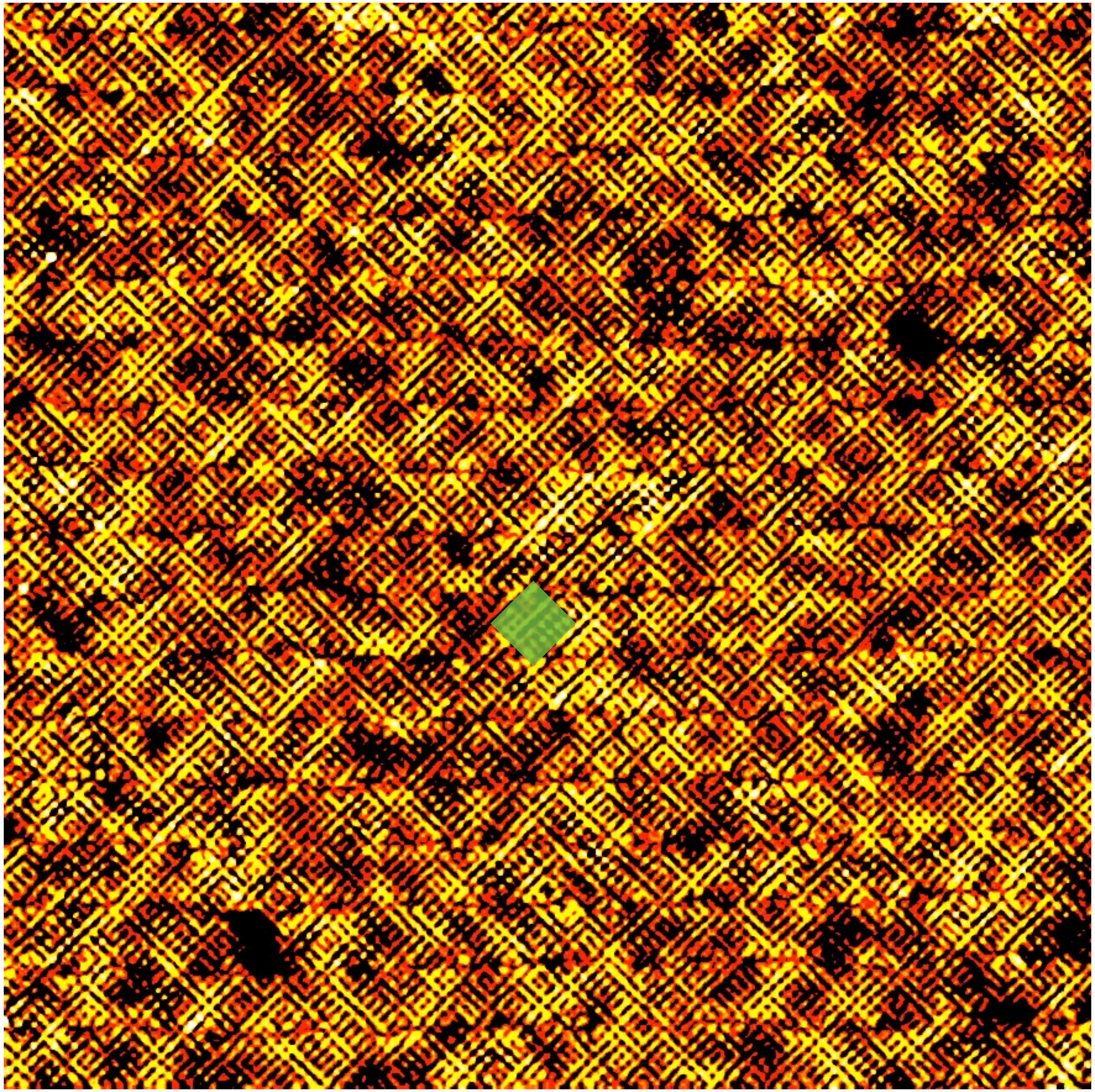

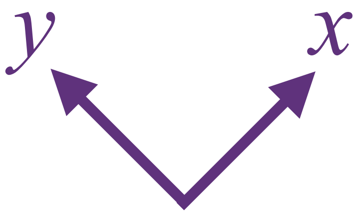

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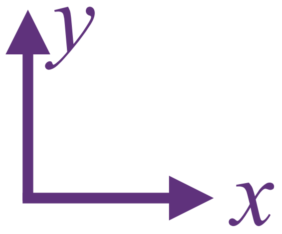

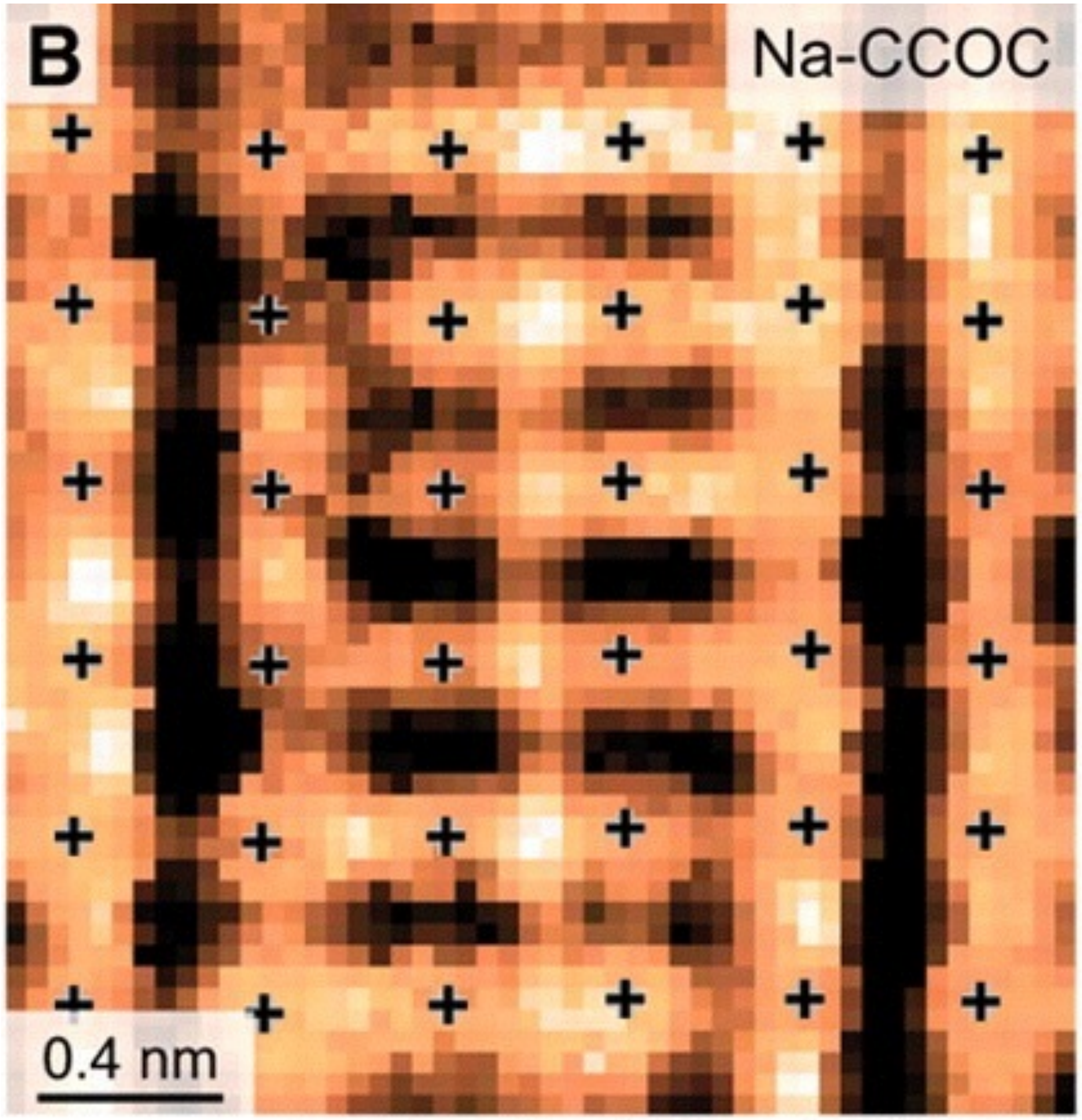

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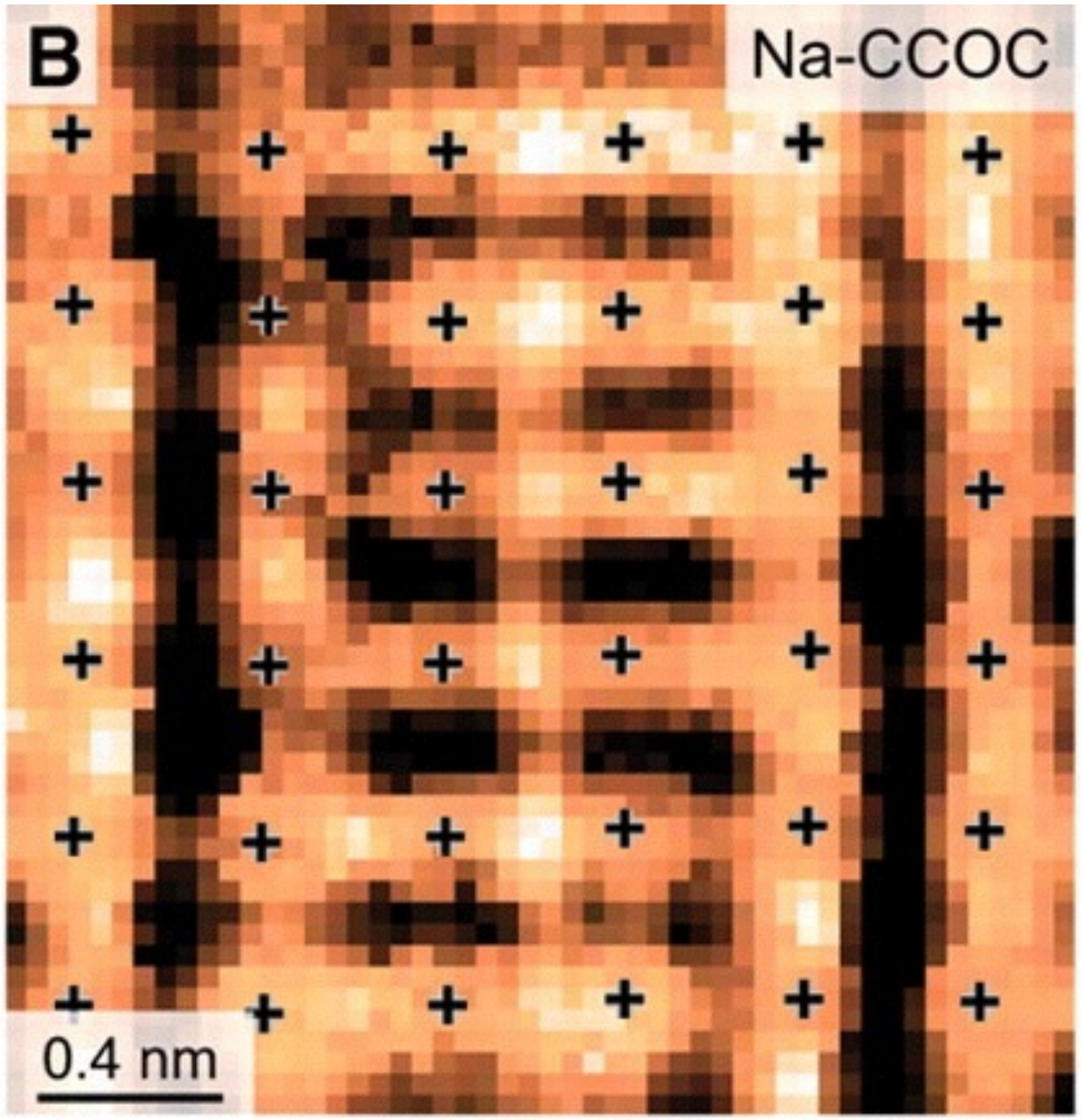

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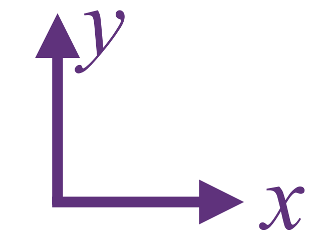
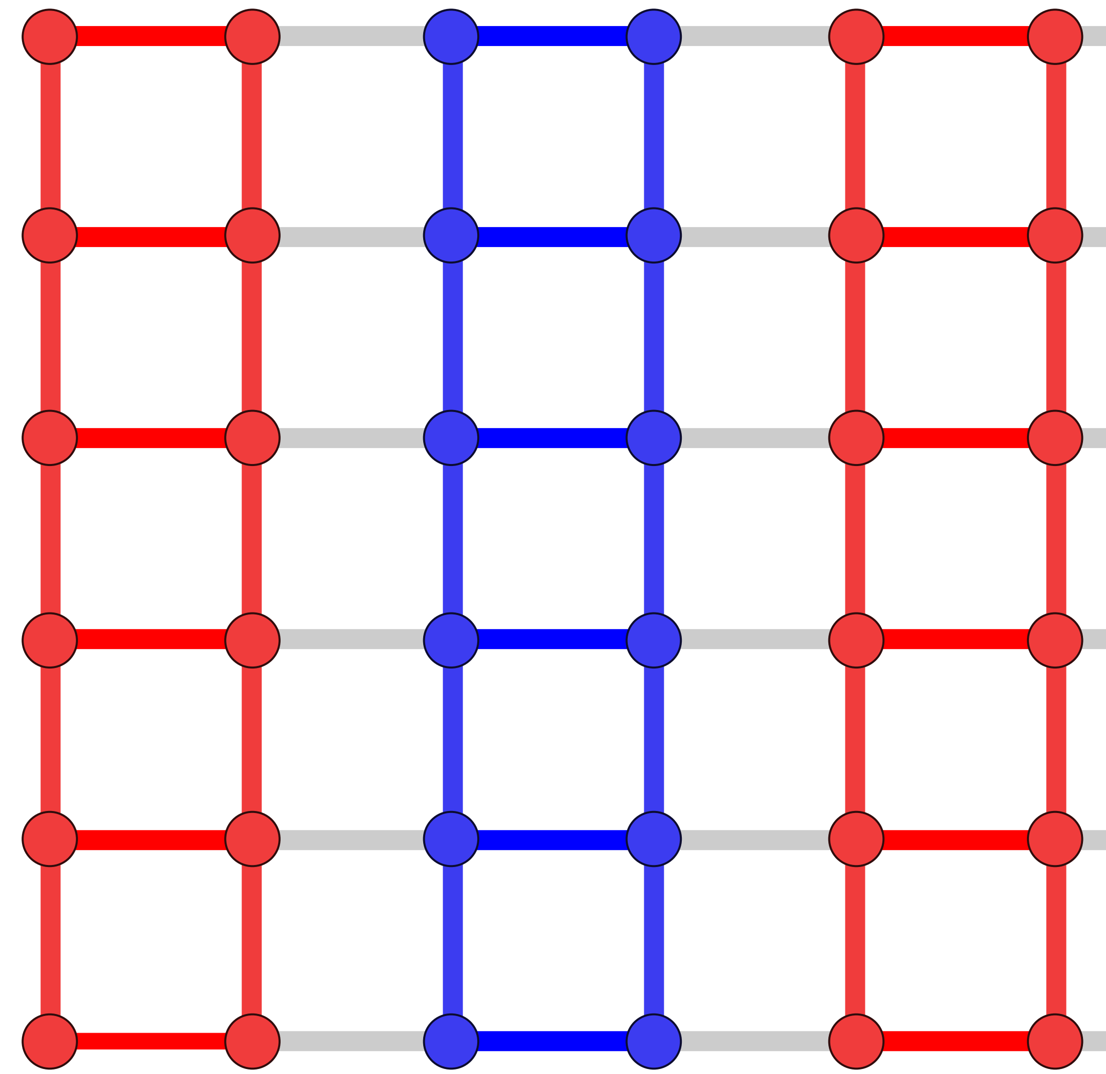
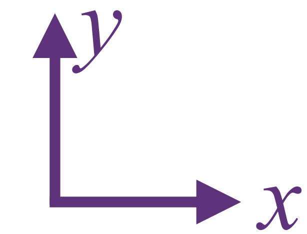
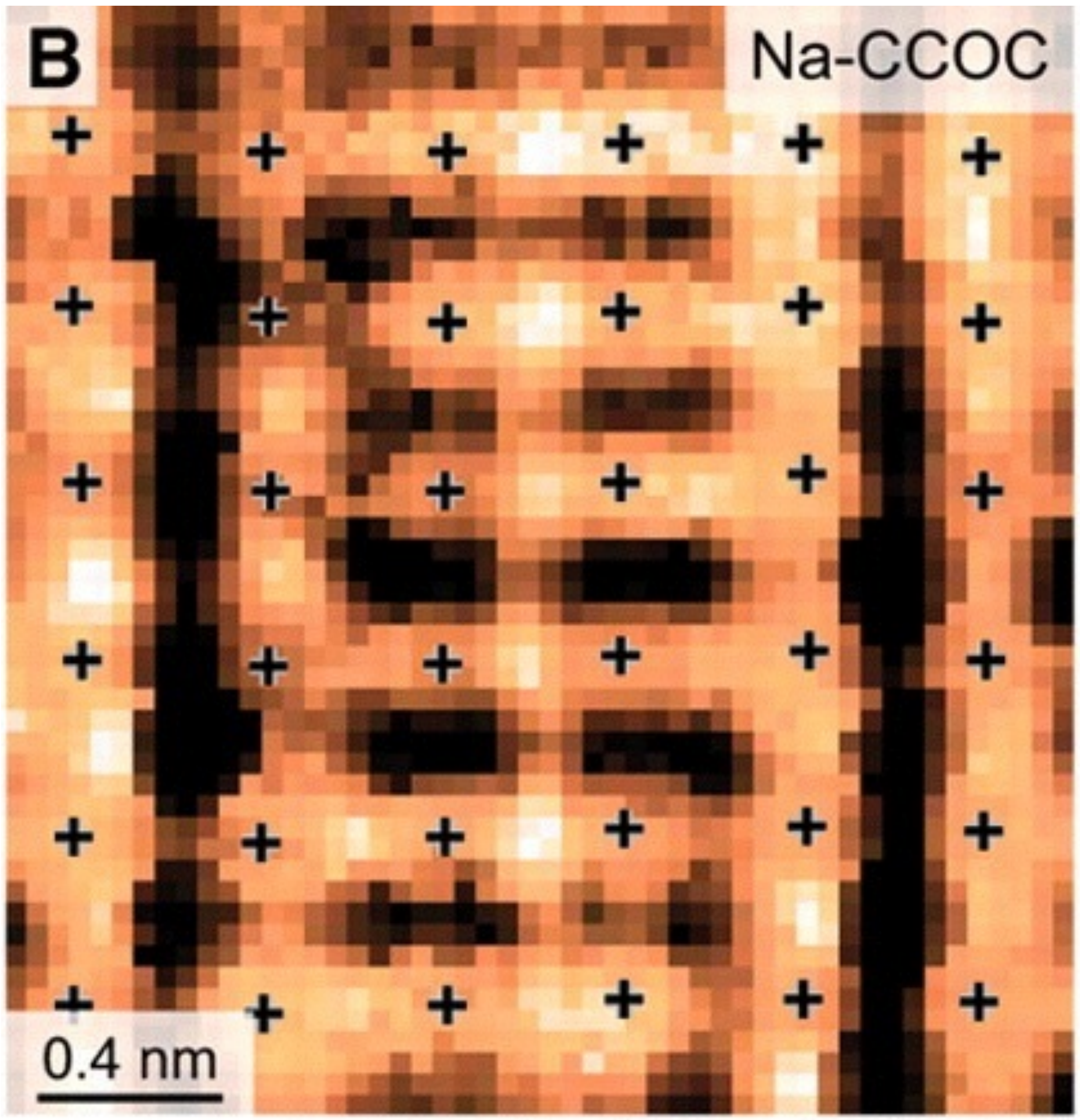




“Stripe” model





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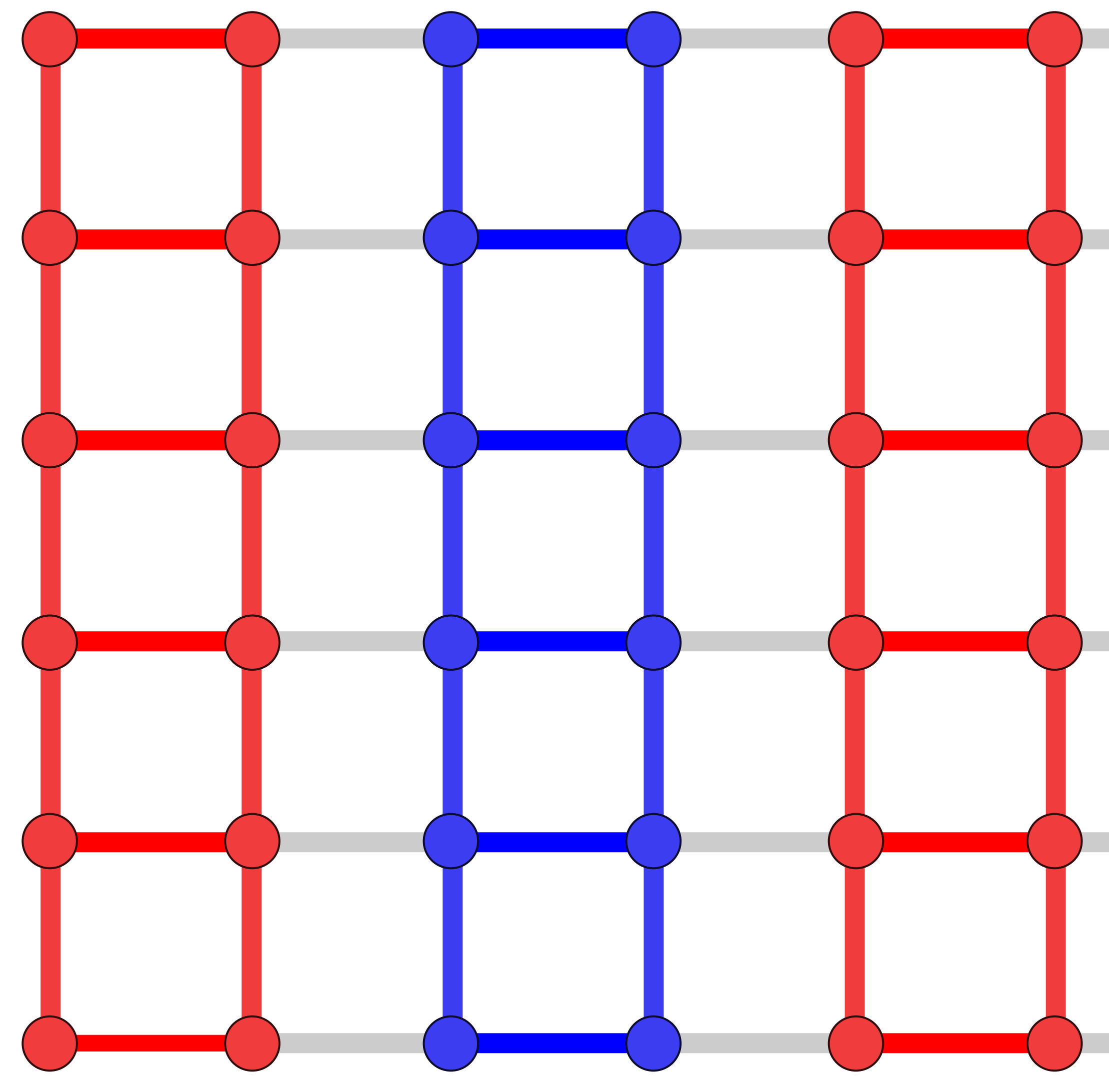

“Stripe” model

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

Charge density wave (CDW) order

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

Nearly constant CDW order parameter

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

$$\left\langle c_\alpha^\dagger(\mathbf{r}_1) c_\alpha(\mathbf{r}_2) \right\rangle$$

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

Nearly constant CDW order parameter

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

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

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

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

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

$$\langle c^\dagger_\alpha(\mathbf{r}_1) c_\alpha(\mathbf{r}_2) \rangle$$

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

Density wave **form factor** (internal particle-hole pair wavefunction)

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

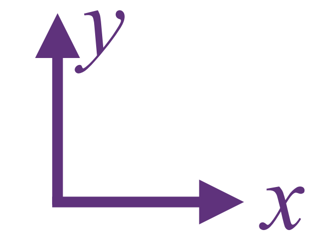
Time-reversal symmetry requires $\mathcal{P}(\mathbf{k}) = \mathcal{P}(-\mathbf{k})$.

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

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

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

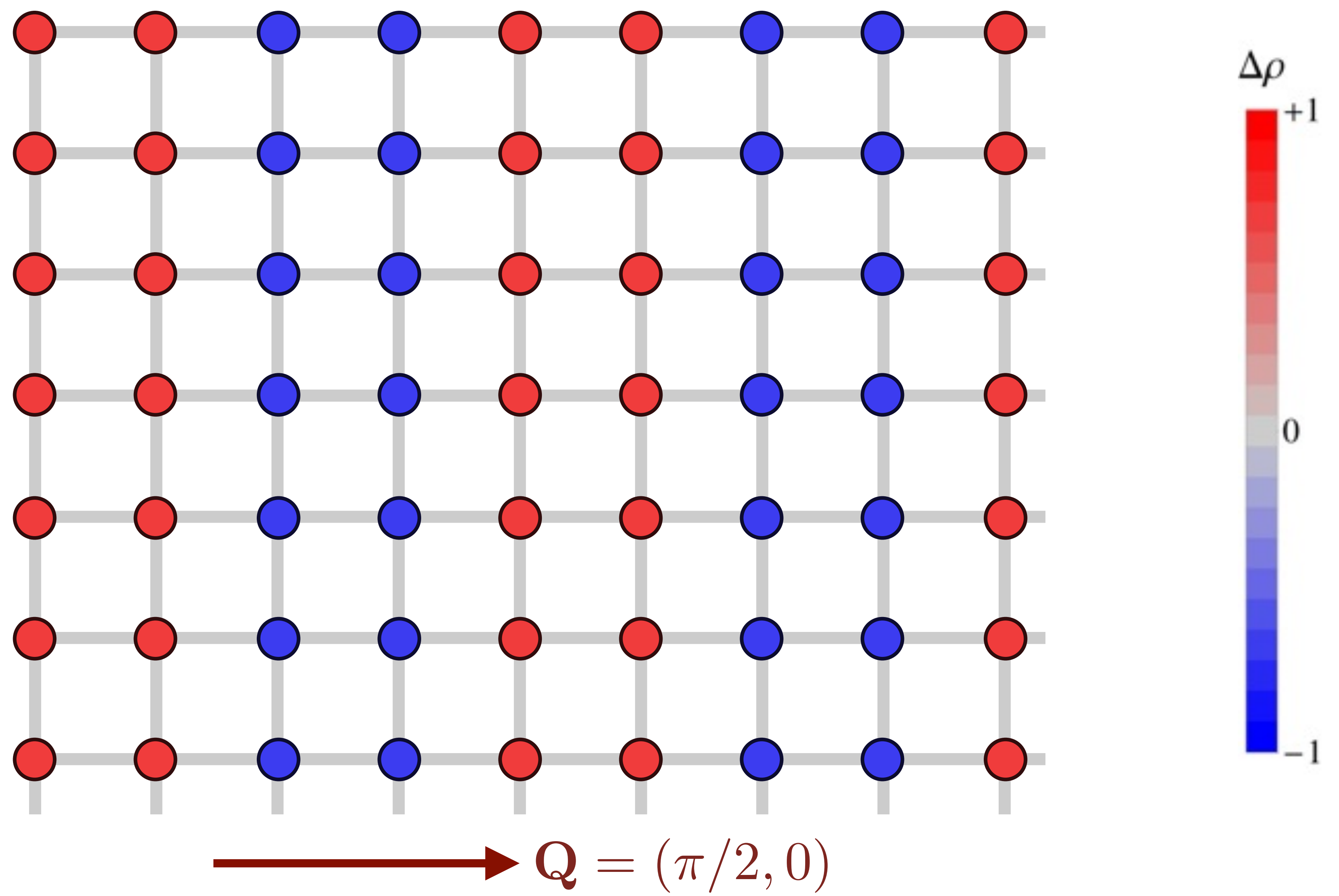
Conventional CDW order: s-form factor



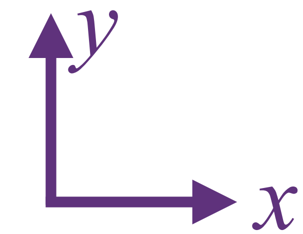
Plot of $P_{ij} = \left\langle c_{i\alpha}^{\dagger} c_{j\alpha} \right\rangle$ for $i = j$, and i, j nearest neighbors.

