Competing order in the cuprates: d-wave bond order and the pseudogap regime

American Physical Society
W40.00001
2:30 PM, Thursday March 6, 2014
Mile High Ballroom 2B-3B

Subir Sachdev

Talk online: sachdev.physics.harvard.edu

PHYSICS
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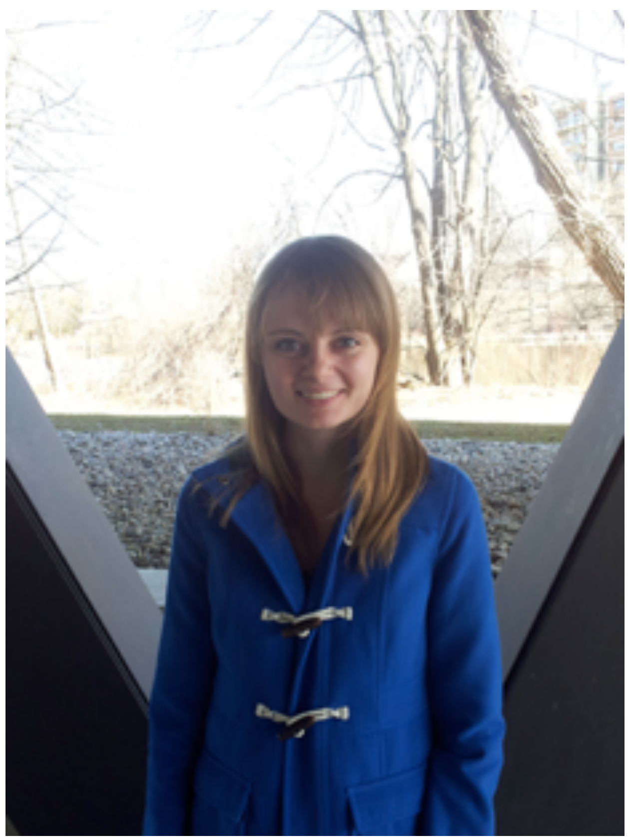
Max Metlitski