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

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



Unconventional DW order: s'-form factor



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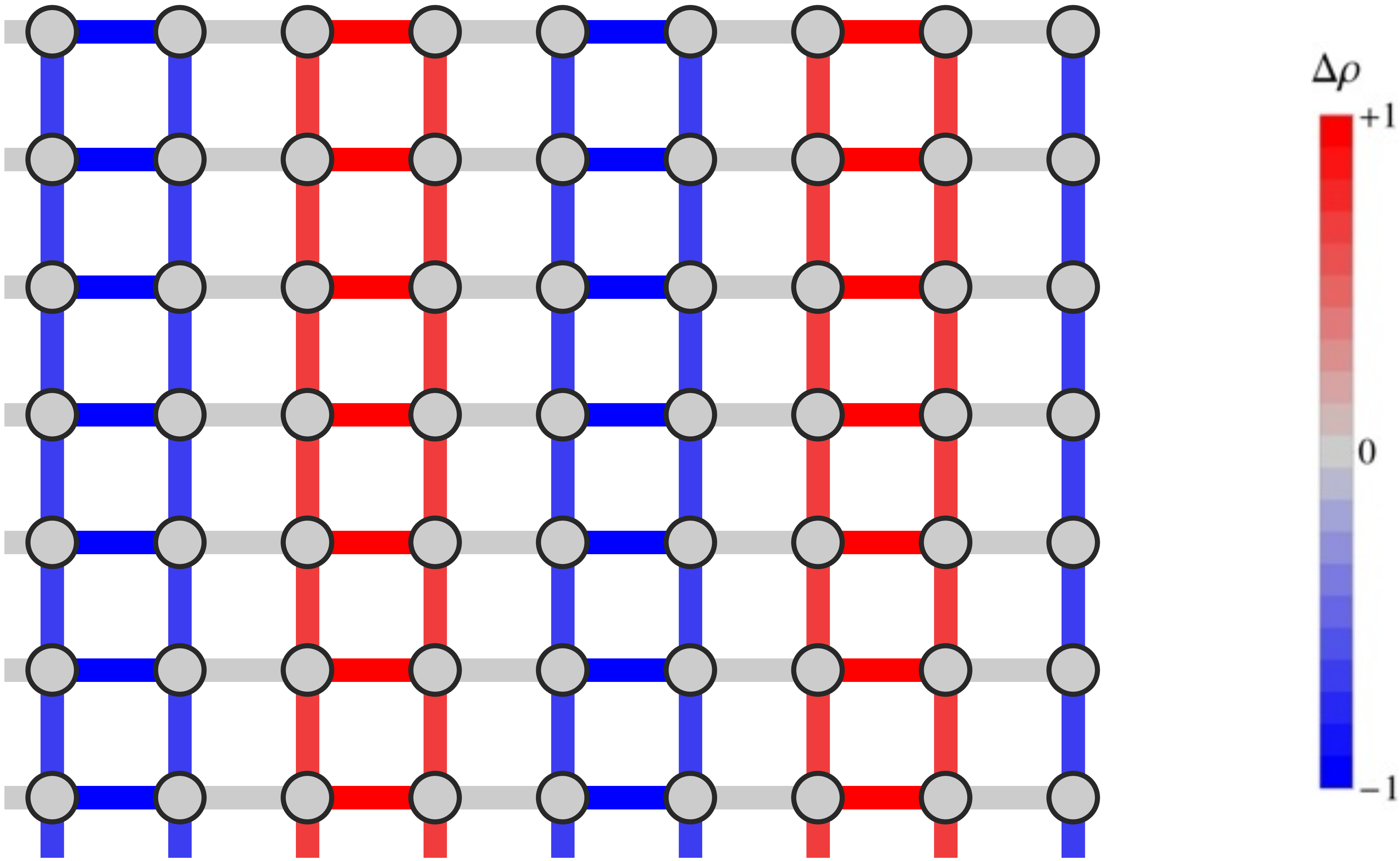
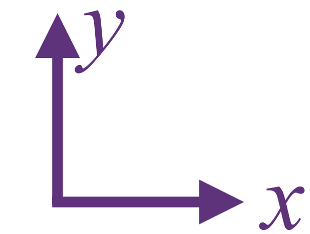
$$\mathcal{P}(\mathbf{k}) = e^{i\phi} \left[\cos(k_x) + \cos(k_y)\right] \quad \text{and} \quad \mathbf{Q} = 2\pi(1/4, 0)$$



$\mathbf{Q} = (\pi/2, 0)$

Unconventional DW order: s'-form factor



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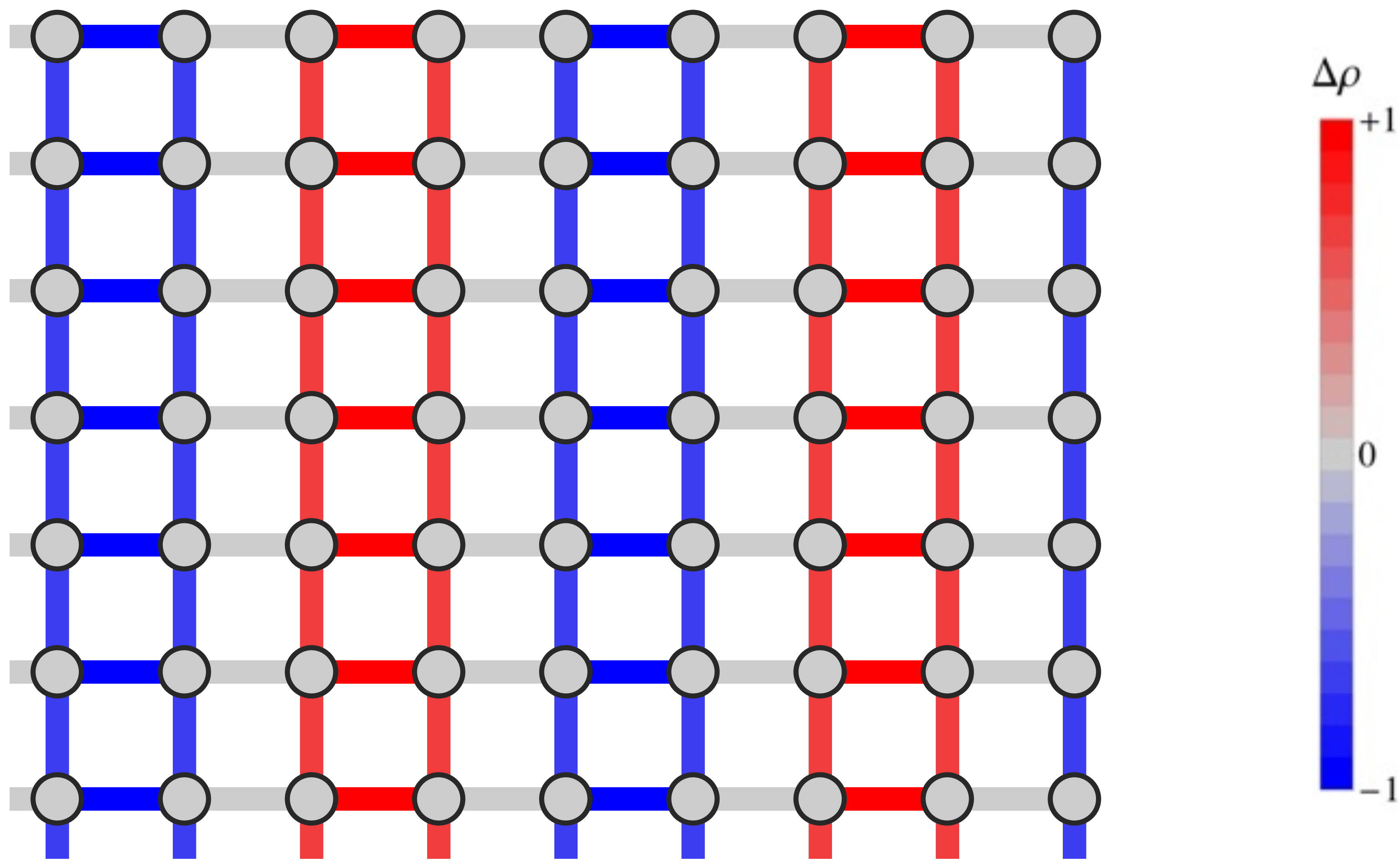
"Stripe" model !



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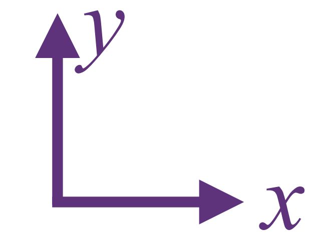
M. H. Fischer, Si Wu, M. Lawler, A. Paramekanti, and Eun-Ah Kim, arXiv:1406.2711

Unconventional DW order: s'-form factor



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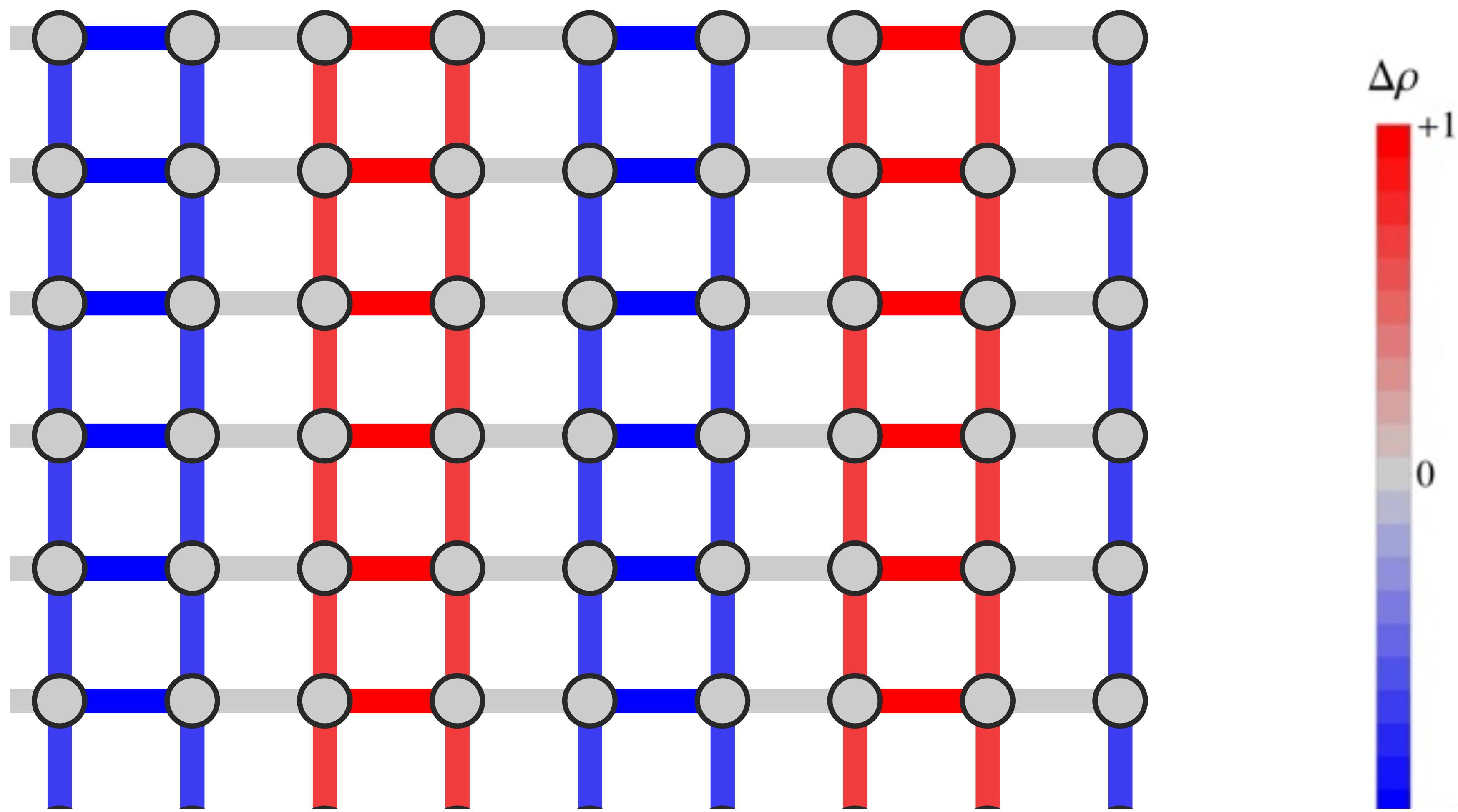
"Stripe" model !

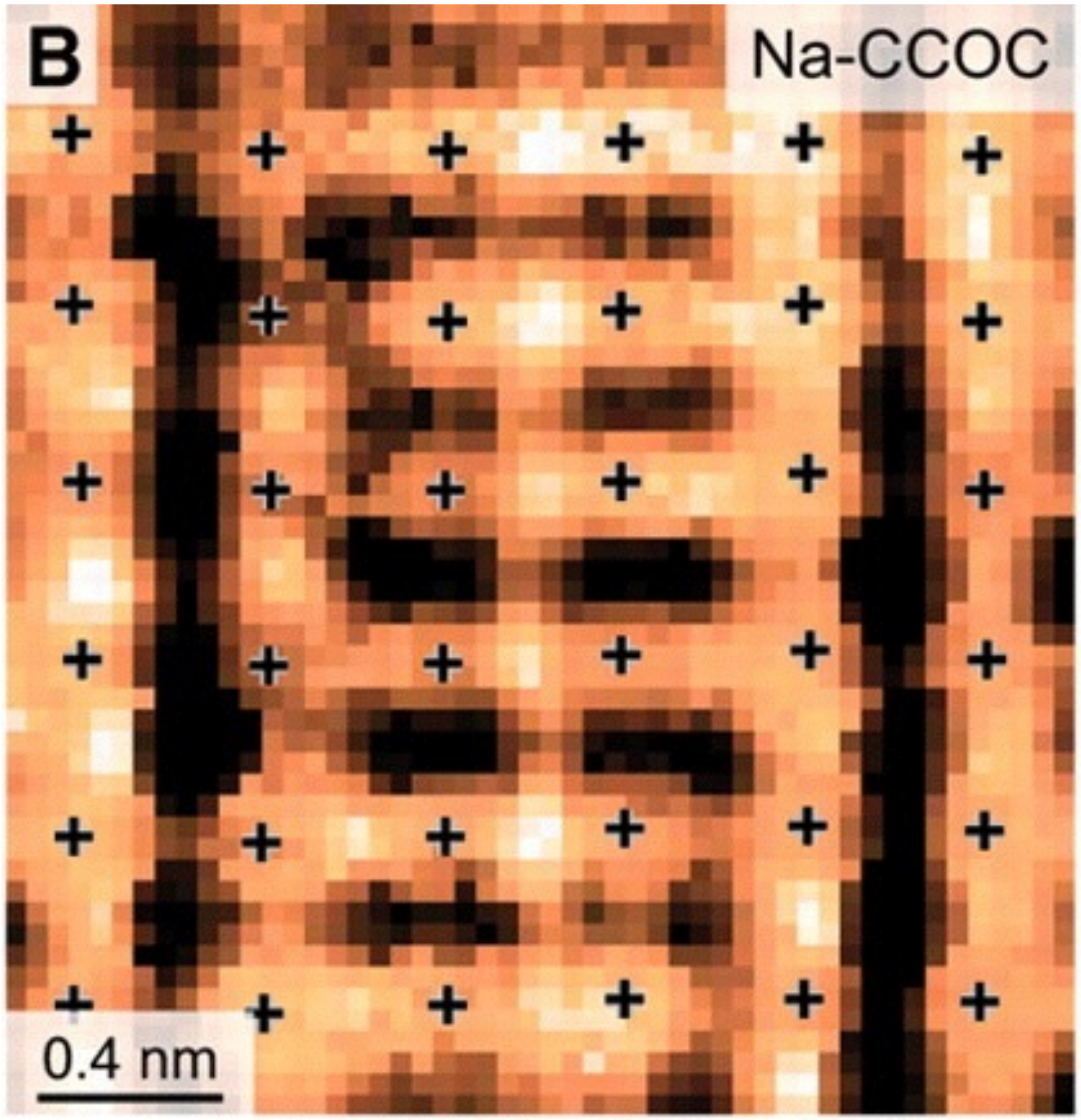
X-ray observations indicate strong s' component in LBCO



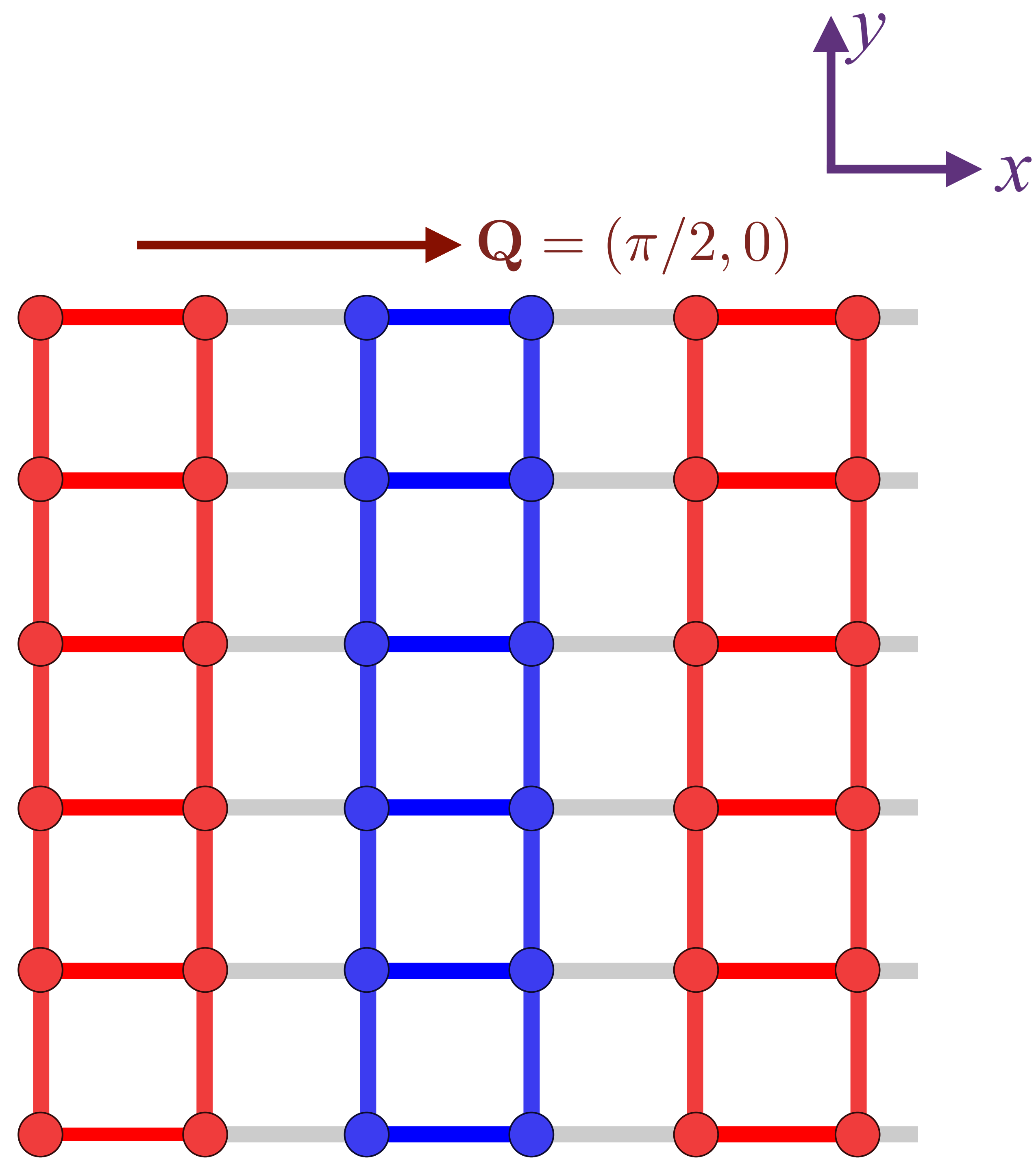
Orbital symmetry of charge density wave order in $La_{1.88}Ba_{0.12}CuO_4$ and $YBa_2Cu_3O_{6.67}$

A. J. Achkar,[1] F. He,[2] R. Sutarto,[2] Christopher McMahon,[1] M. Zwiebler,[3] M. Hücker,[4] G. Gu,[4] Ruixing Liang,[5] D. A. Bonn,[5] W. N. Hardy,[5] J. Geck,[3] and D. G. Hawthorn[1]

M. H. Fischer, Si Wu, M. Lawler, A. Paramekanti, and Eun-Ah Kim, arXiv:1406.2711



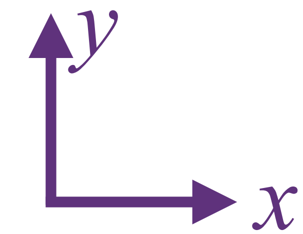
Y. Kohsaka *et al.*, SCIENCE **315**, 1380 (2007)



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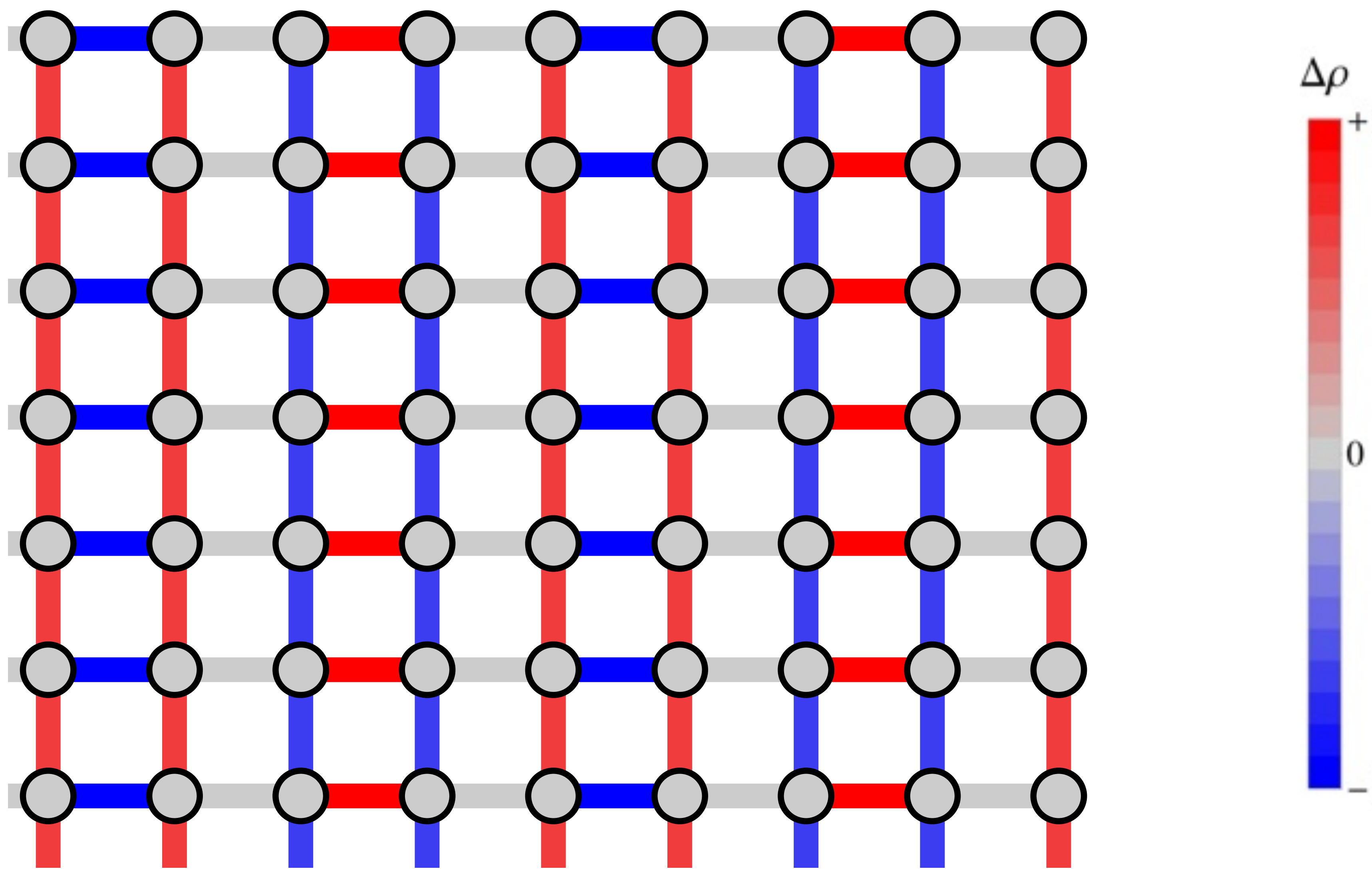
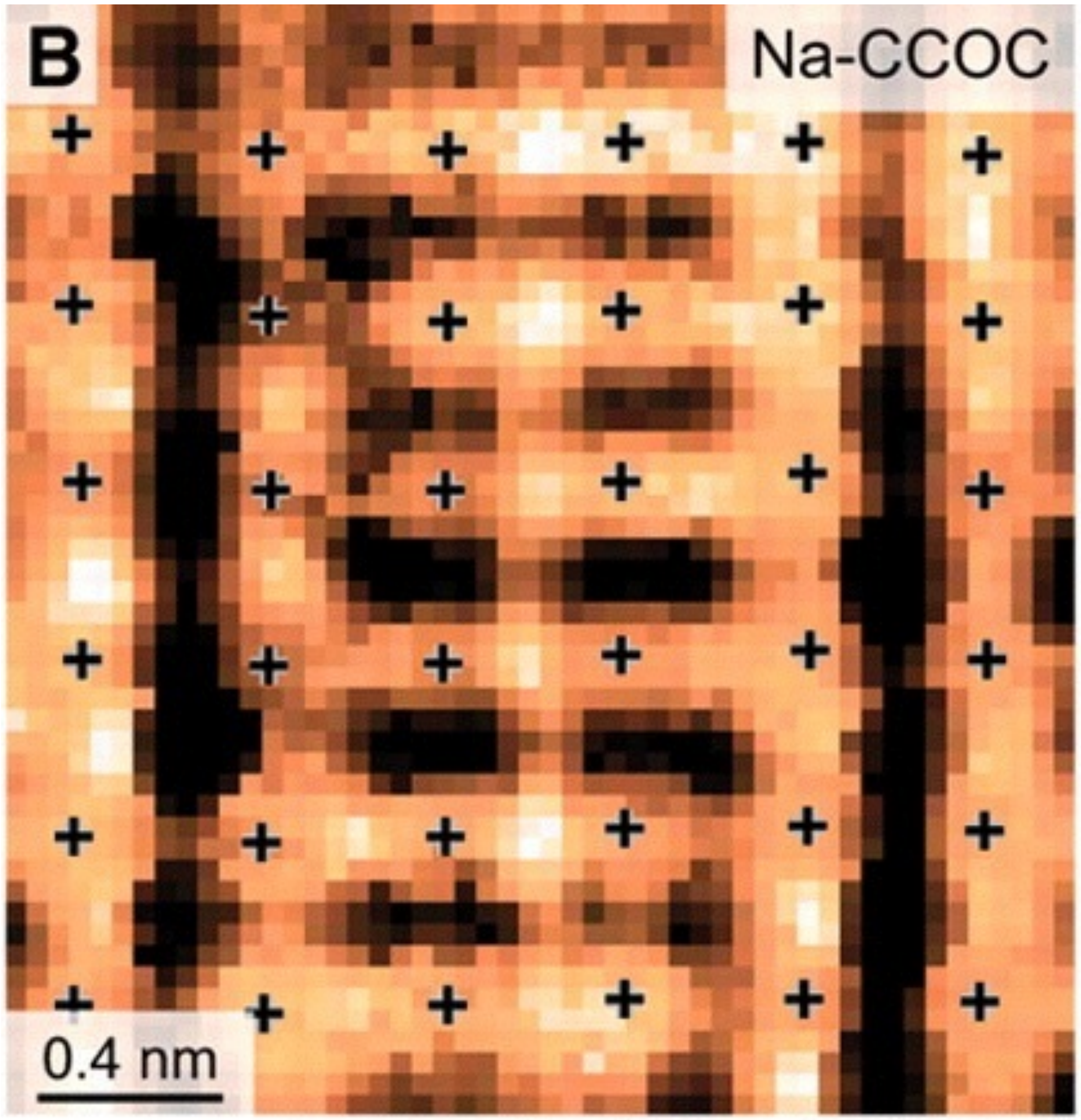
Density wave on horizontal bonds has a phase-shift of π relative to the wave on vertical bonds



$\mathbf{Q} = (\pi/2, 0)$

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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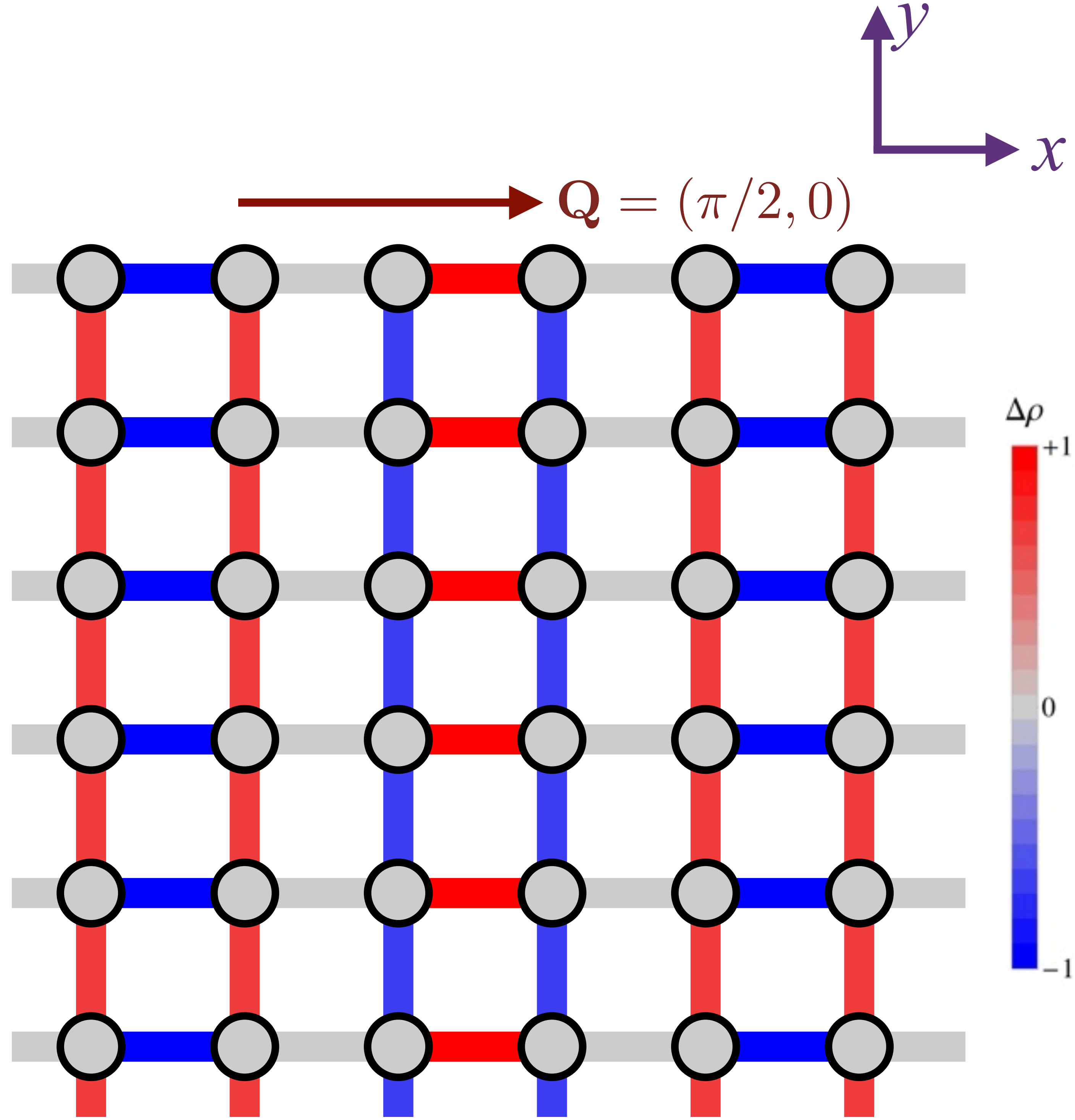

d-form factor density wave order

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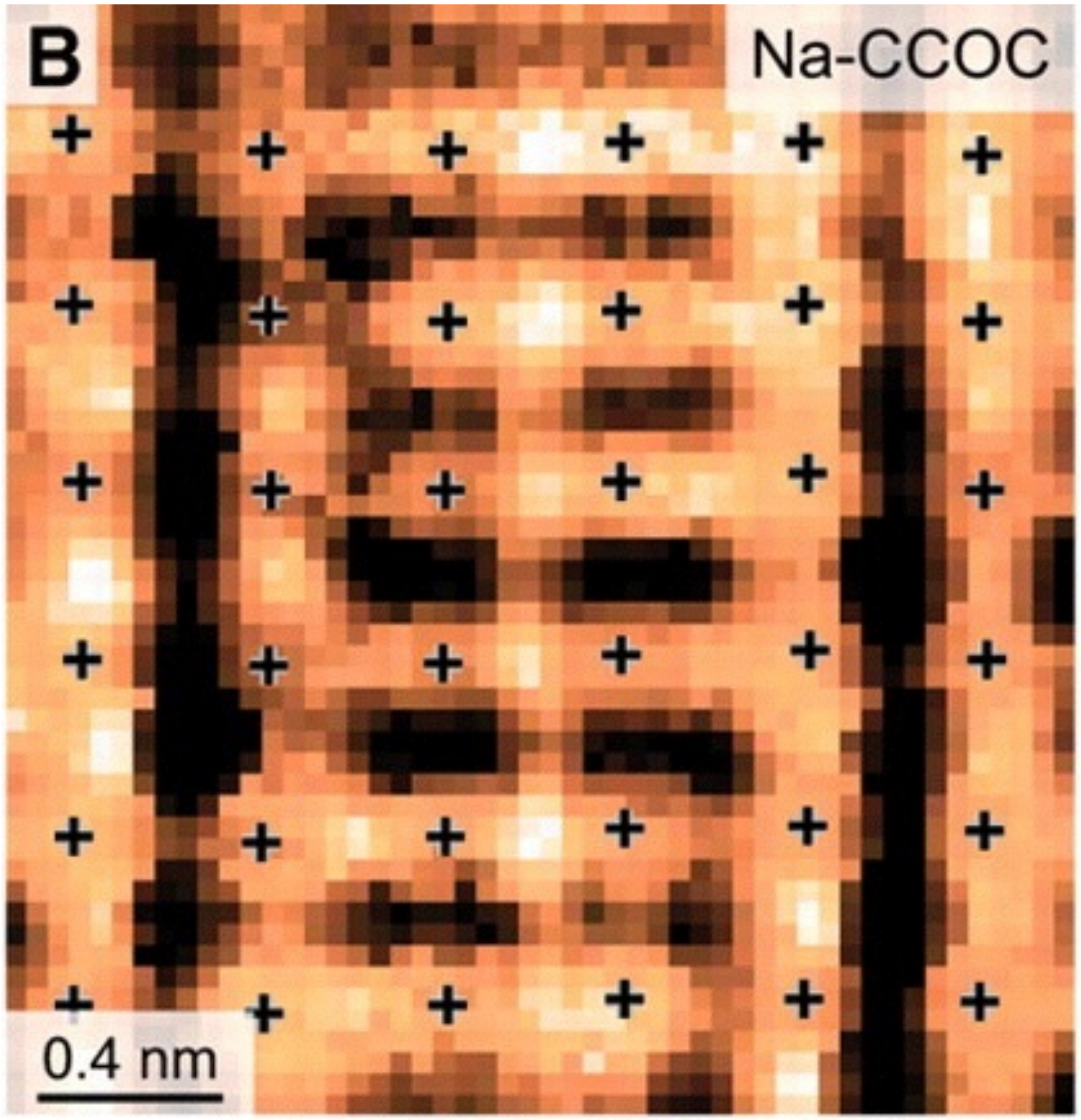

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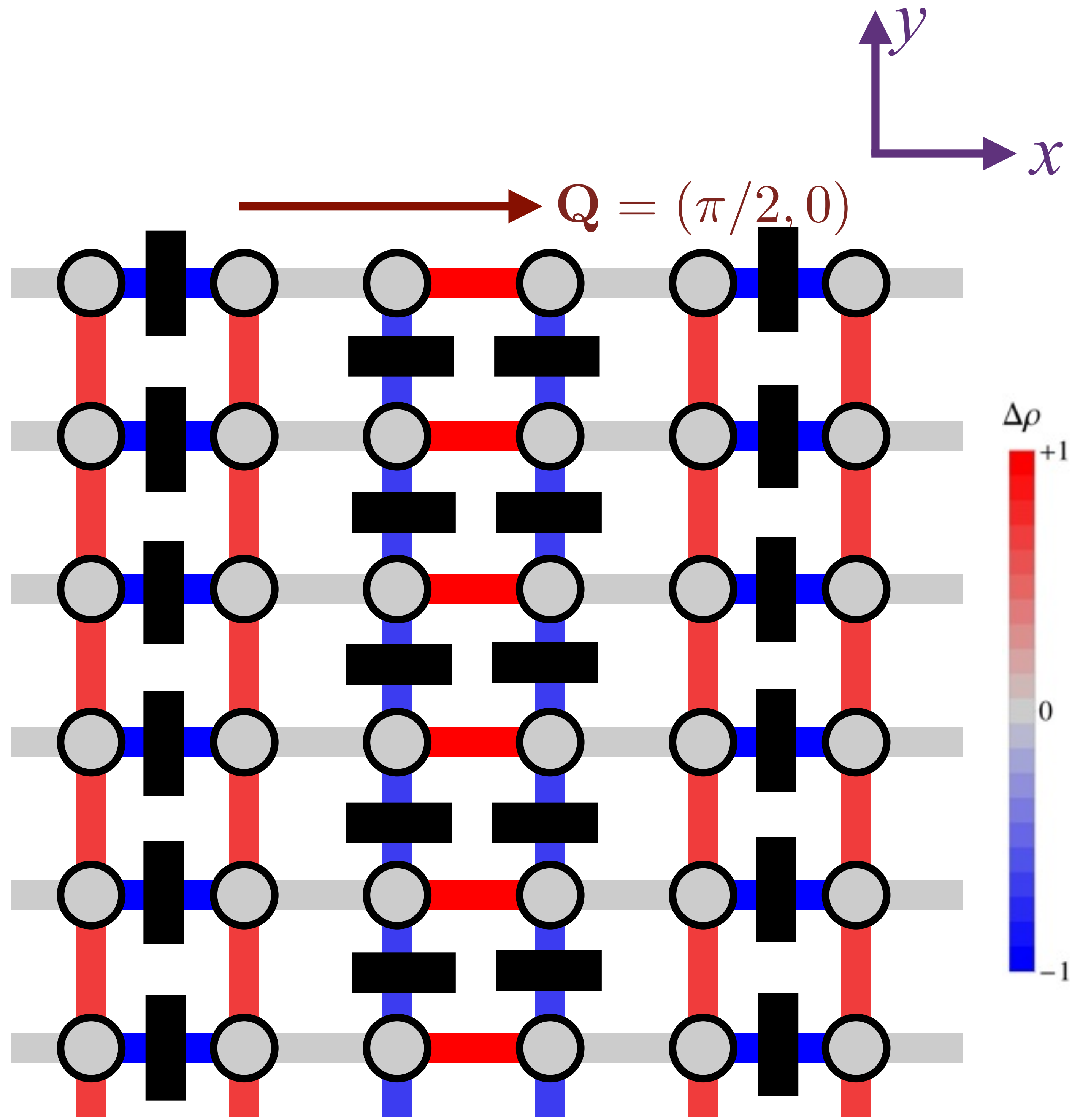

d-form factor density wave order

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

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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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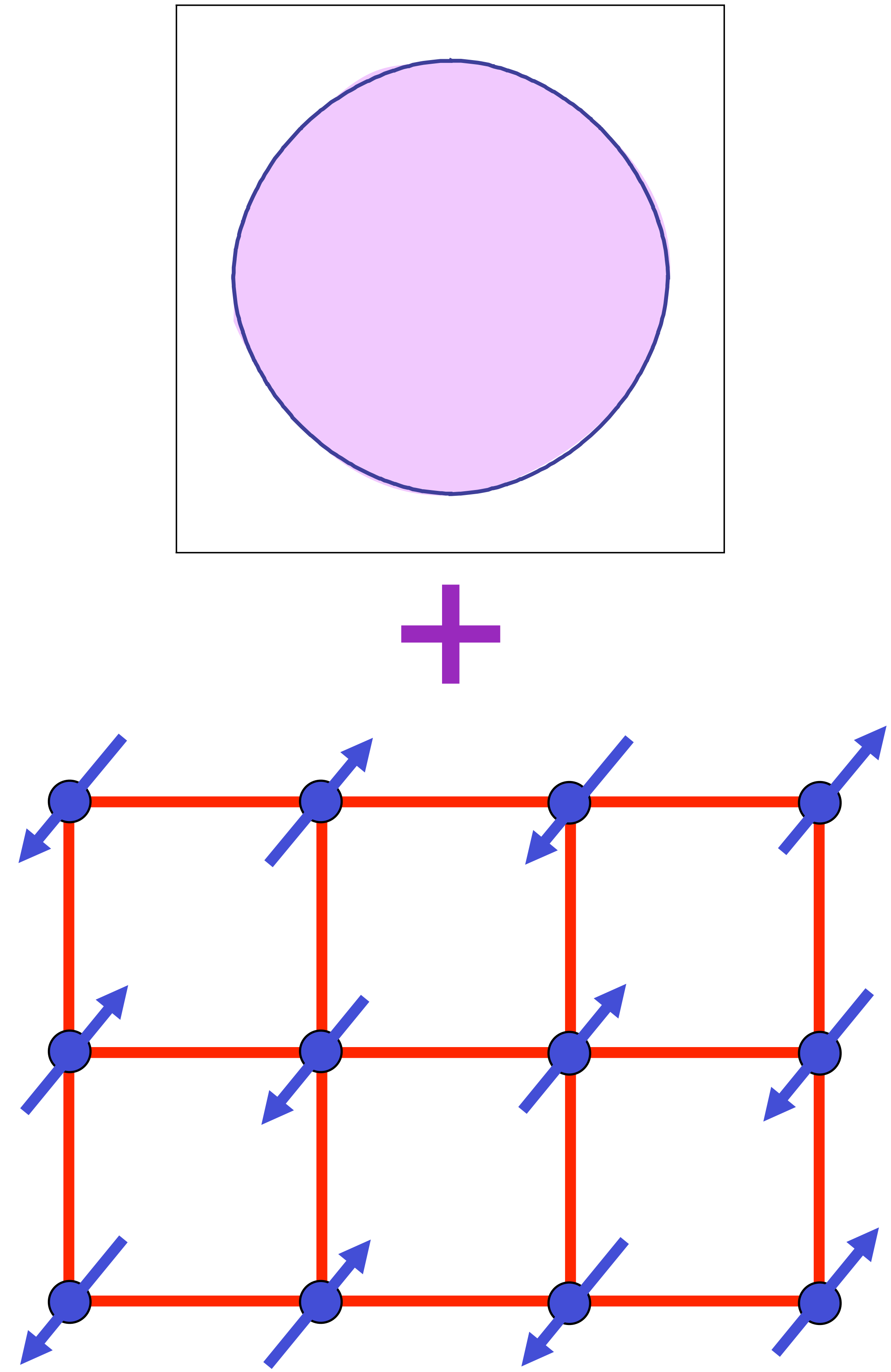
Fermi surface+antiferromagnetism

Metal with "large"
Fermi surface



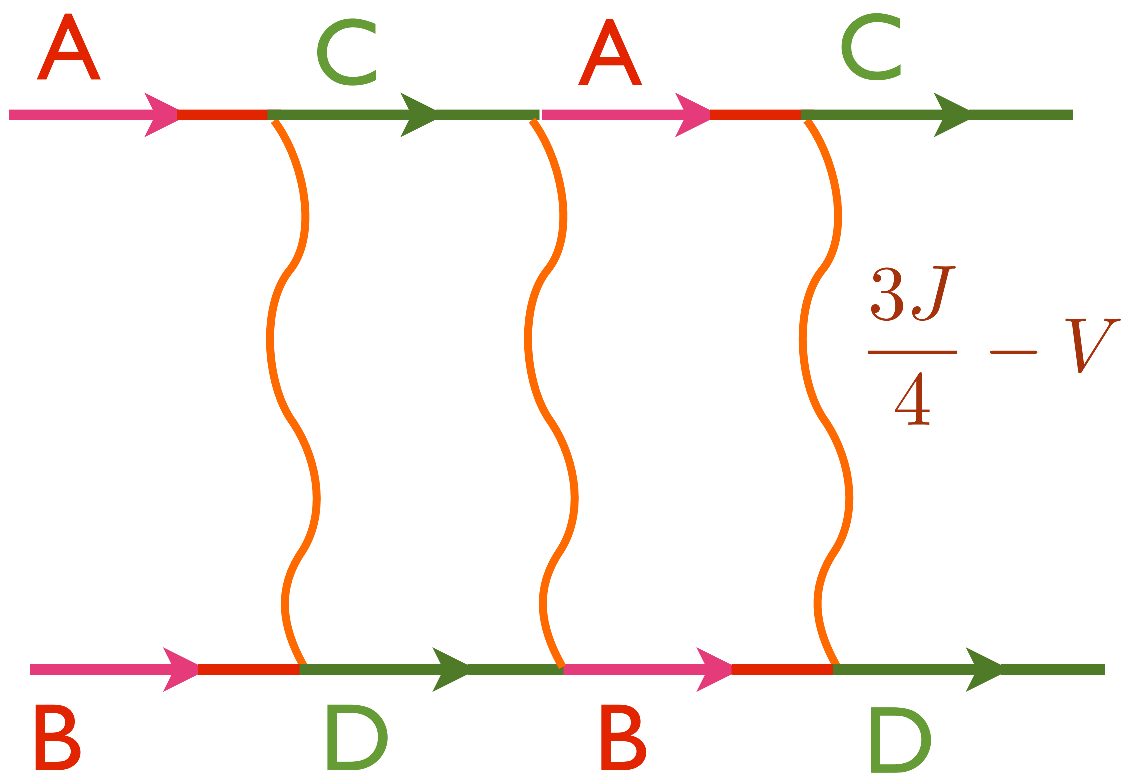
The electron spin polarization obeys

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

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

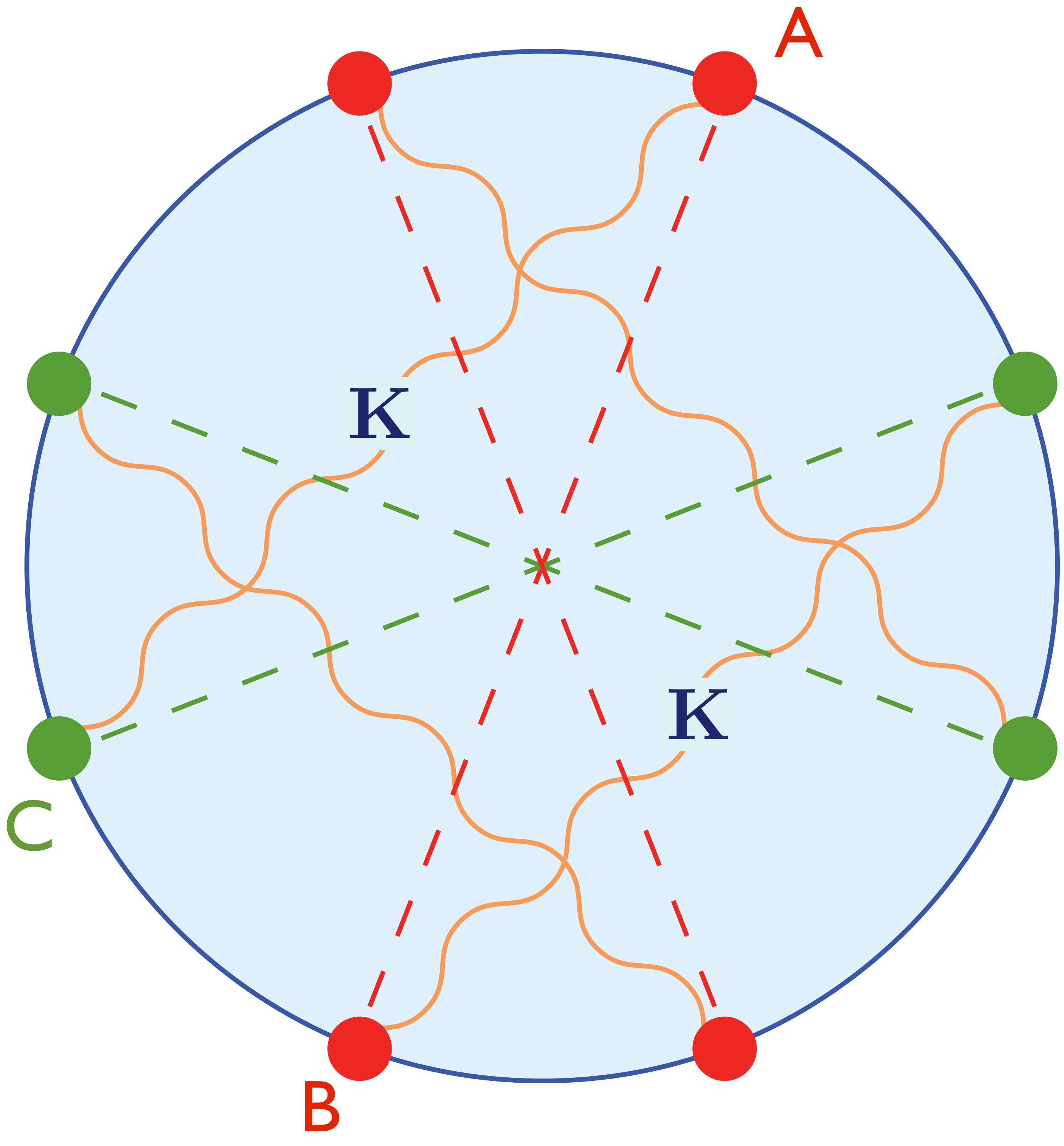
Pairing "glue" from antiferromagnetic fluctuations