Rolando La Placa

Andrea Allais

Johannes Bauer



Lauren Hayward

Roger Melko

David Hawthorn

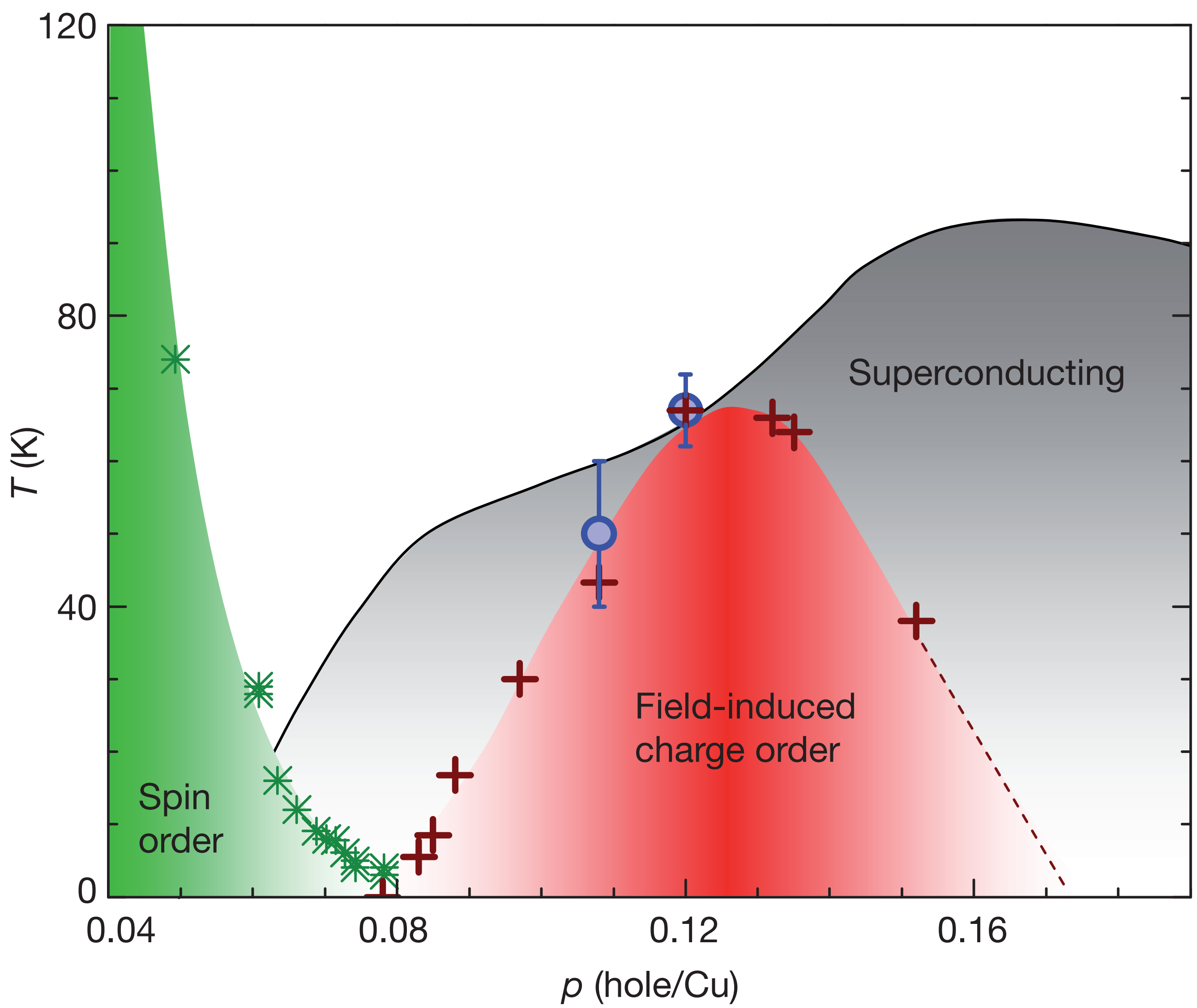
Debanjan Chowdhury

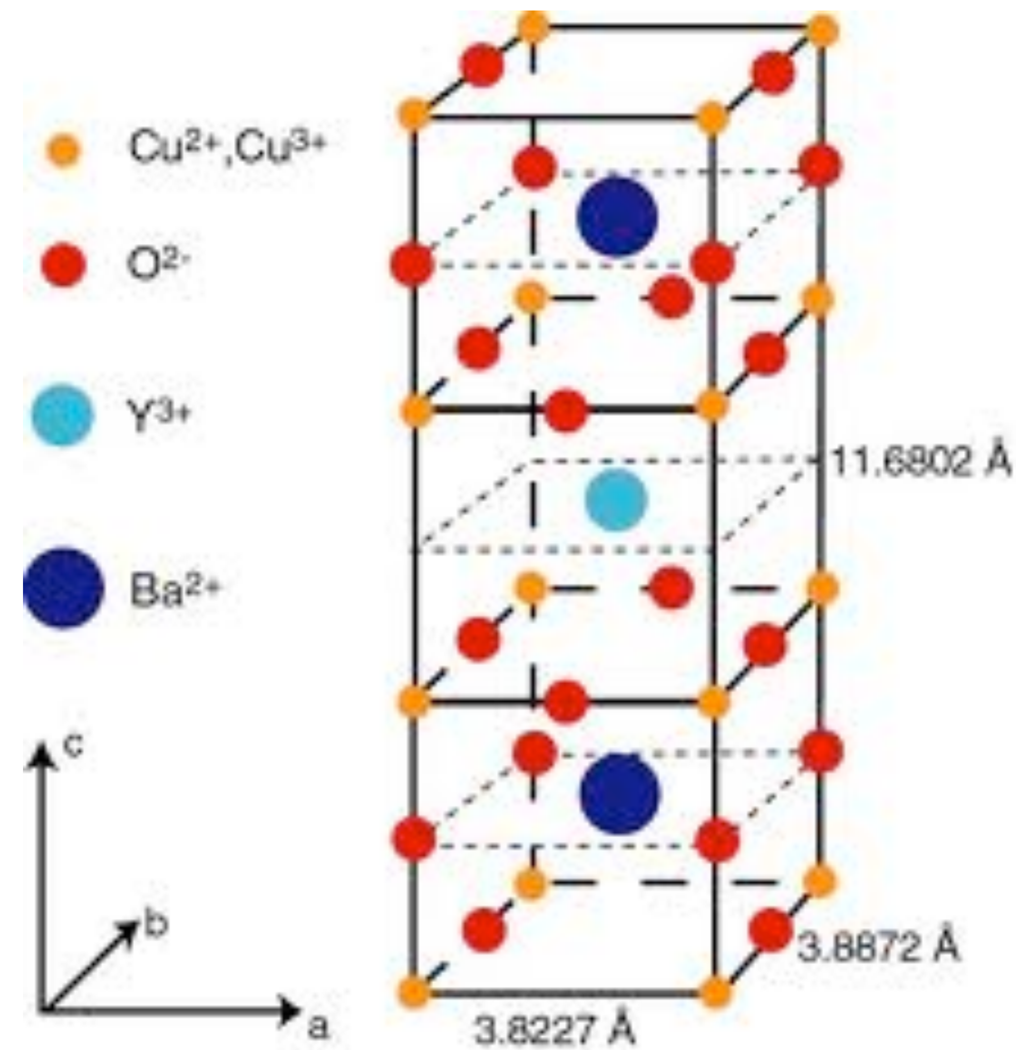
Jay Deep Sau

Magnetic-field-induced charge-stripe order in the high-temperature superconductor $YBa_2Cu_3O_y$