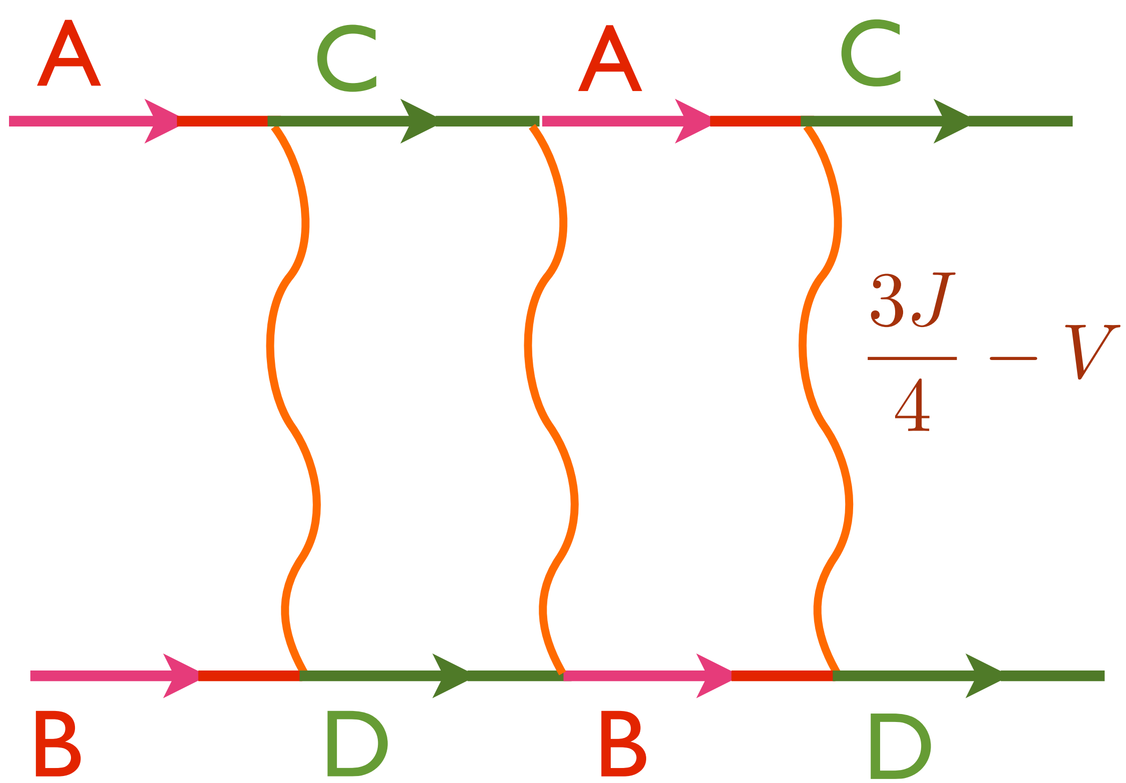
$$H = -\sum_{i,j} t_{ij} c^\dagger_{i\alpha} c_{j\alpha} + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + V \sum_{\langle ij \rangle} n_i n_j + \ldots$$



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)

Pairing "glue" from antiferromagnetic fluctuations





V. J. Emery, *J. Phys. (Paris) Colloq.* **44**, C3-977 (1983)
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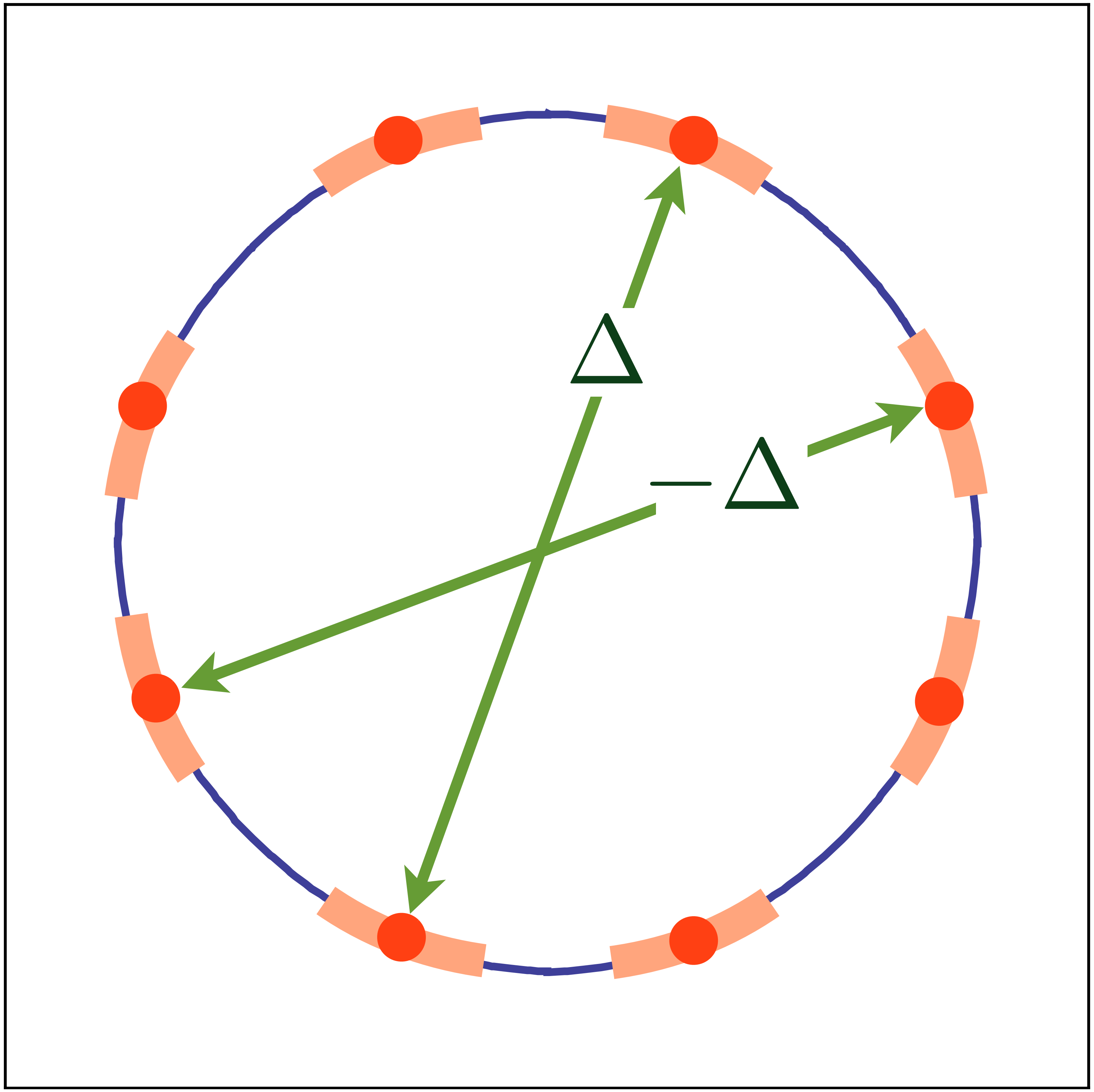
$$\left\langle c^{\dagger}_{\mathbf{k}\alpha} c^{\dagger}_{-\mathbf{k}\beta} \right\rangle = \varepsilon_{\alpha\beta} \Delta (\cos k_x - \cos k_y)$$



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

$$\Psi_{i\uparrow} = \left(\begin{array}{c} c_{i\uparrow} \\ c^\dagger_{i\downarrow} \end{array} \right) \quad , \quad \Psi_{i\downarrow} = \left(\begin{array}{c} c_{i\downarrow} \\ -c^\dagger_{i\uparrow} \end{array} \right)$$

Then we can write

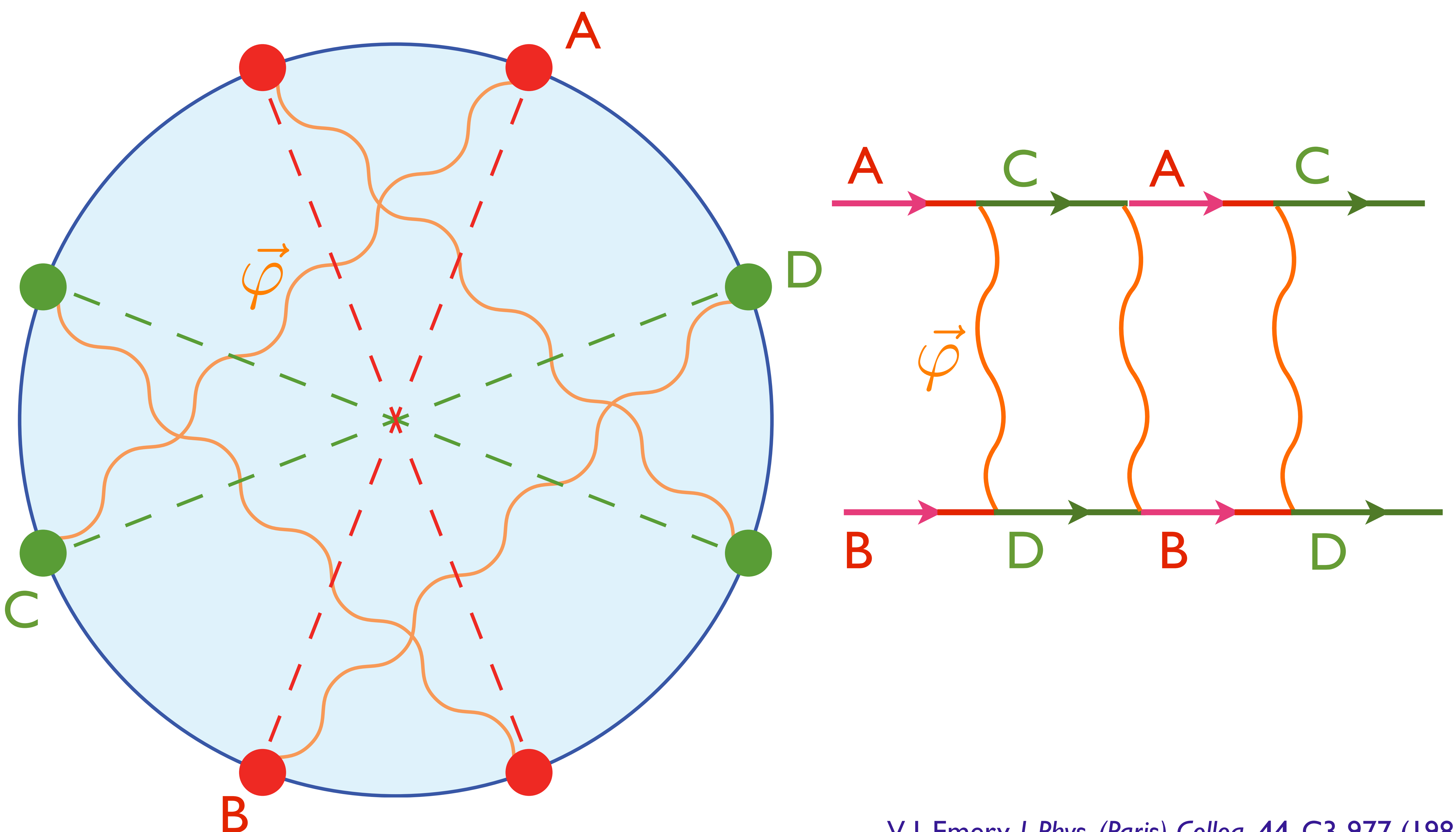
$$H_J = \frac{1}{8} \sum_{i<j} J_{ij} \left(\Psi^\dagger_{i\alpha a} \vec{\sigma}_{\alpha\beta} \Psi_{i\beta a} \right) \cdot \left(\Psi^\dagger_{j\gamma b} \vec{\sigma}_{\gamma\delta} \Psi_{j\delta b} \right)$$

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



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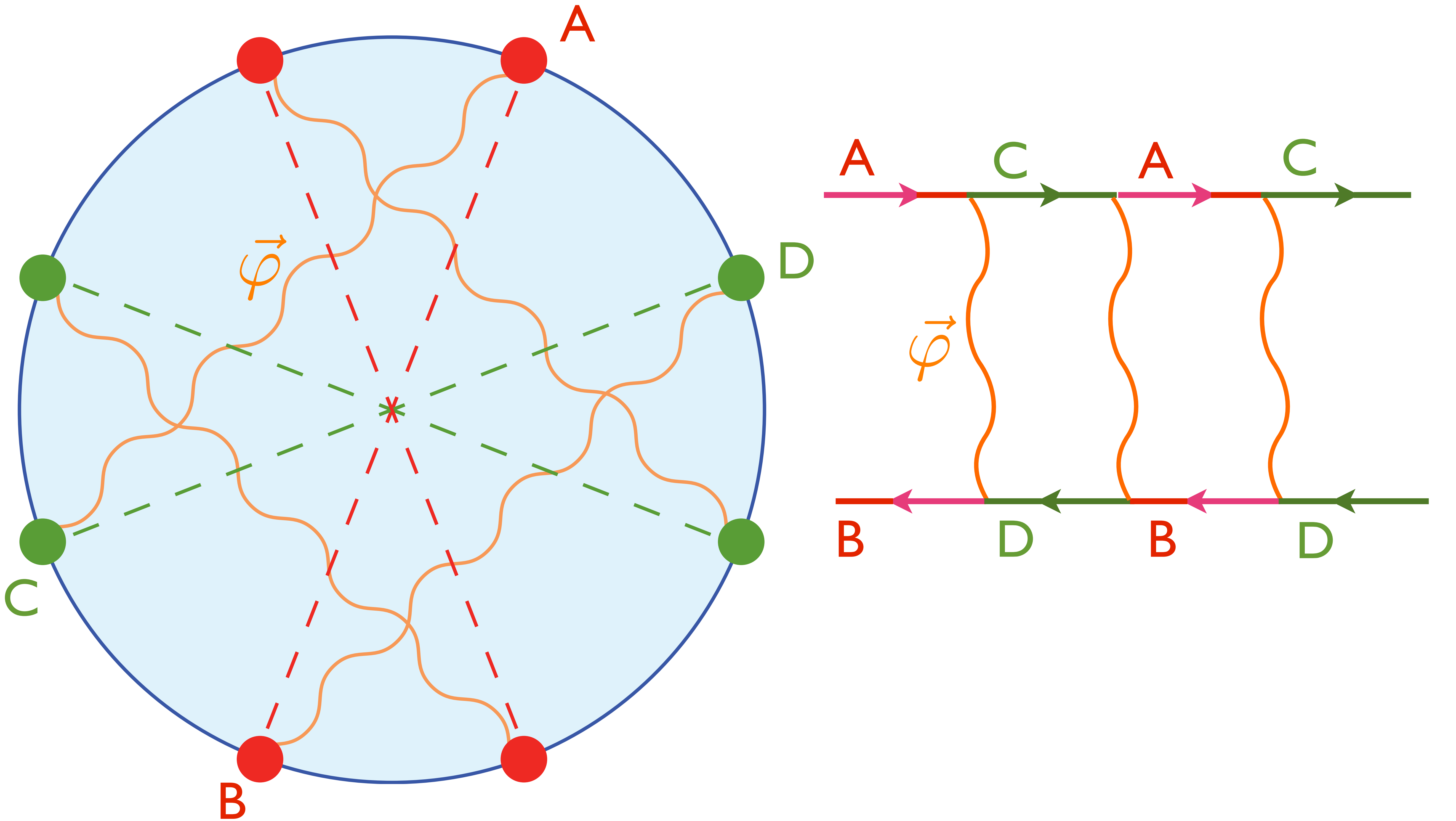
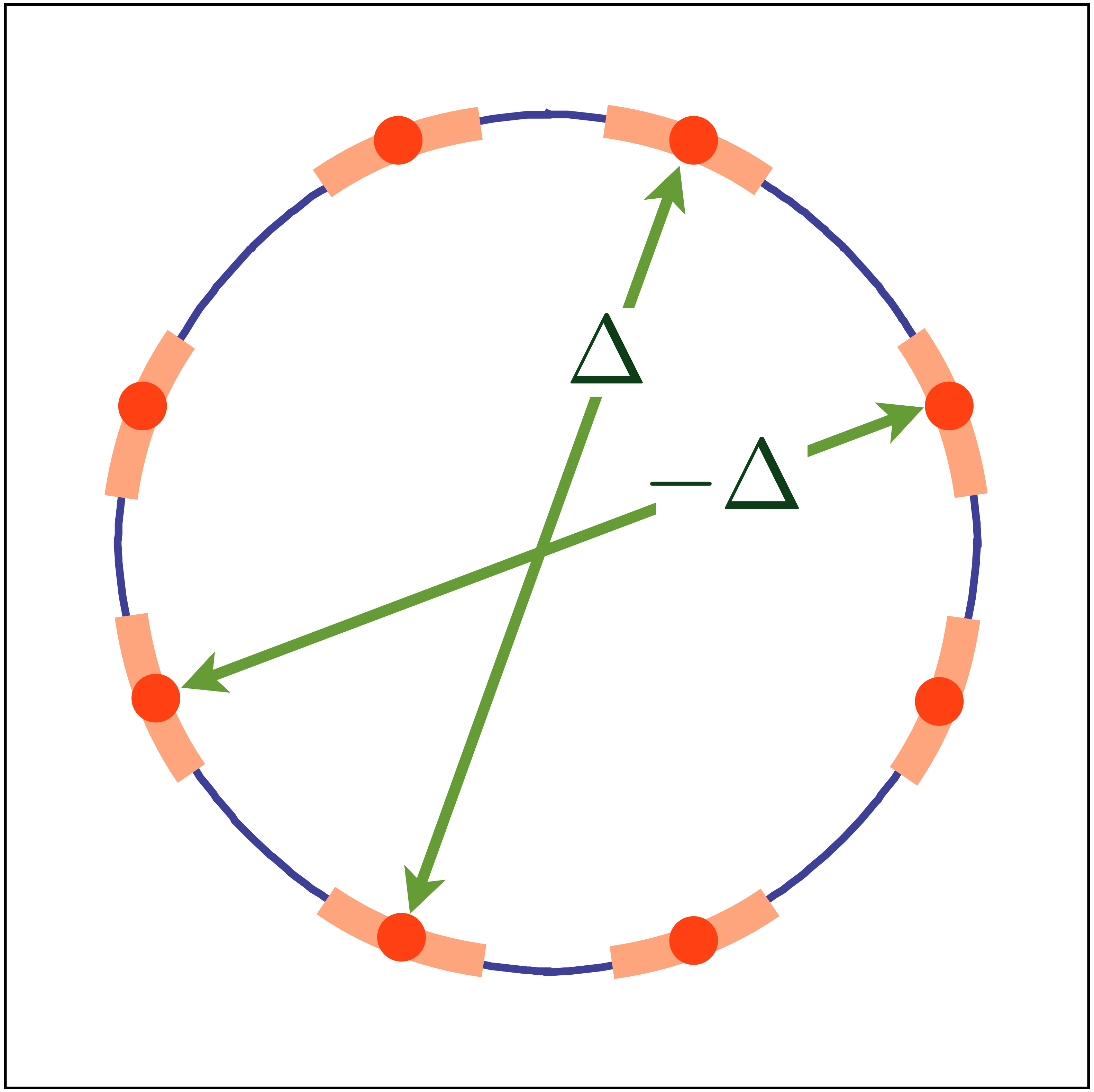
K. Miyake, S. Schmitt-Rink, and C. M.Varma, *Phys. Rev. B* **34**, 6554 (1986)
S. Raghu, S.A. Kivelson, and D.J. Scalapino, *Phys. Rev. B* **81**, 224505 (2010)

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



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

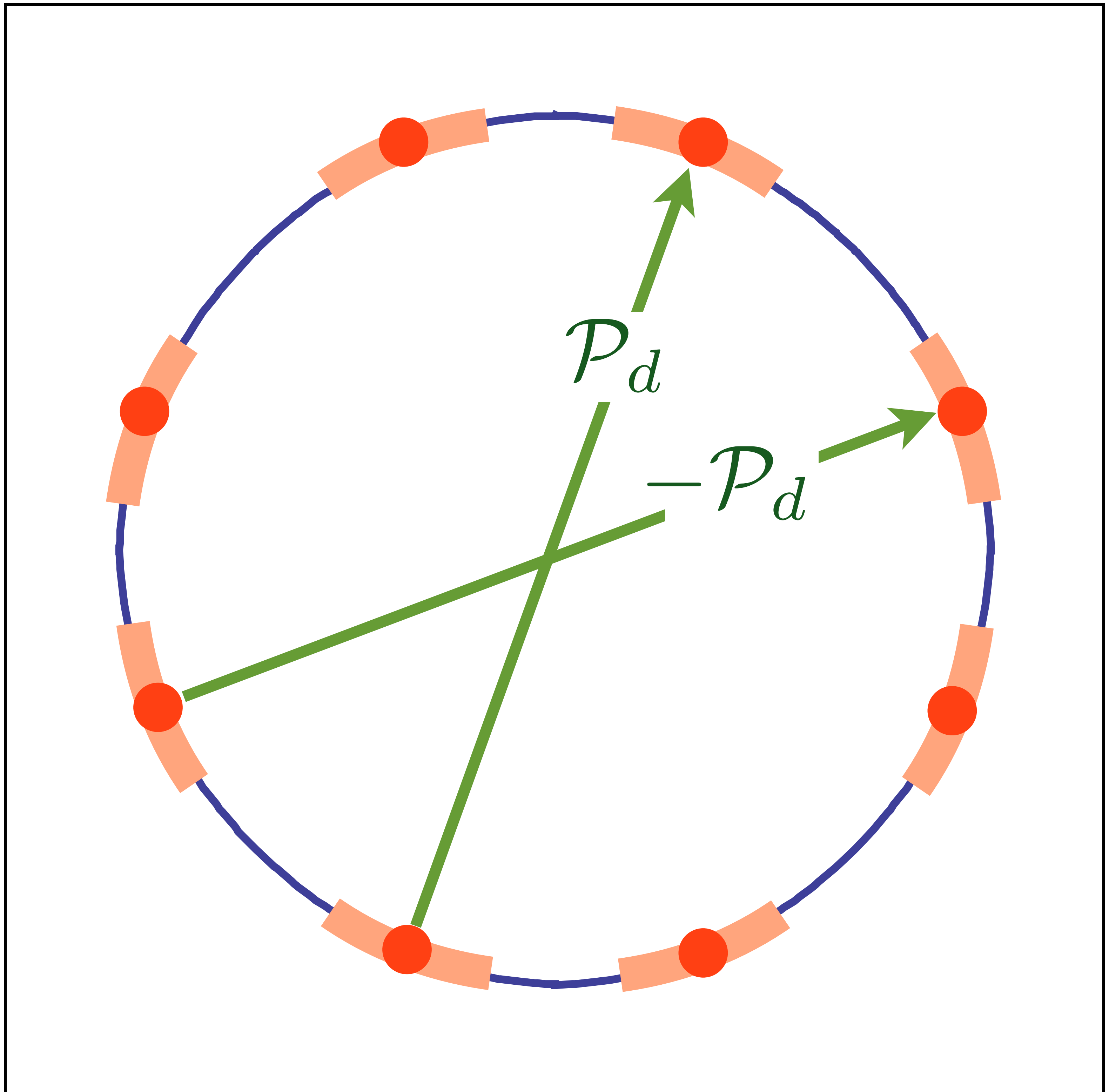
$$\left\langle c^\dagger_{\mathbf{k}\alpha} c^\dagger_{-\mathbf{k}\beta} \right\rangle = \varepsilon_{\alpha\beta} \Delta (\cos k_x - \cos k_y)$$



Unconventional pairing at *and near* hot spots

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

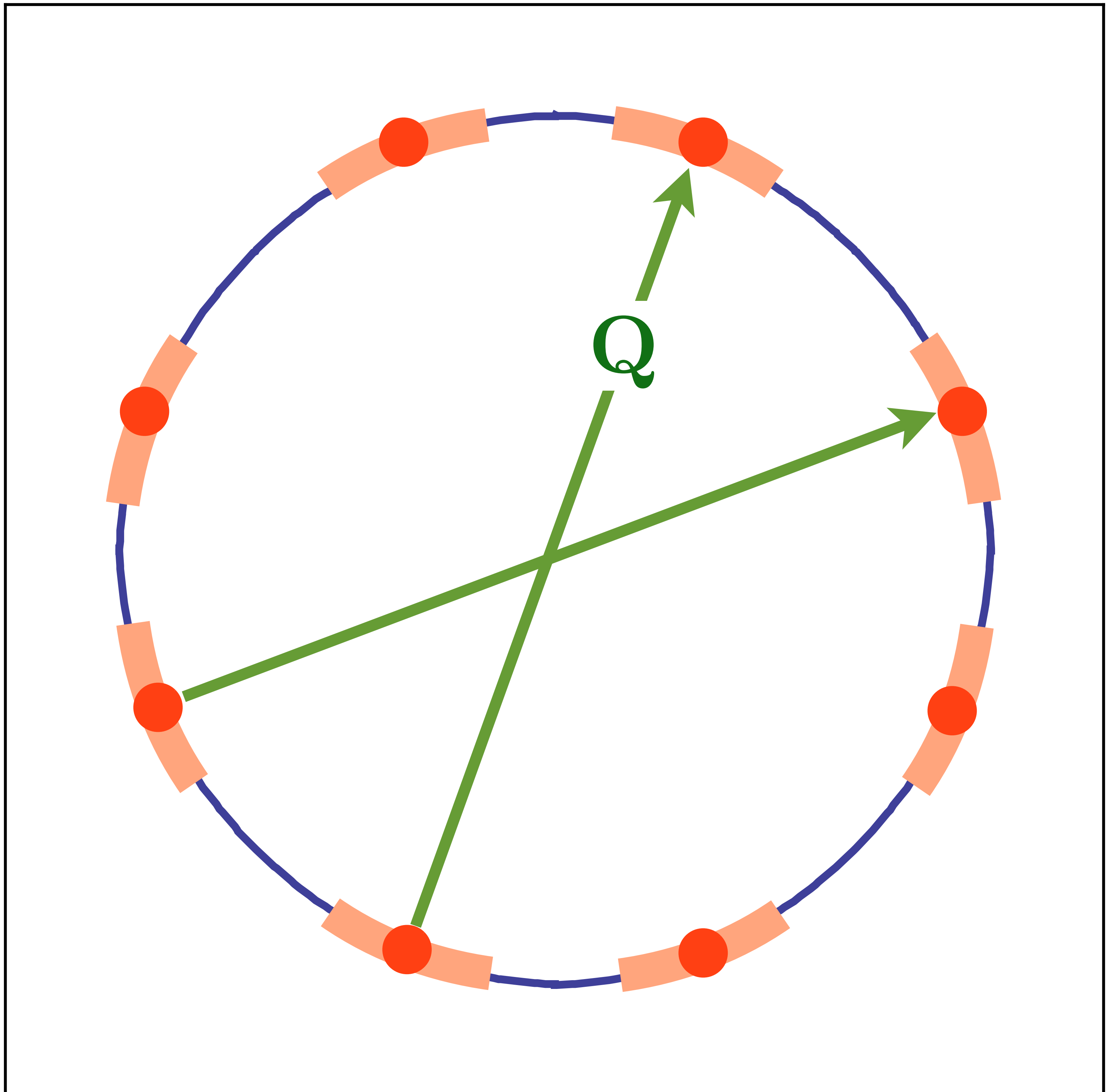
After pseudospin rotation on *half* the hot-spots



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

"*d*-form factor" density wave

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



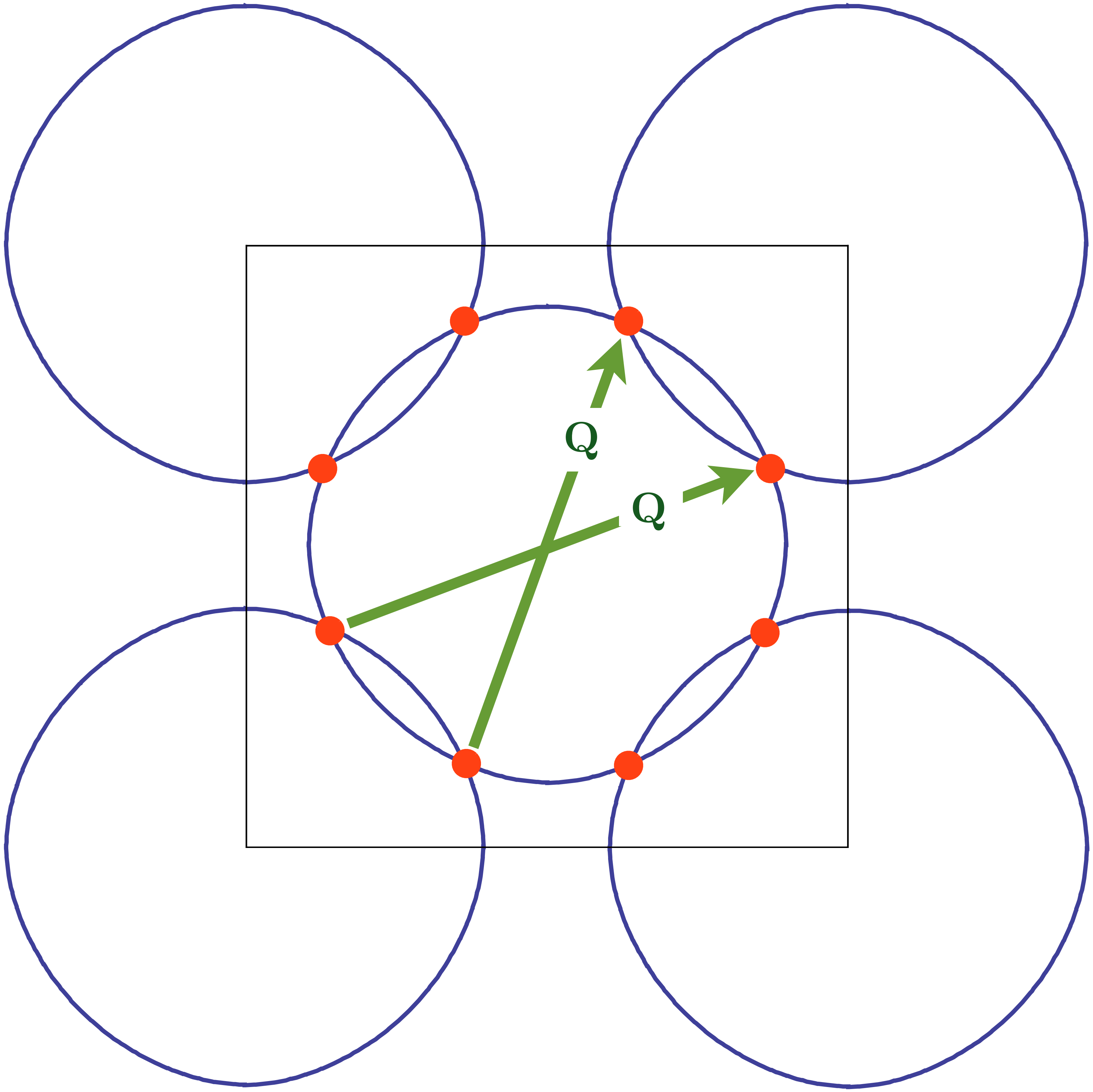
$\mathbf{Q}$ is '$2k_F$' wavevector

After pseudospin rotation on *half* the hot-spots

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

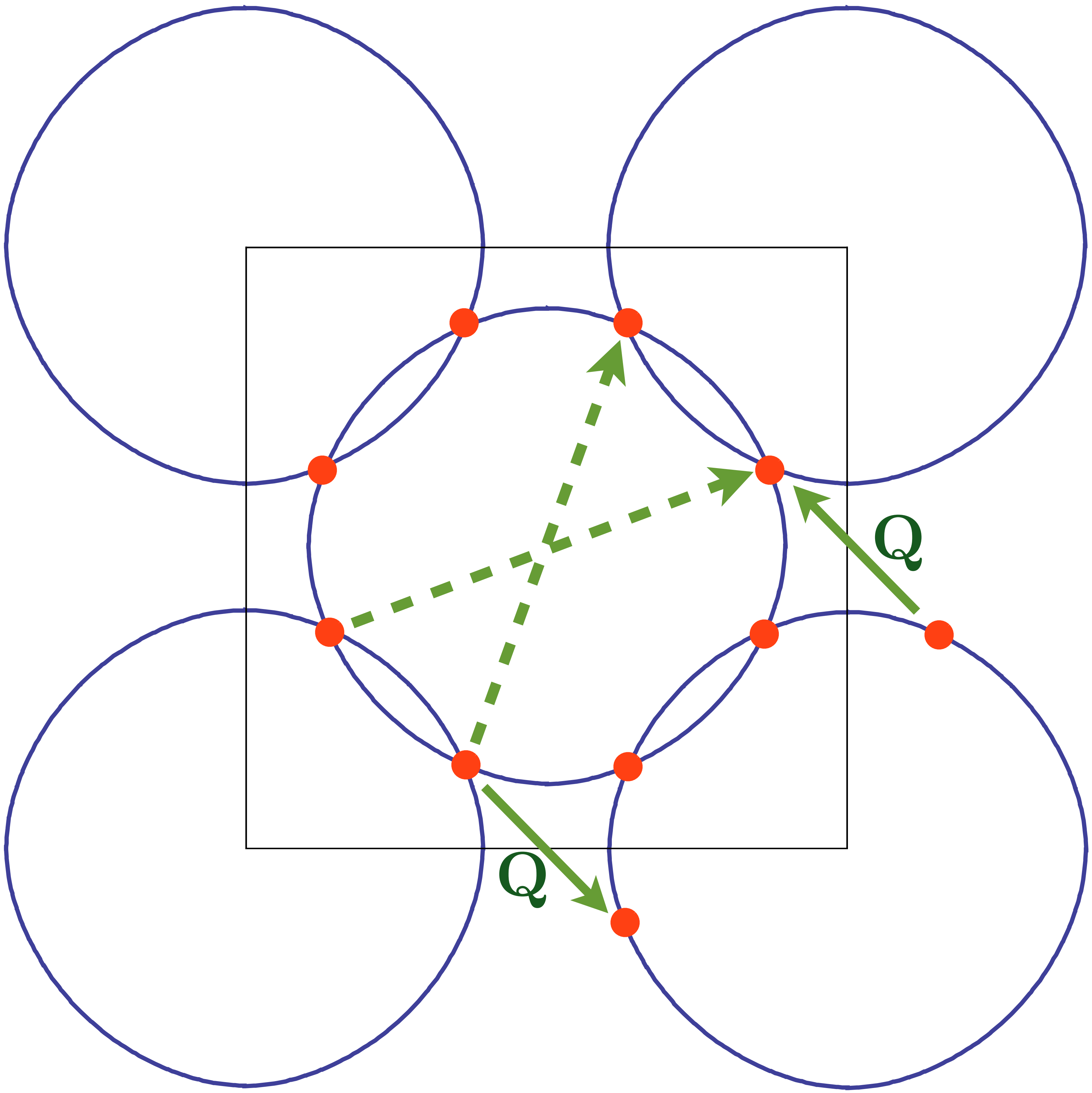
"*d*-form factor" density wave

d-form factor density wave



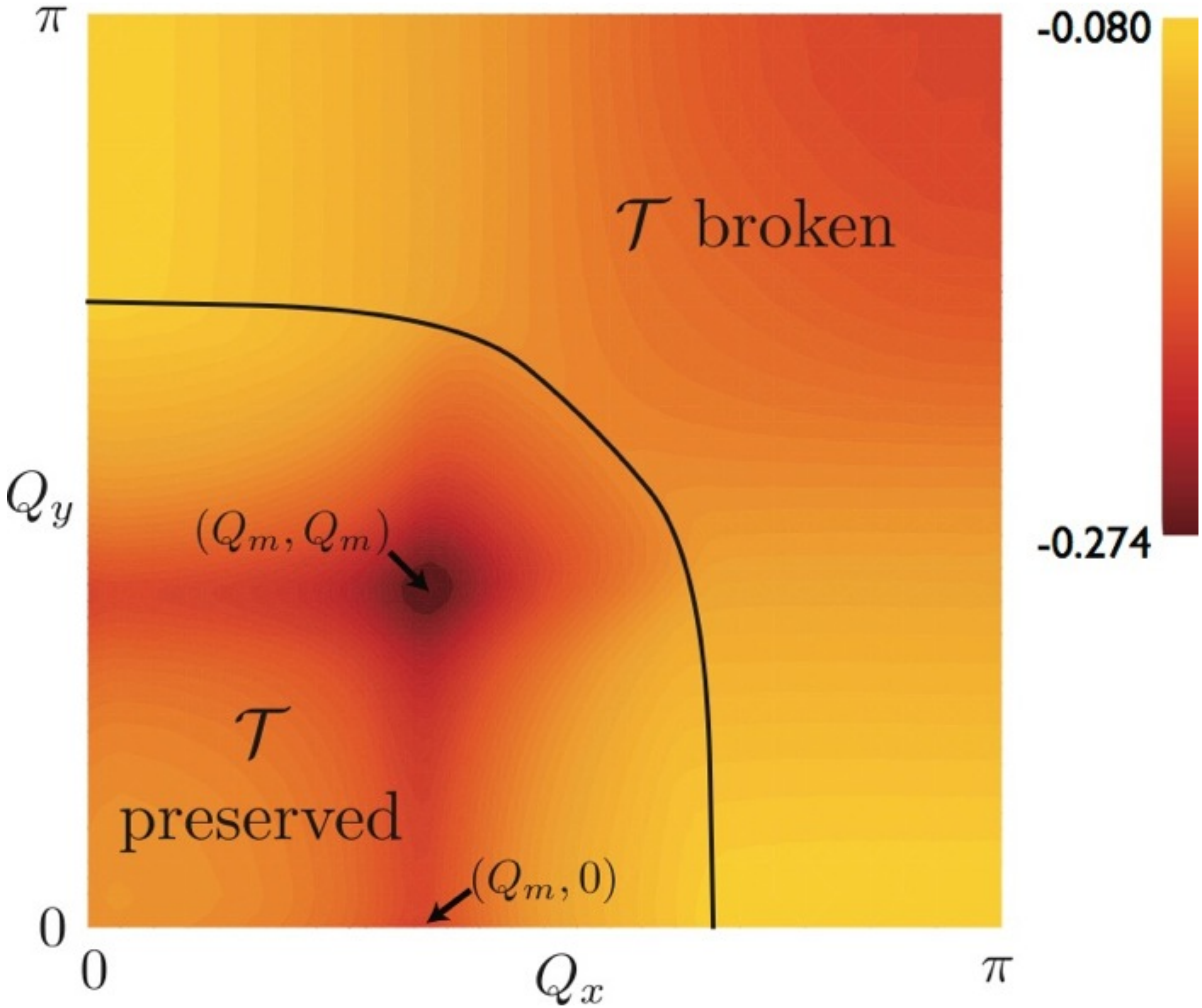
$$\left\langle c^{\dagger}_{\mathbf{k}-\mathbf{Q}/2,\alpha} c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \right\rangle = \mathcal{P}_d(\cos k_x - \cos k_y)$$

d-form factor density wave



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

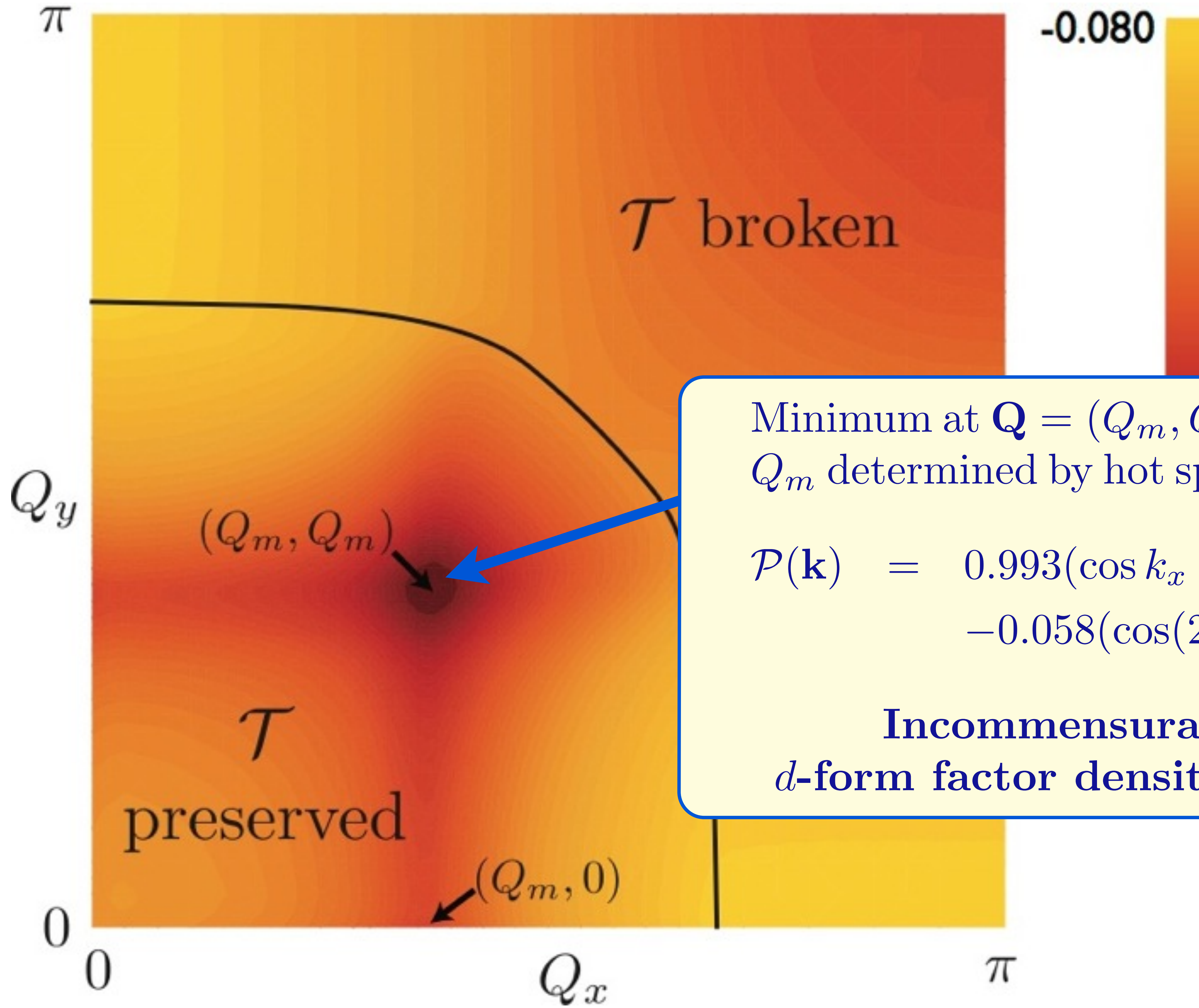
S. Sachdev and R. La Placa, Phys. Rev. Lett. 111, 027202 (2013); A. Allais, J. Bauer, and S. Sachdev, arXiv:1402.6311



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

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

S. Sachdev and R. La Placa, Phys. Rev. Lett. **111**, 027202 (2013); A. Allais, J. Bauer, and S. Sachdev, arXiv:1402.6311



Minimum at $\mathbf{Q} = (Q_m, Q_m)$ (with Q_m determined by hot spots) with

$$\mathcal{P}(\mathbf{k}) = 0.993(\cos k_x - \cos k_y) - 0.058(\cos(2k_x) - \cos(2k_y))$$

Incommensurate
d-form factor density wave

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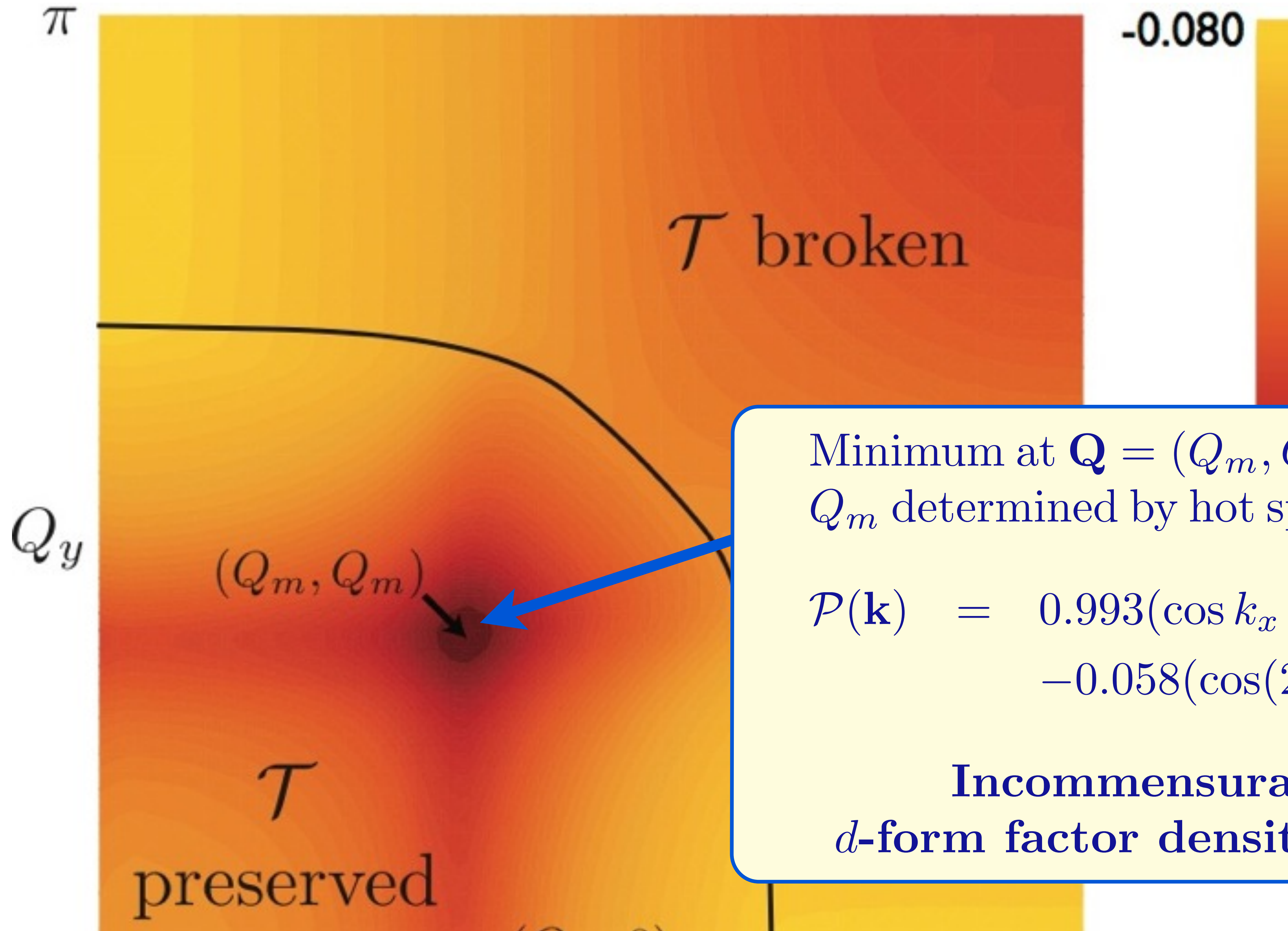

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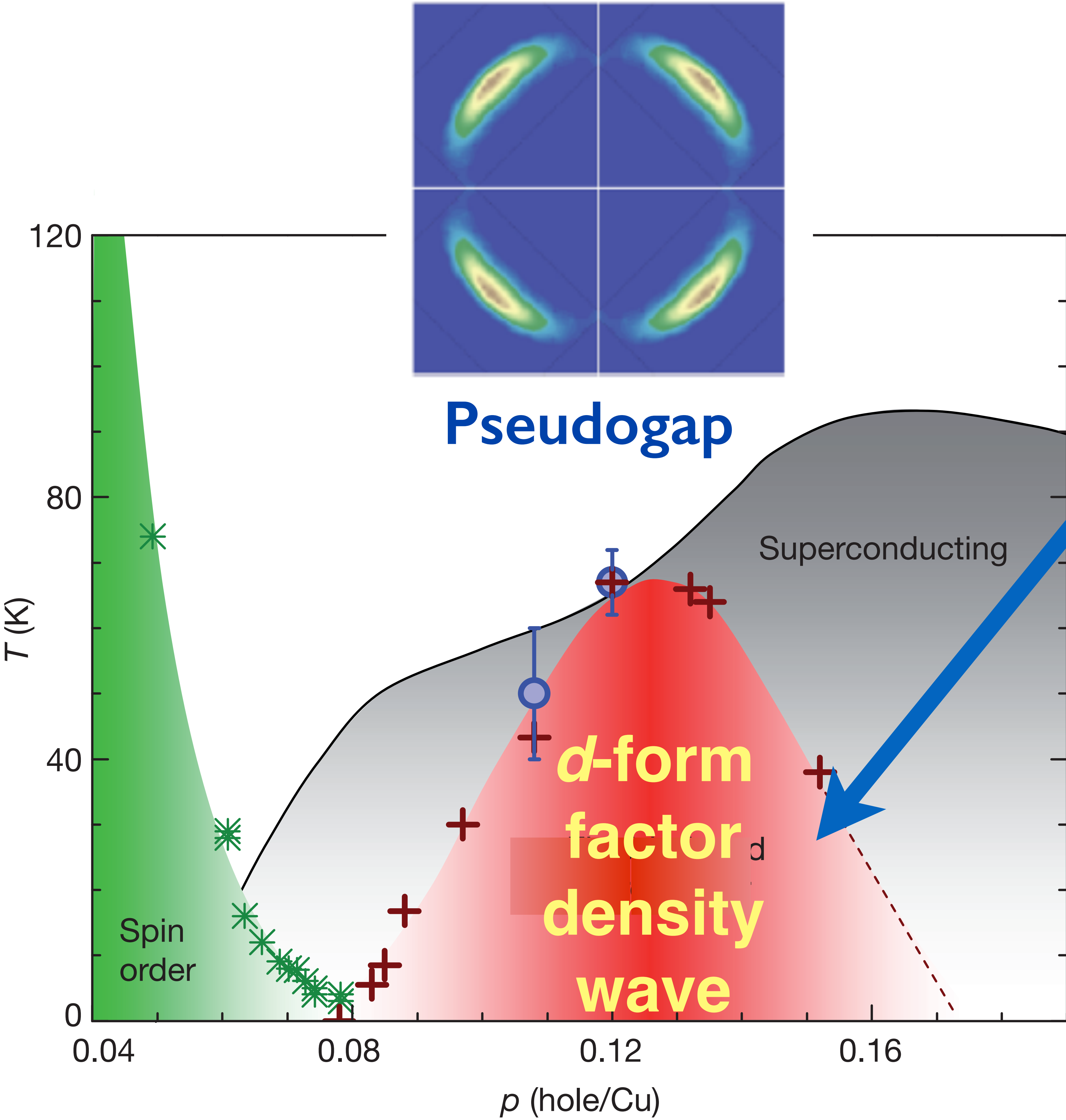
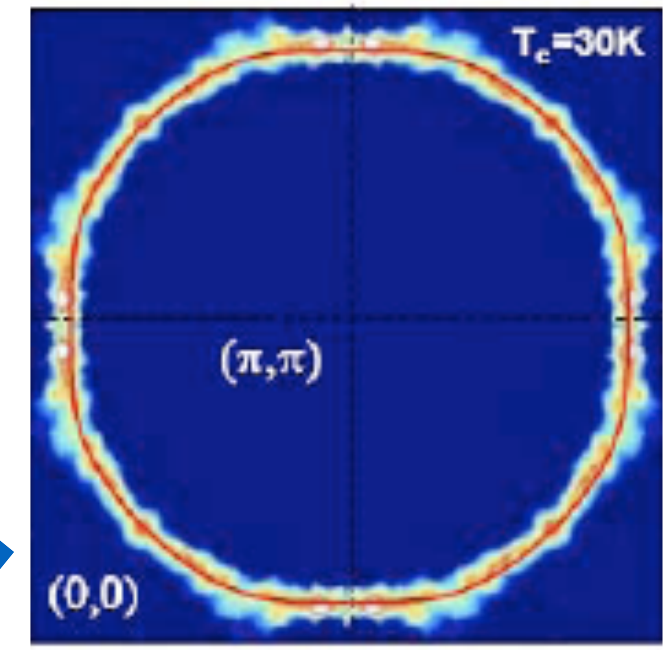
$$\mathcal{P}(\mathbf{k}) = 0.993(\cos k_x - \cos k_y) - 0.058(\cos(2k_x) - \cos(2k_y))$$

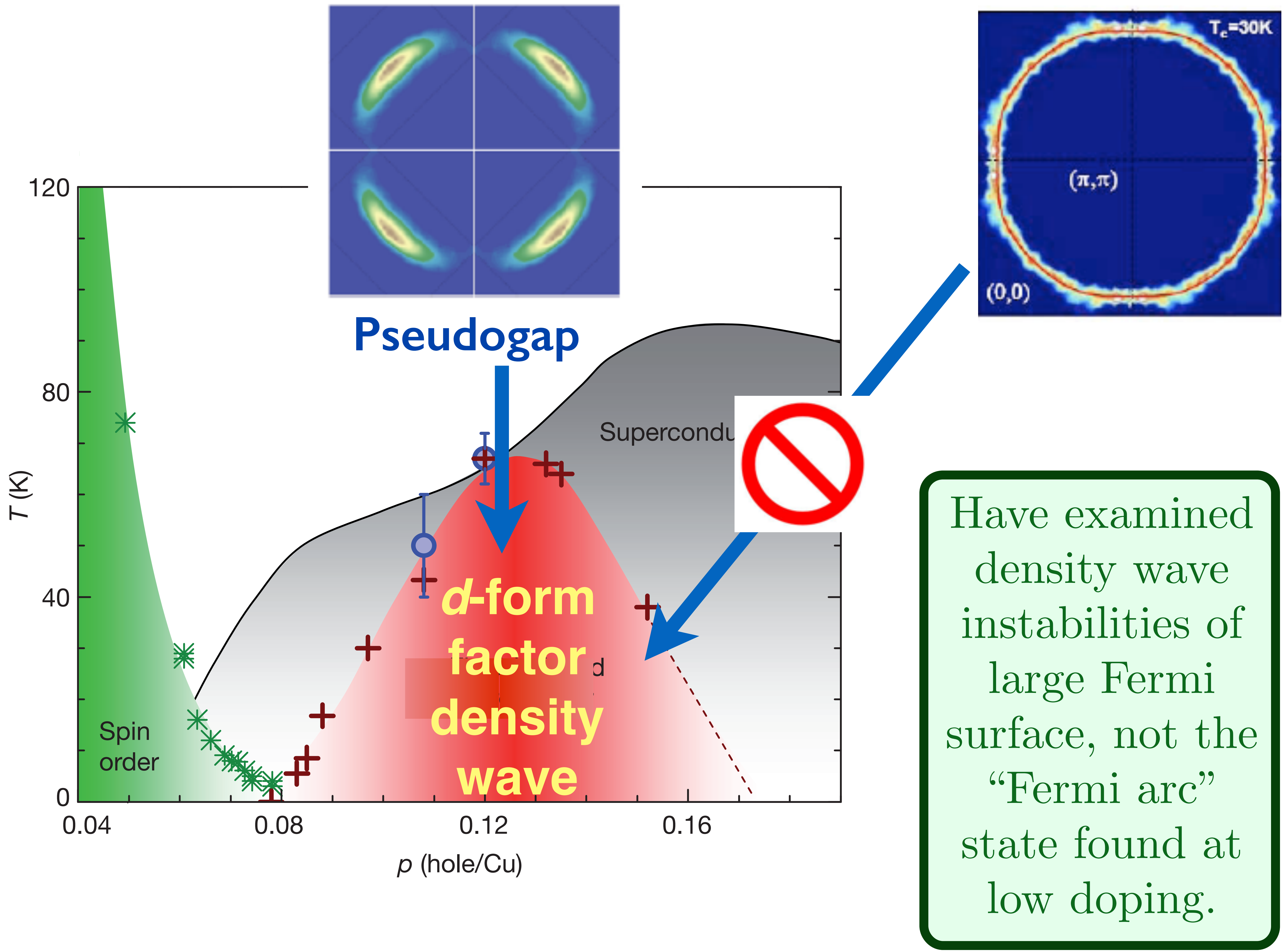
Incommensurate
***d*-form factor density wave**

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.



Pseudogap
Tc=30K
(π,π)
(0,0)
Superconduc
120
80
40
0
T (K)
0.04
0.08
0.12
0.16
p (hole/Cu)
Spin
order
d-form
factor
density
wave
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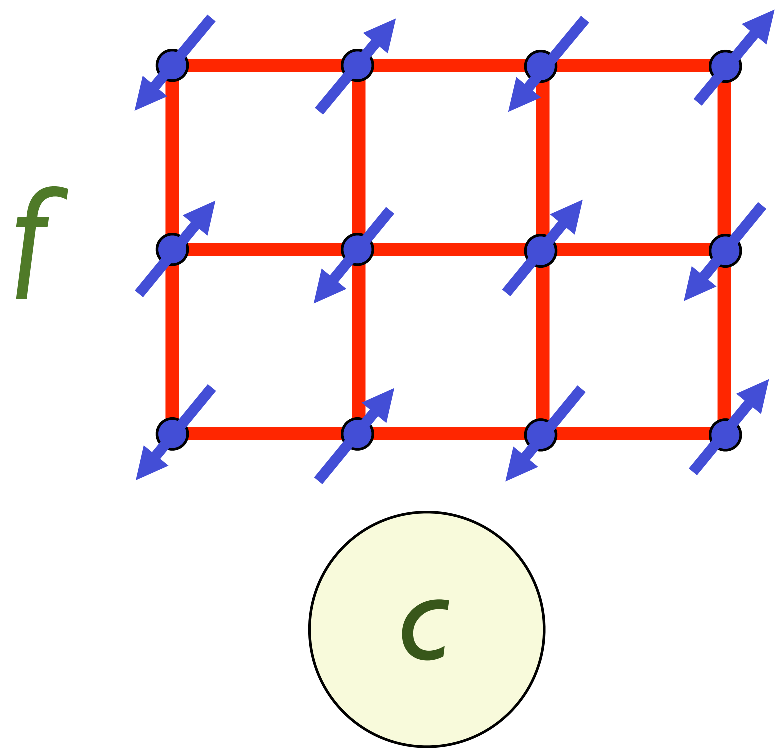
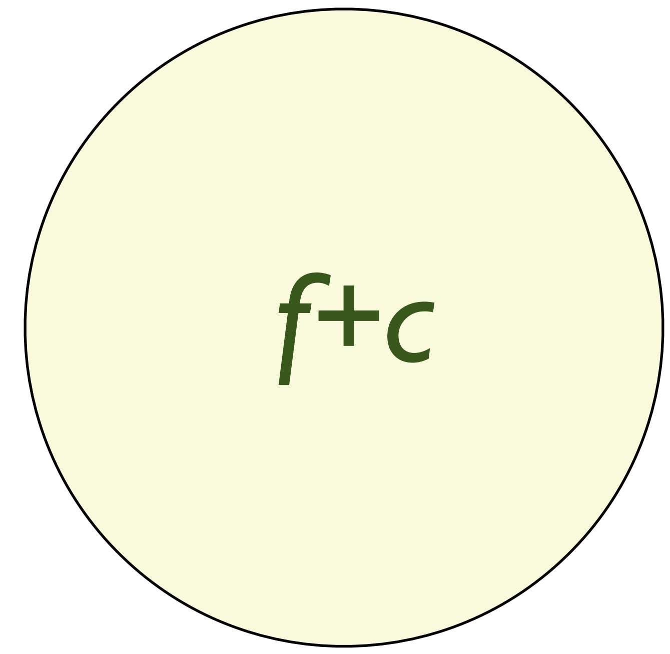
Magnetic order and the heavy Fermi liquid in the Kondo lattice



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

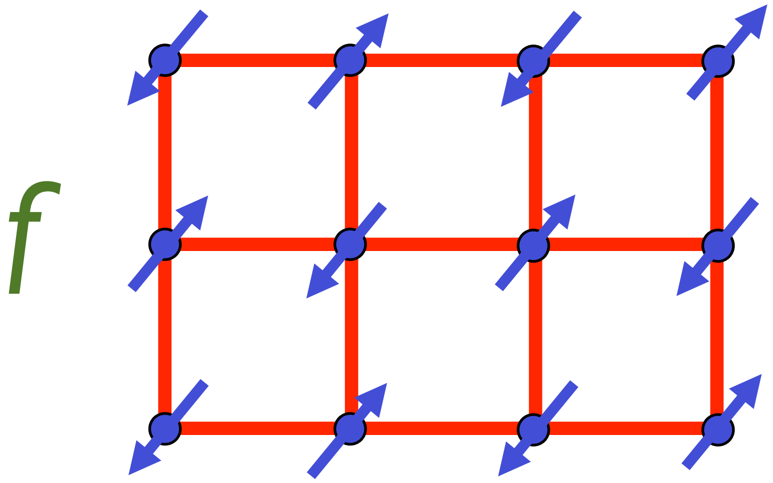
Magnetic Metal:
f-electron moments
and
c-conduction electron
Fermi surface

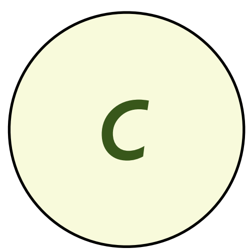


$$\langle \vec{\varphi} \rangle = 0$$

Heavy Fermi liquid
with "large" Fermi
surface of
hydridized *f* and
c-conduction
electrons

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





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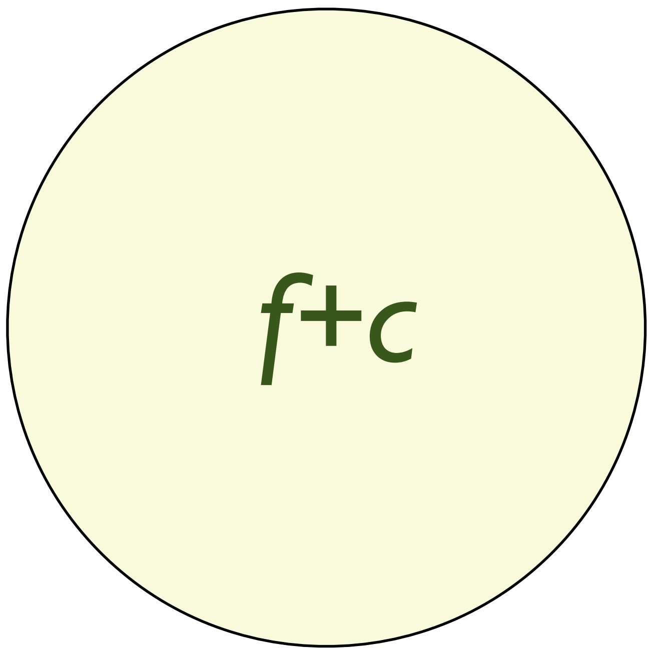

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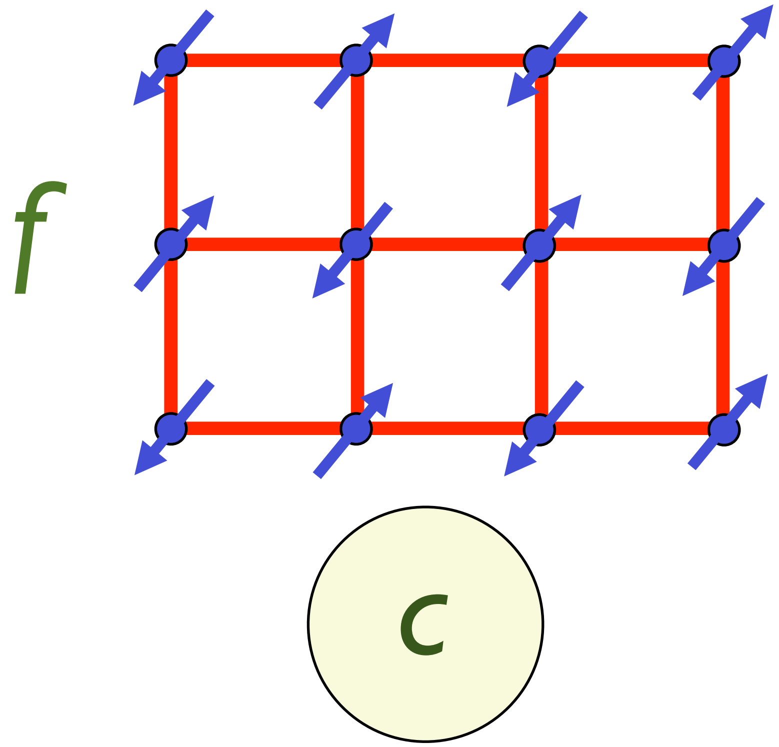

$\langle \vec{\varphi} \rangle \neq 0$

Magnetic Metal:
f-electron moments
and
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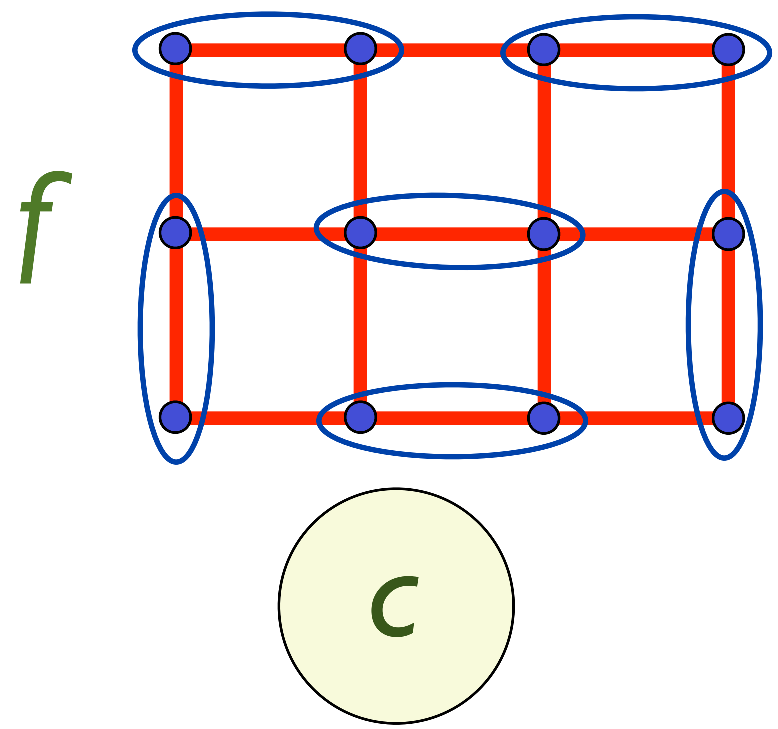
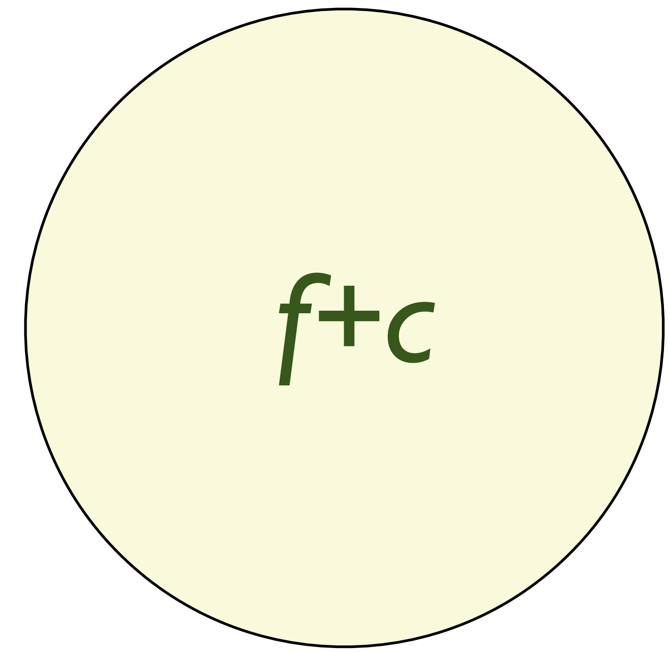


$\langle \vec{\varphi} \rangle = 0$

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



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

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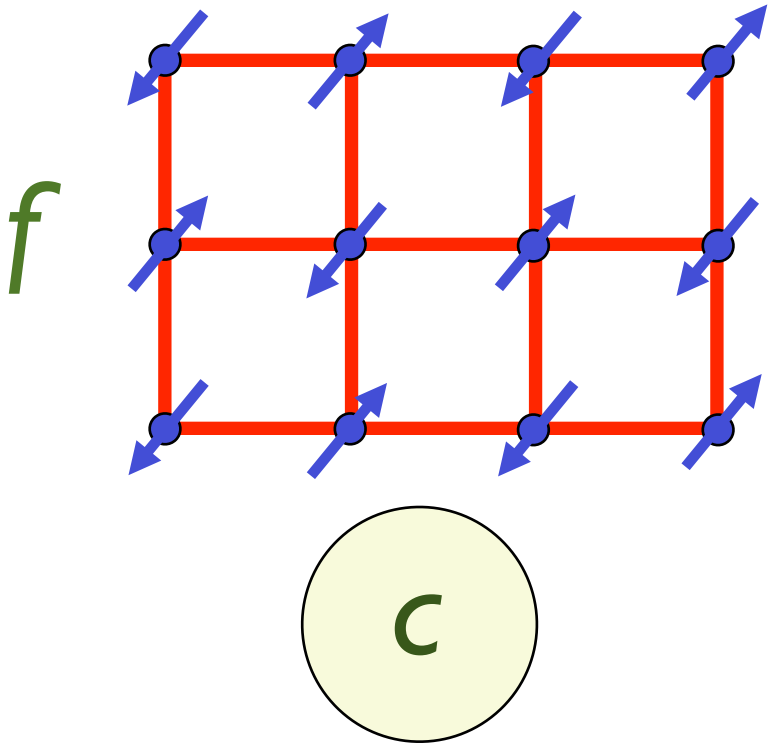

$\langle \vec{\varphi} \rangle \neq 0$

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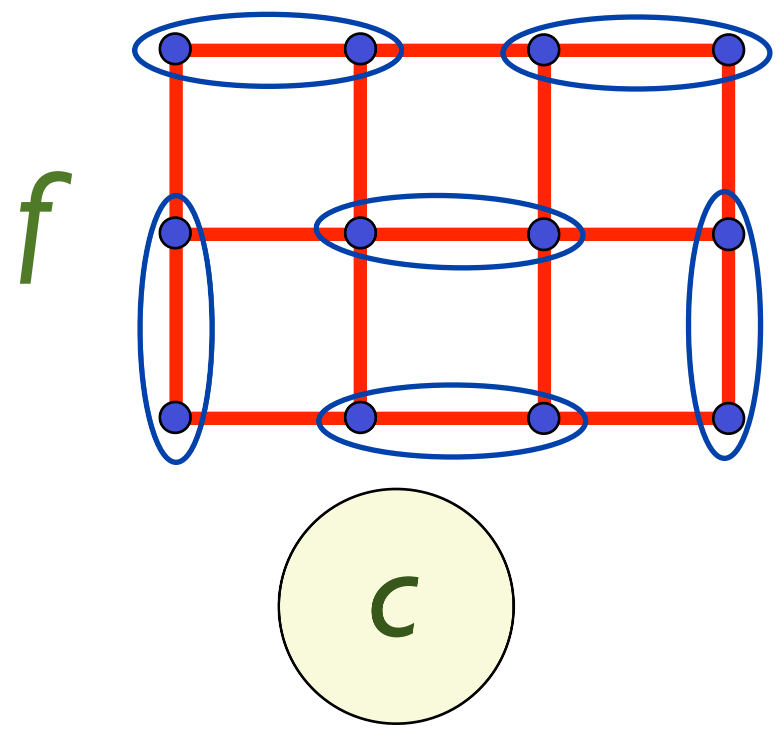
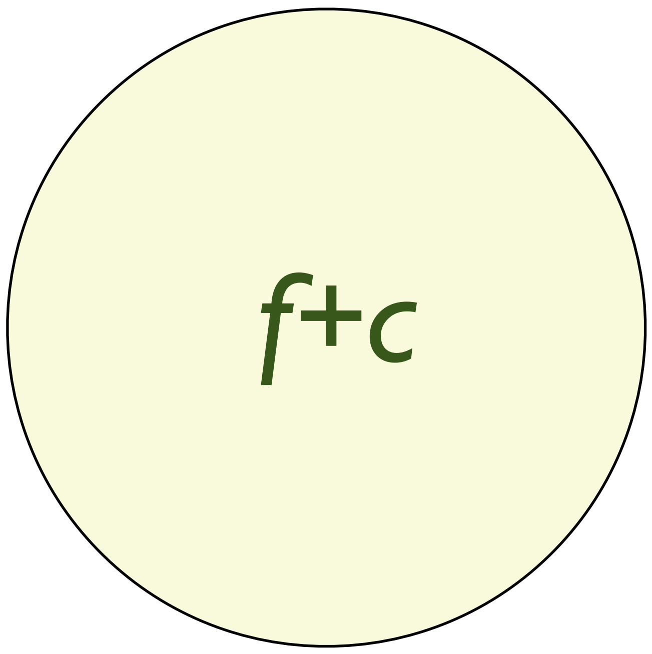


$\langle \vec{\varphi} \rangle = 0$

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

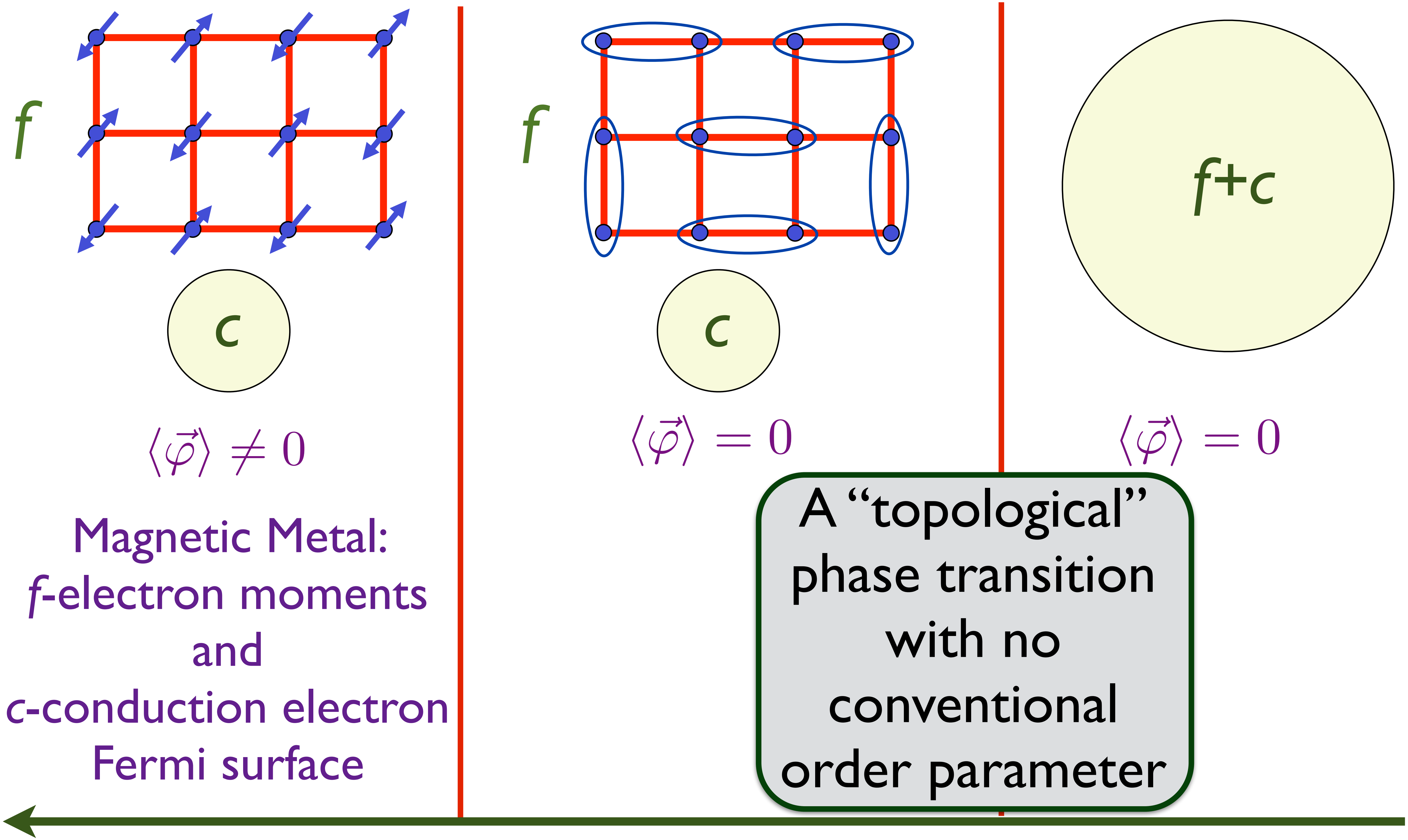


$\langle \vec{\varphi} \rangle = 0$

Heavy Fermi liquid with "large" Fermi surface of hydridized *f* and *c*-conduction electrons

T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

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



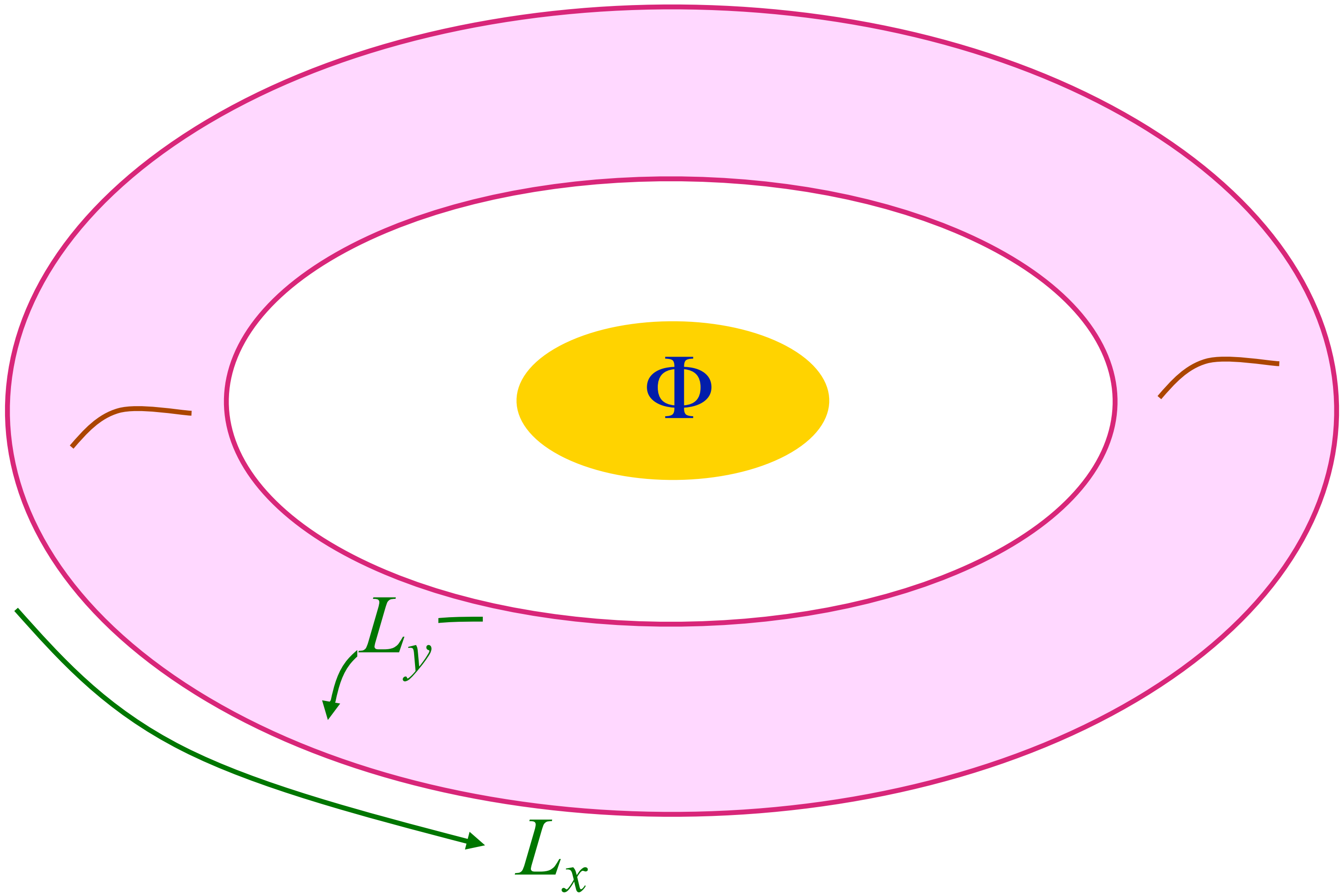
T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

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.

T. Senthil, M. Vojta, and S. Sachdev, *Phys. Rev. B* **69**, 035111 (2004)

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



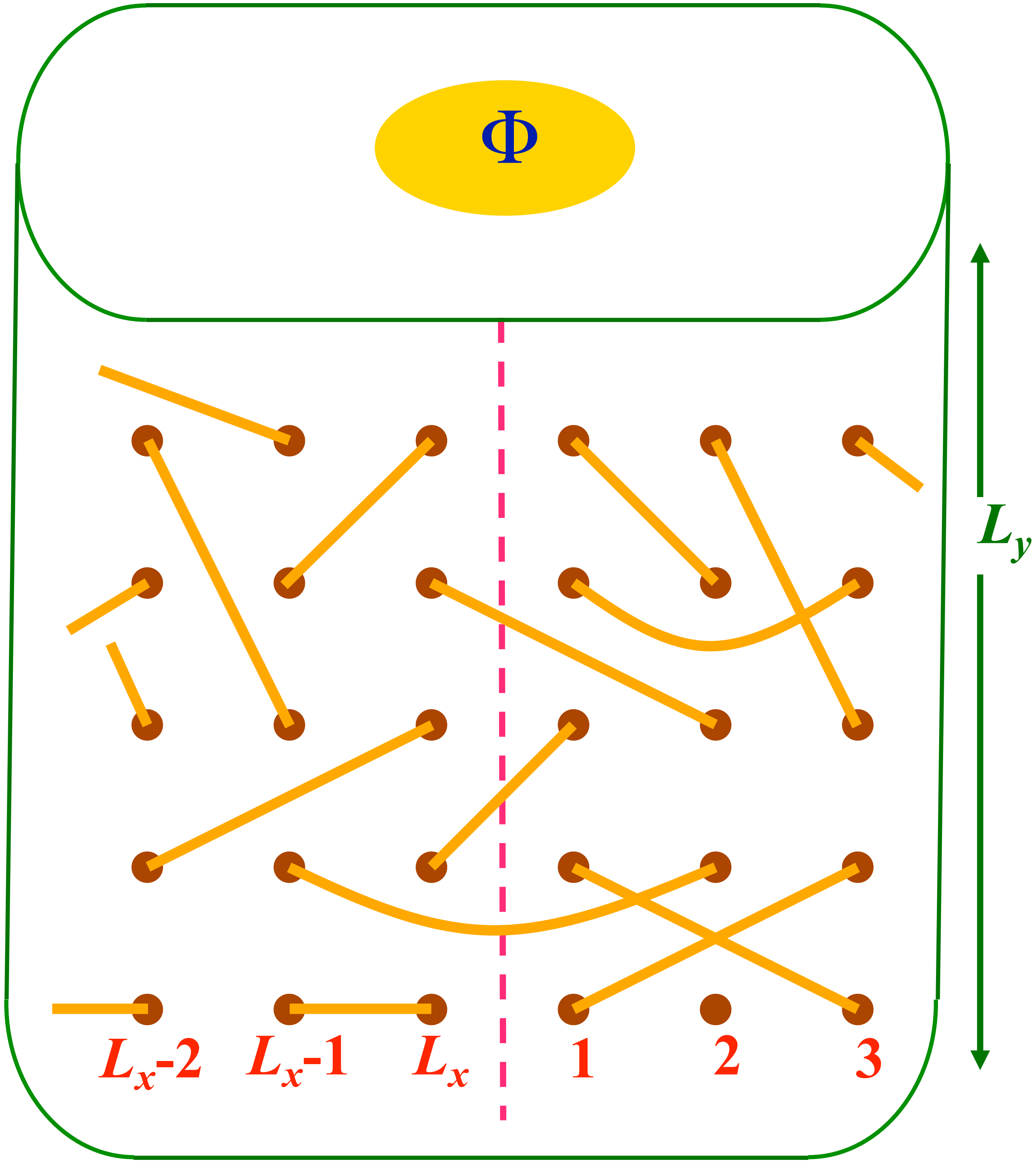
Unit cell a_x, a_y.
L_x/a_x, L_y/a_y
coprime integers

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.

M. Oshikawa, *Phys. Rev. Lett.* **84**, 3370 (2000).

Effect of flux-piercing on a spin liquid

$$|D\rangle =$$

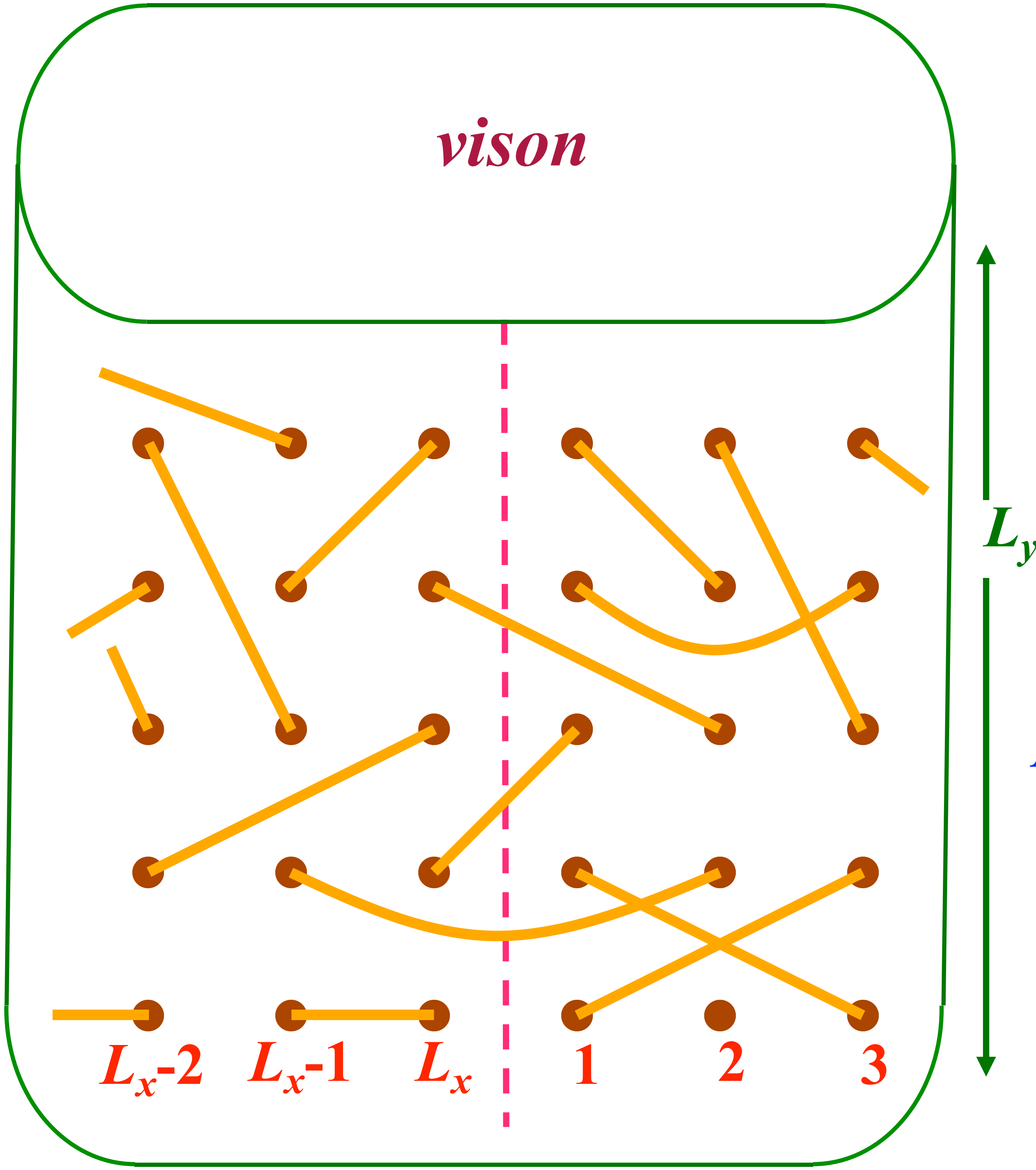


N. E. Bonesteel, *Phys. Rev.* B **40**, 8954 (1989).
G. Misguich, C. Lhuillier, M. Mambrini, and P. Sindzingre, *Eur. Phys. J.* B **26**, 167 (2002).

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

Effect of flux-piercing on a spin liquid

$$\left| D \right\rangle =$$



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

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

After flux insertion $\left| D \right\rangle \Rightarrow$

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

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.

T. Senthil, M. Vojta, and S. Sachdev, *Phys. Rev. B* **69**, 035111 (2004)

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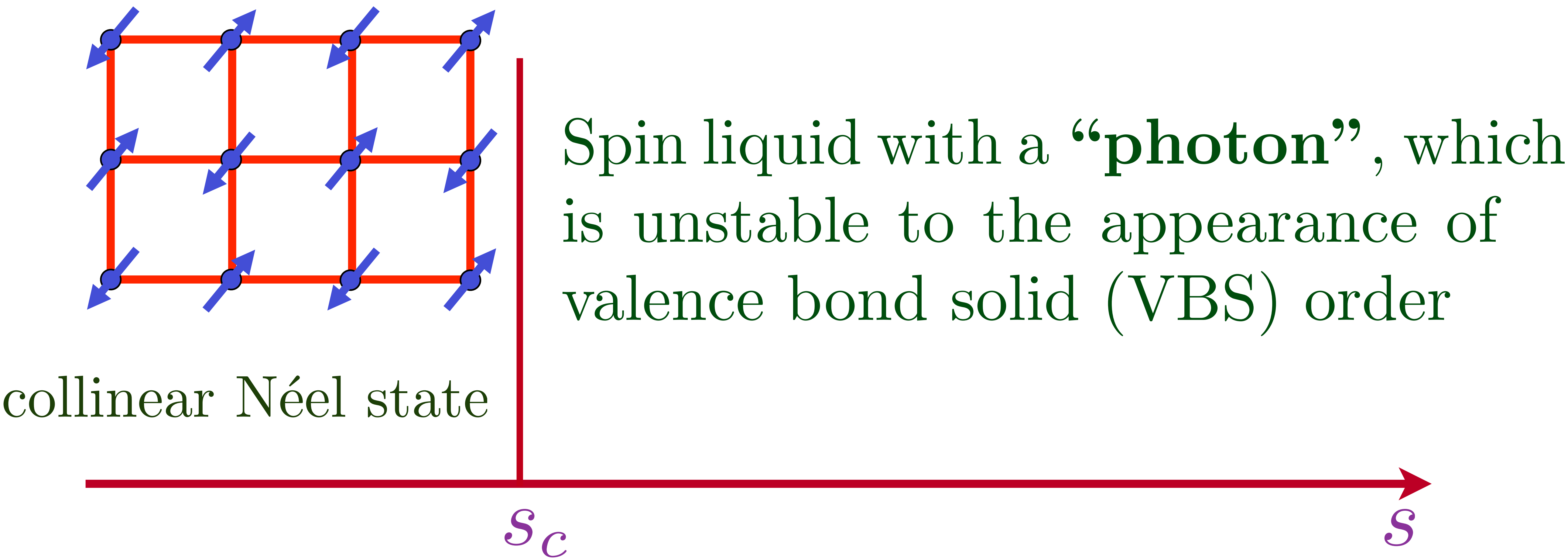
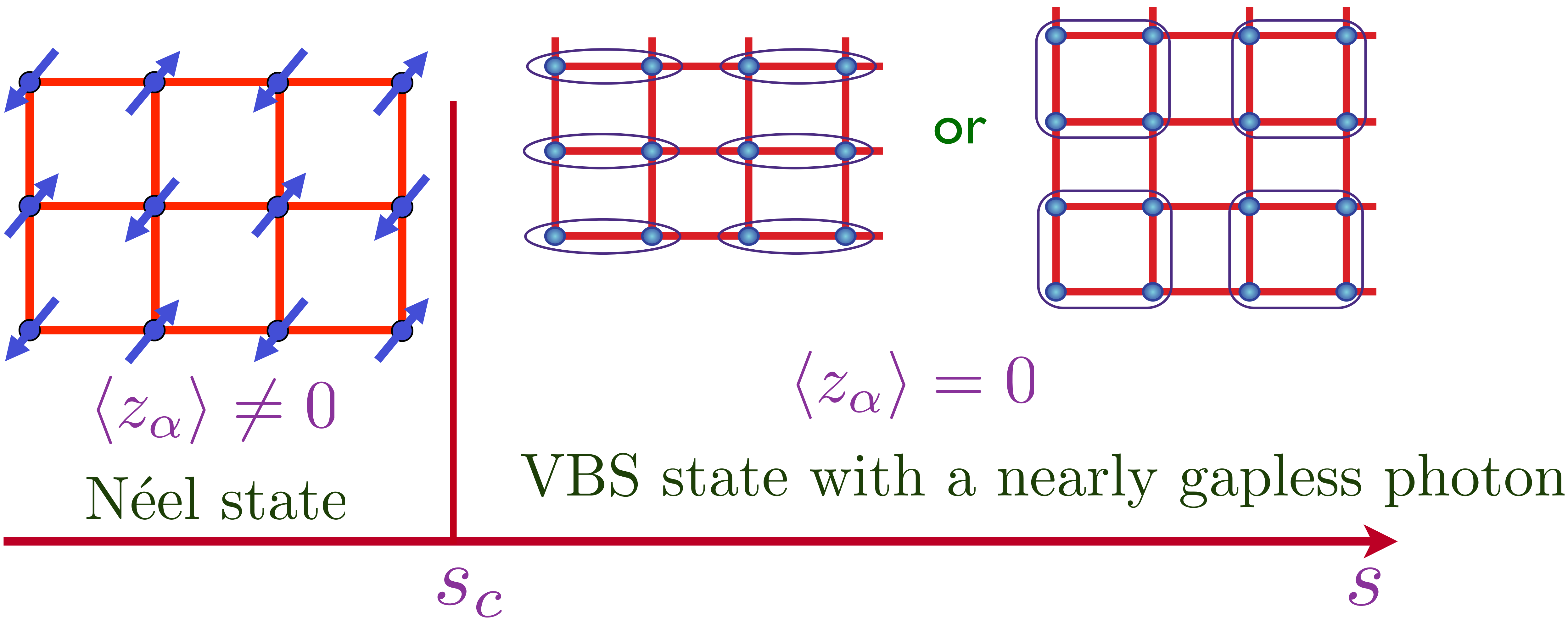
Quantum “disordering” magnetic order



N. Read and S. Sachdev, *Phys. Rev. Lett*. **62**, 1694 (1989).

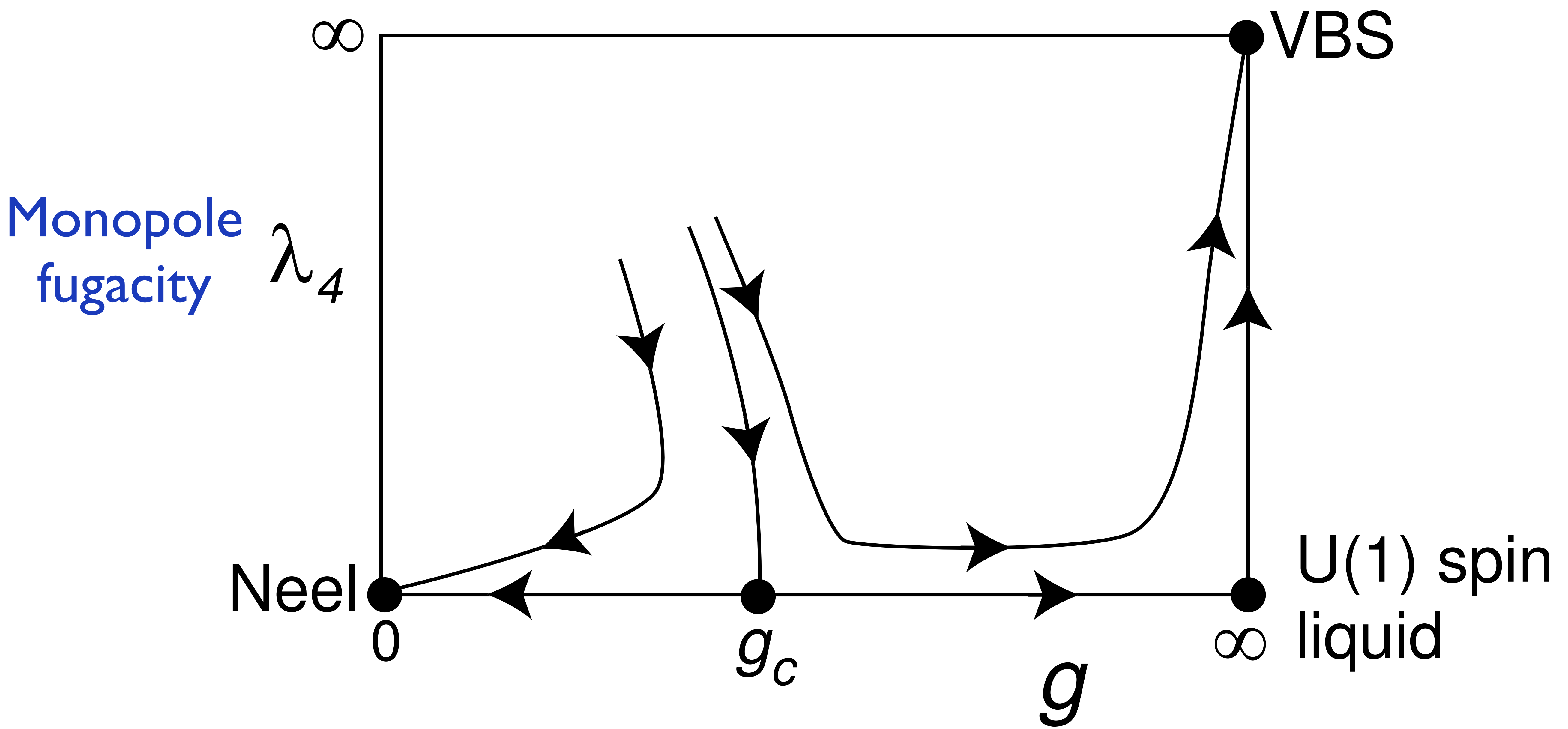
Neel-VBS quantum transition



Critical theory for photons and deconfined spinons:

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

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).



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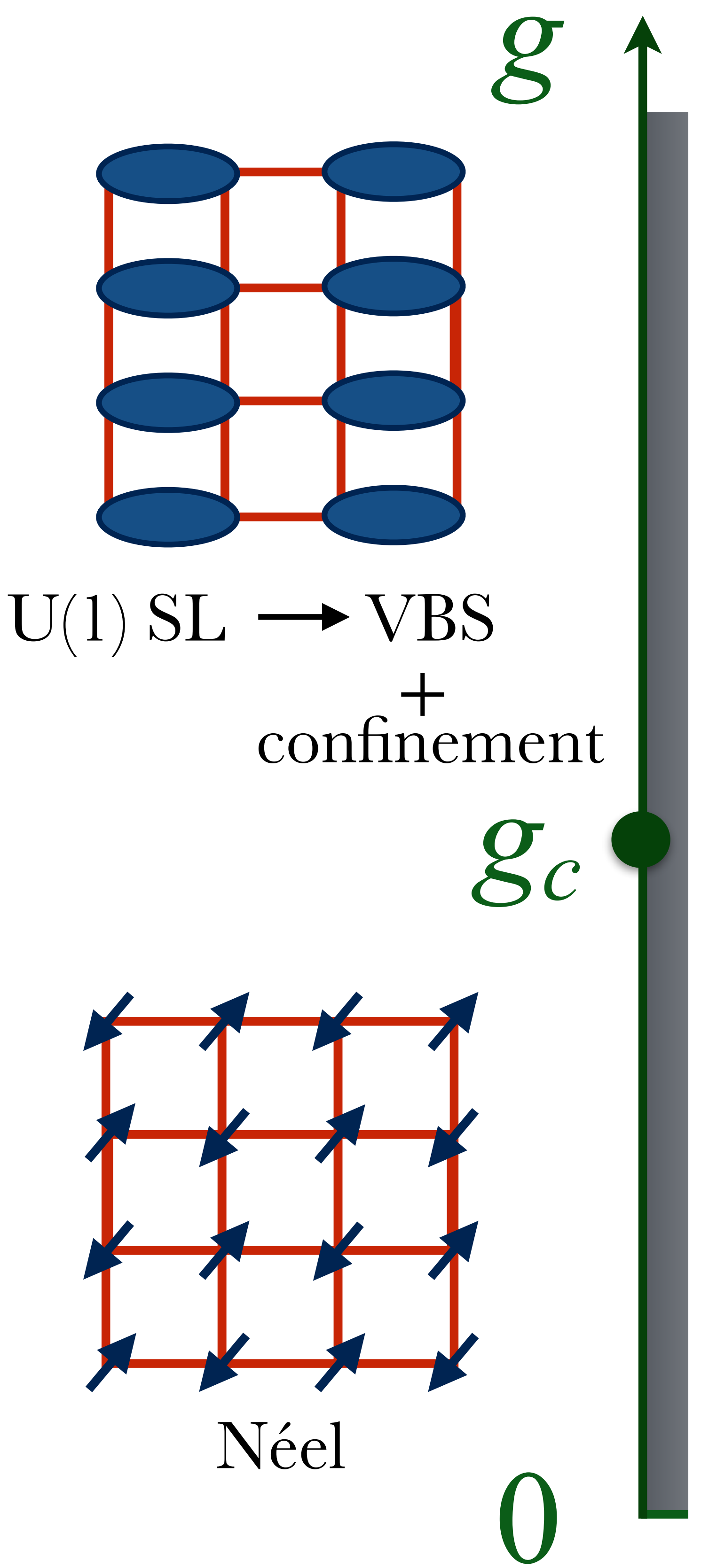

g
U(1) SL → VBS
+
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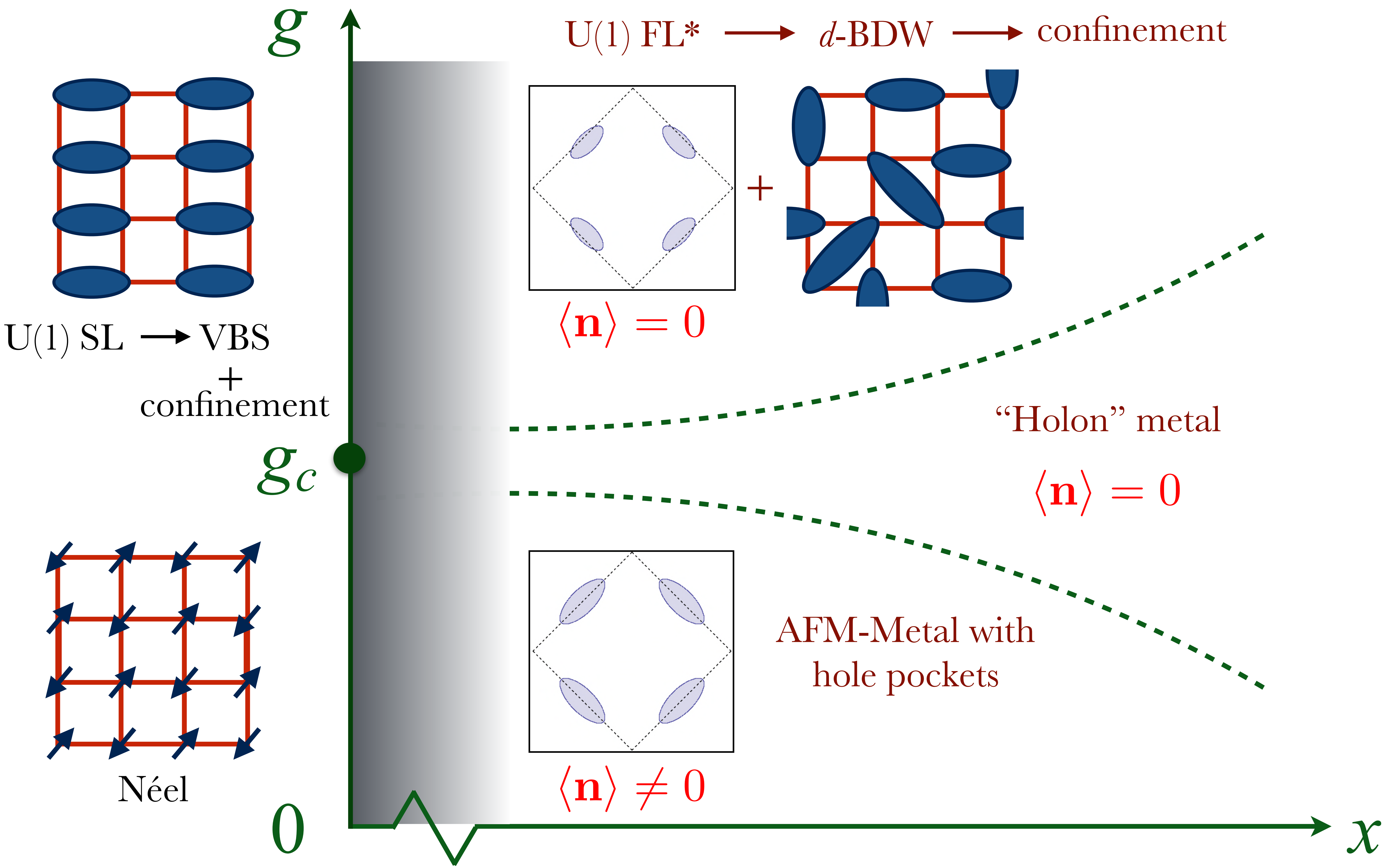

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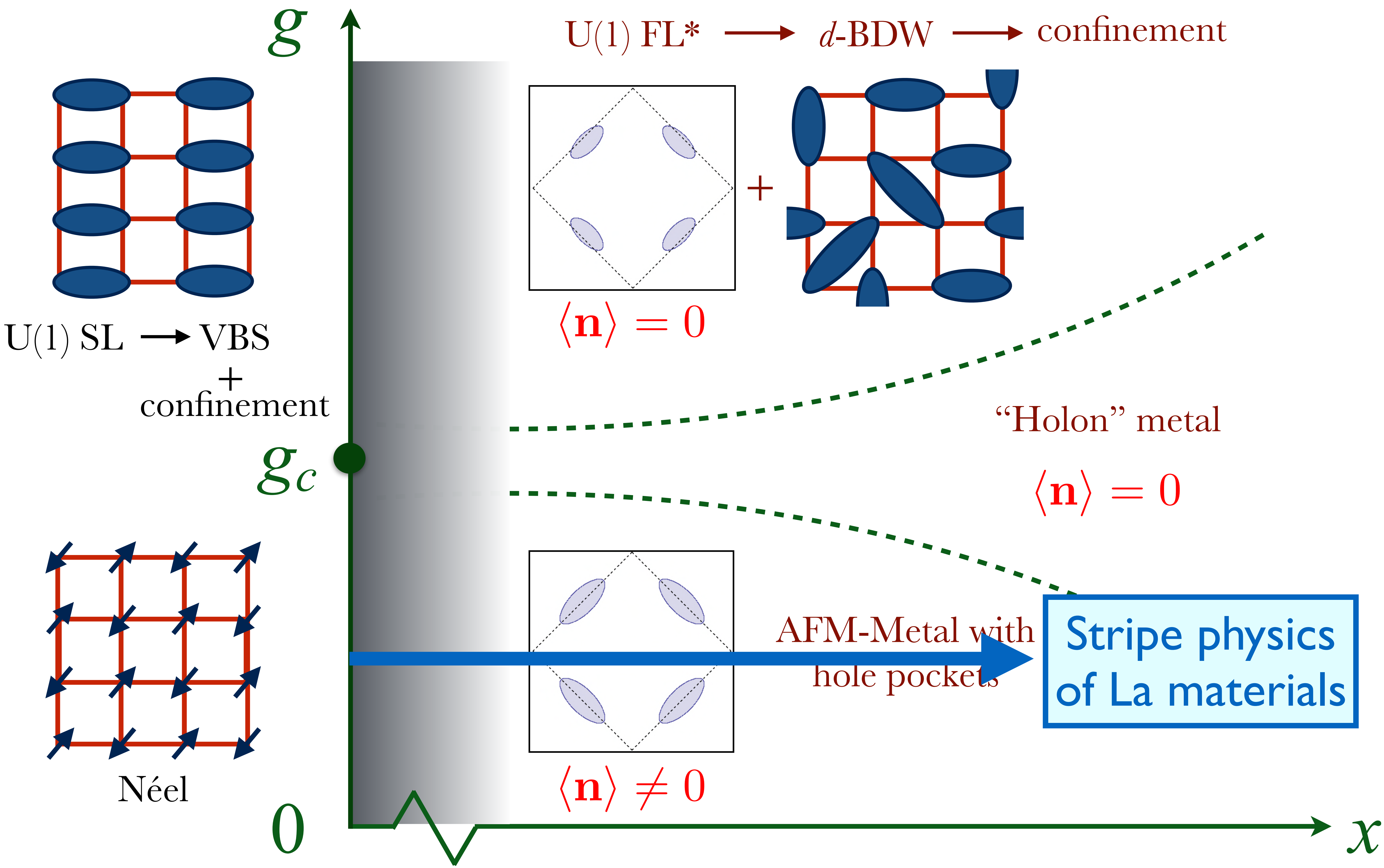

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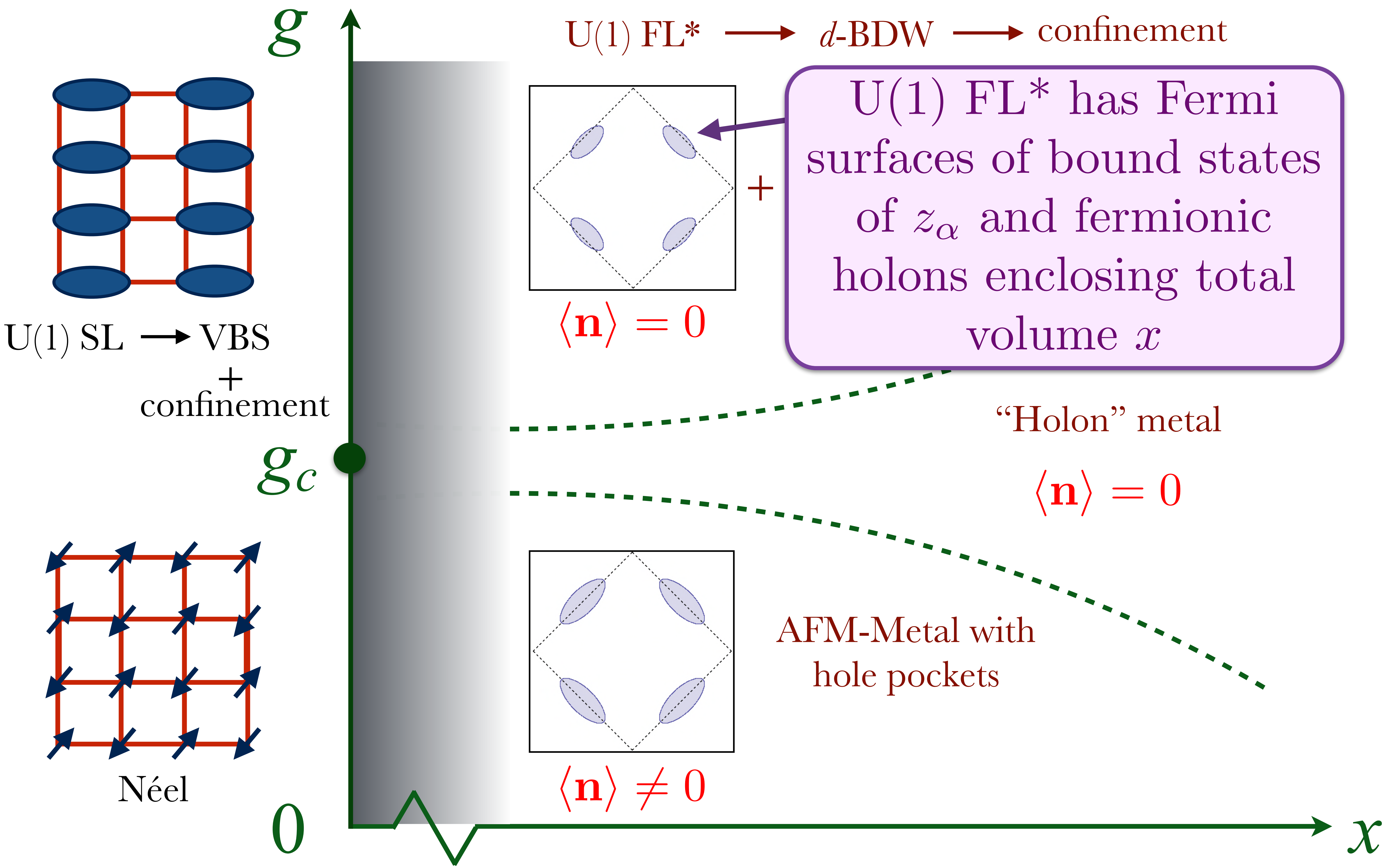

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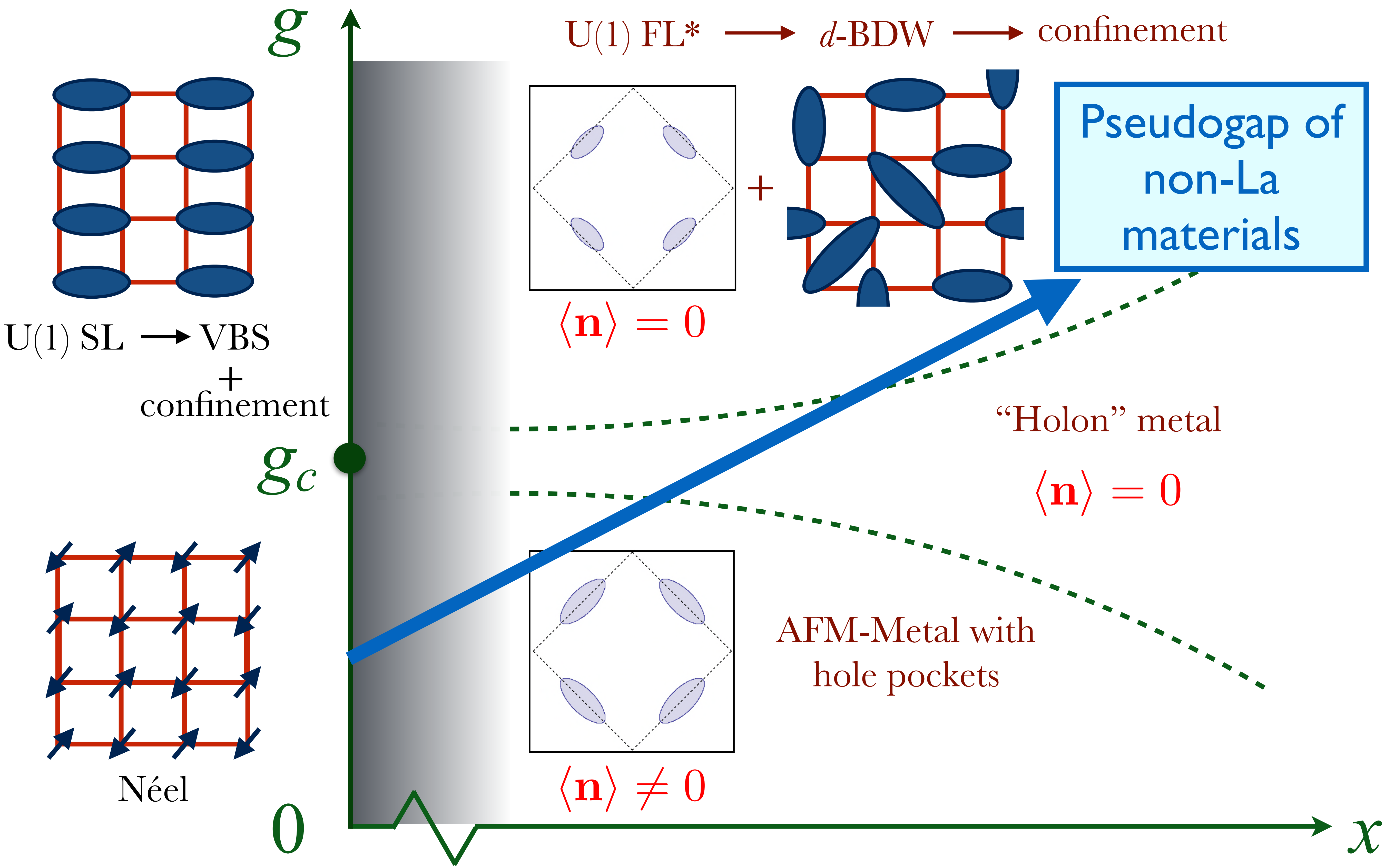

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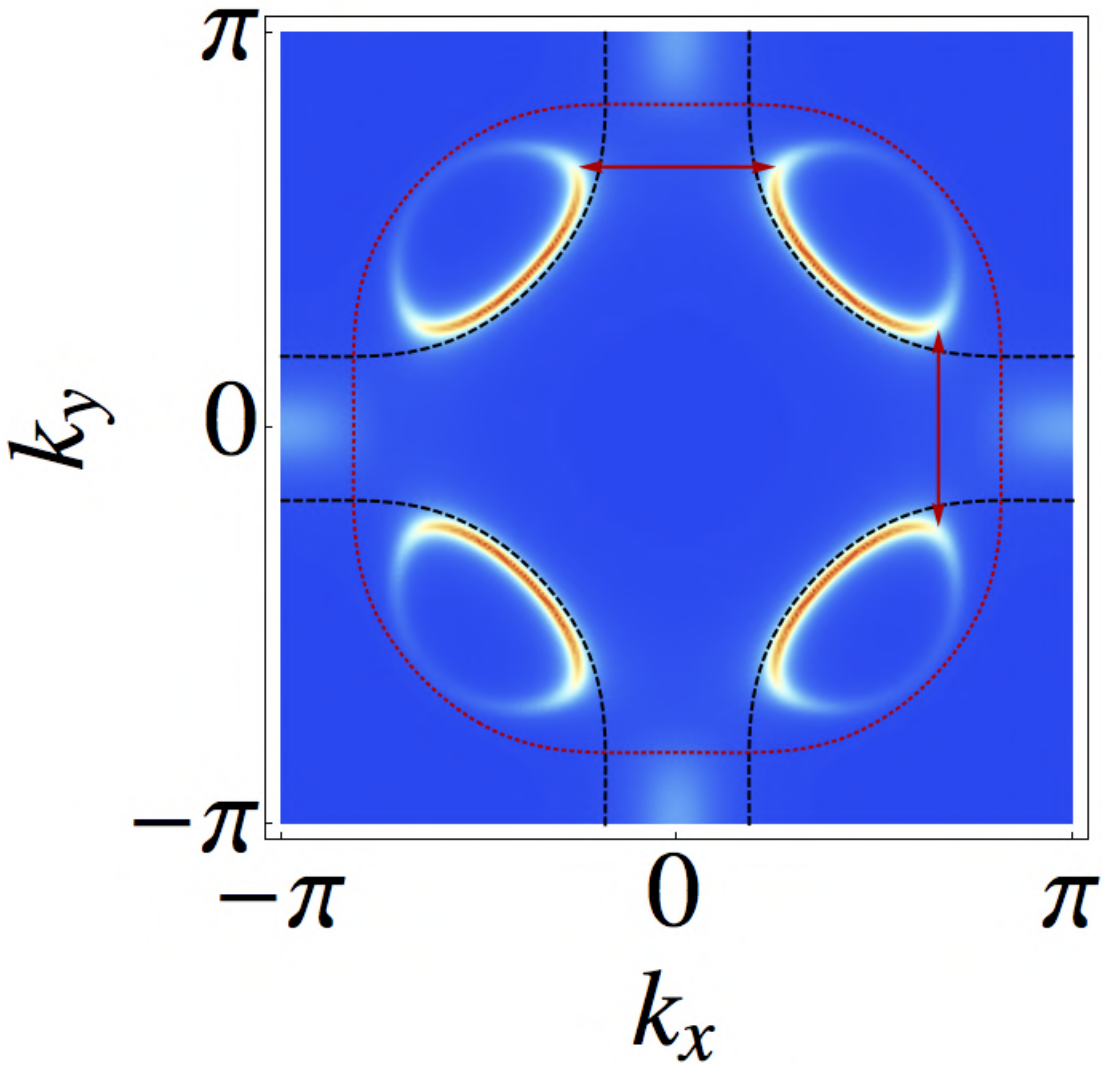

Electron spectral function of FL*

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.

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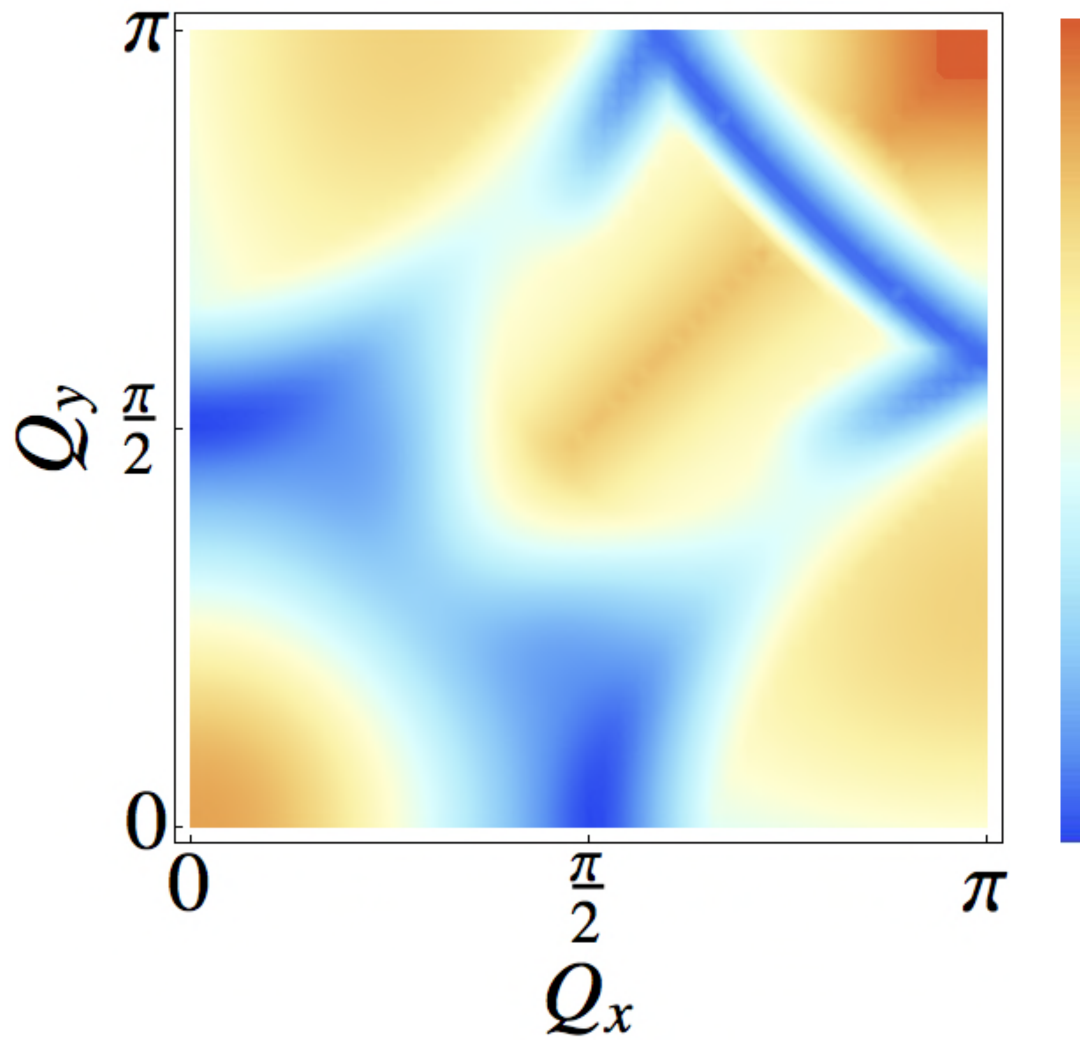

Eigenvalues of spin-singlet, time-reversal-preserving particle-hole propagator

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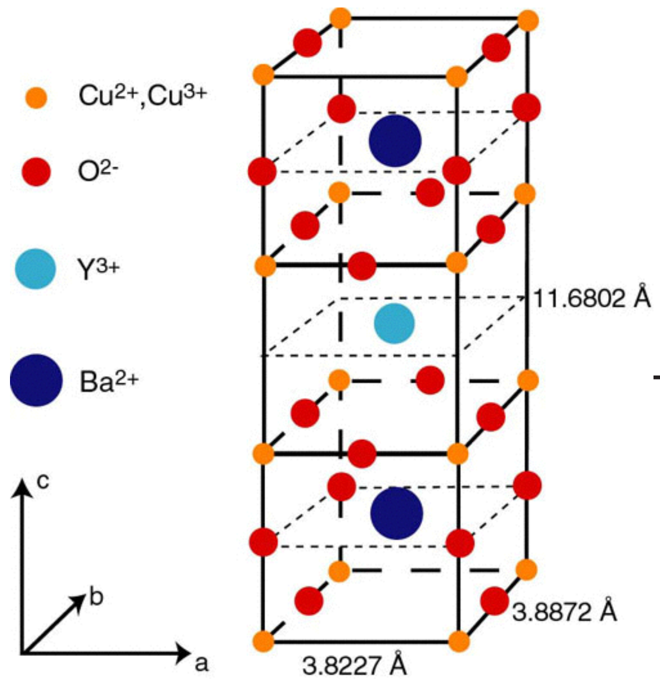
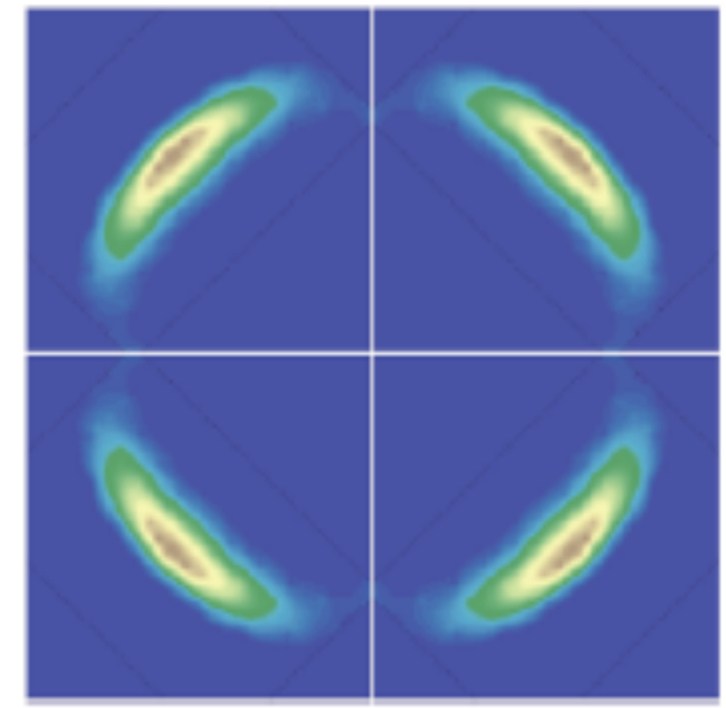
3. Is the *d*-form factor an unexpected window into the spin-liquid physics of the pseudogap ?





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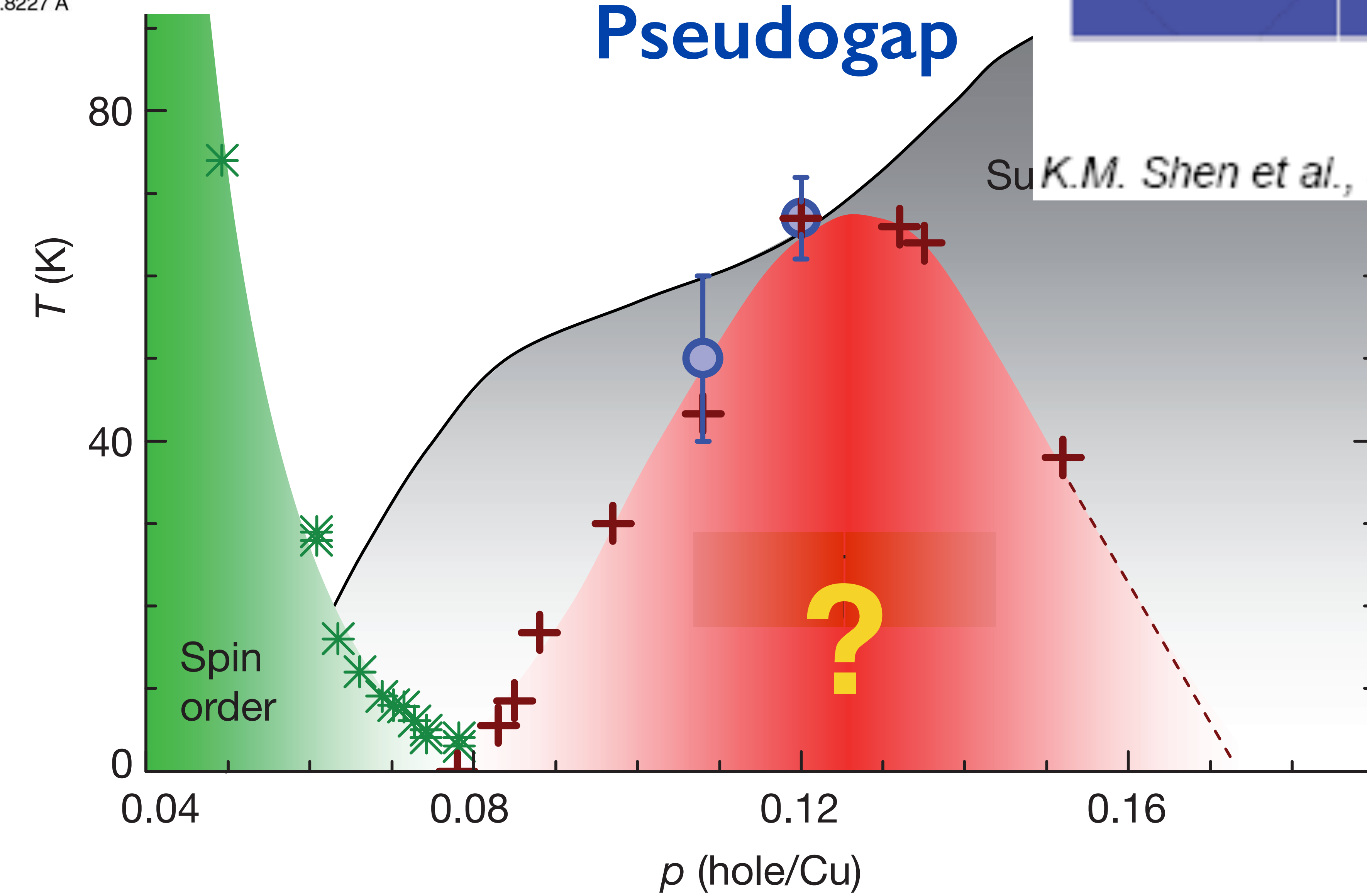

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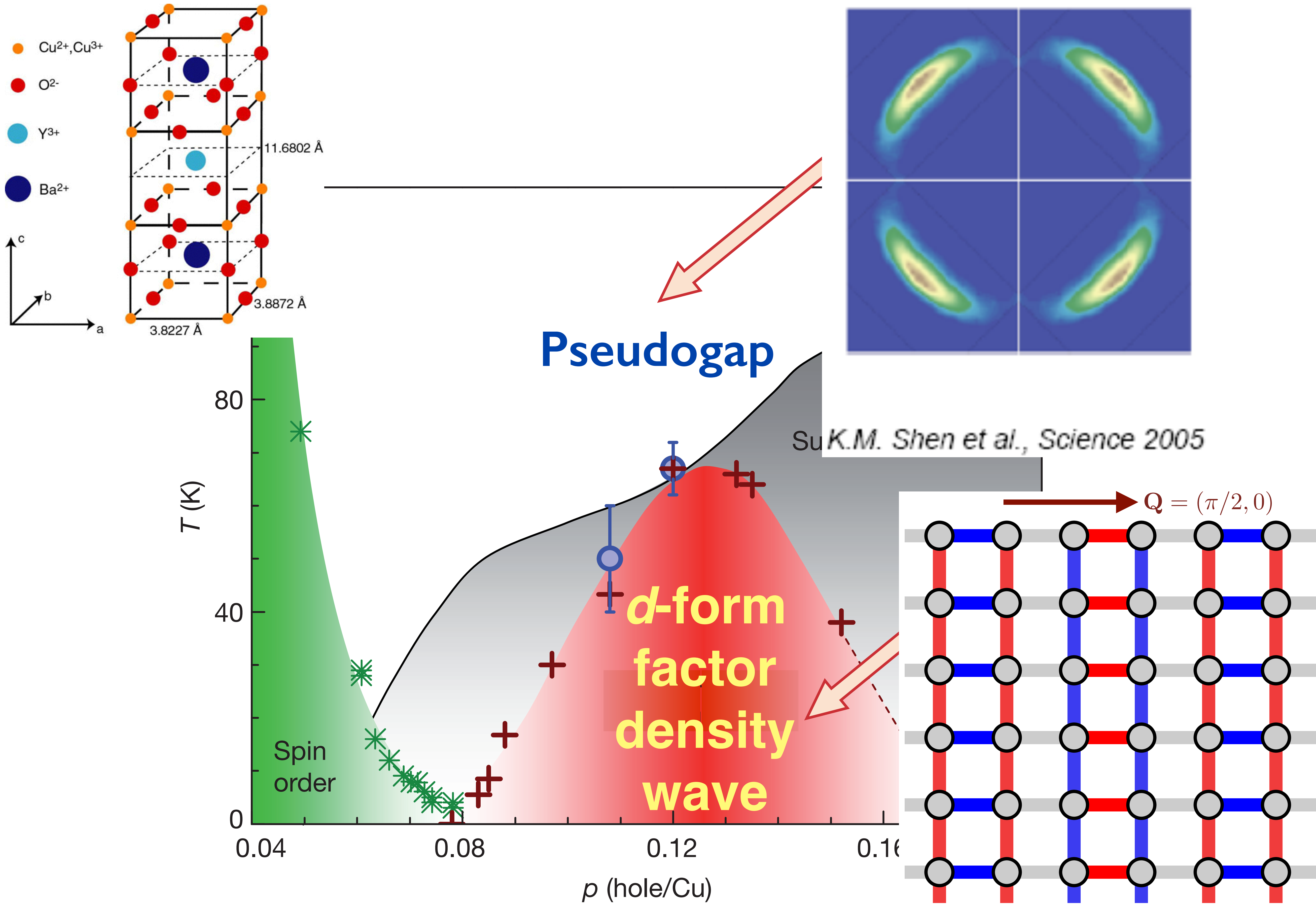

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