Tao Wu[1], Hadrien Mayaffre[1], Steffen Krämer[1], Mladen Horvatić[1], Claude Berthier[1], W. N. Hardy[2,3], Ruixing Liang[2,3], D. A. Bonn[2,3] & Marc-Henri Julien[1]

8 SEPTEMBER 2011 | VOL 477 | NATURE | 191





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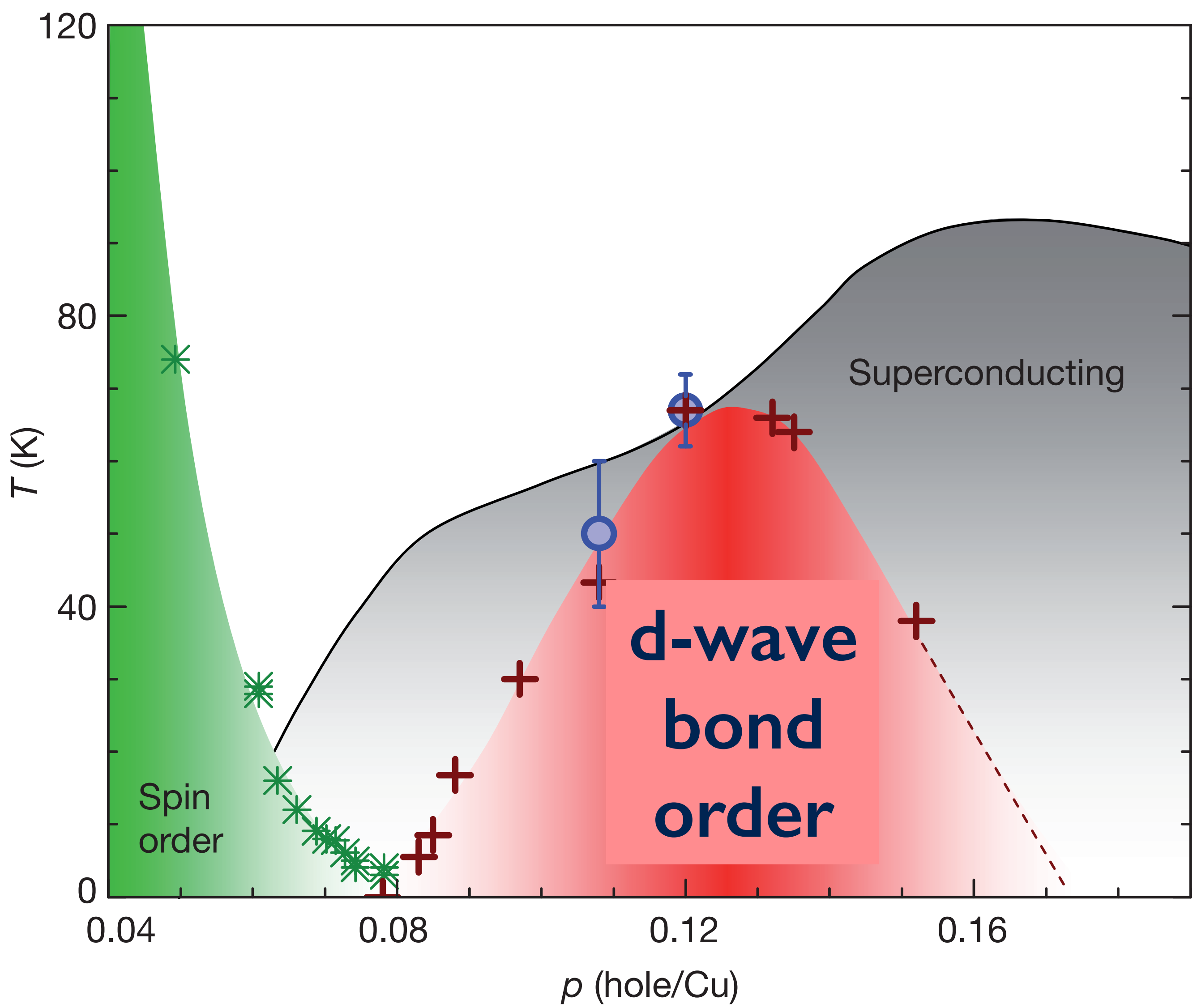
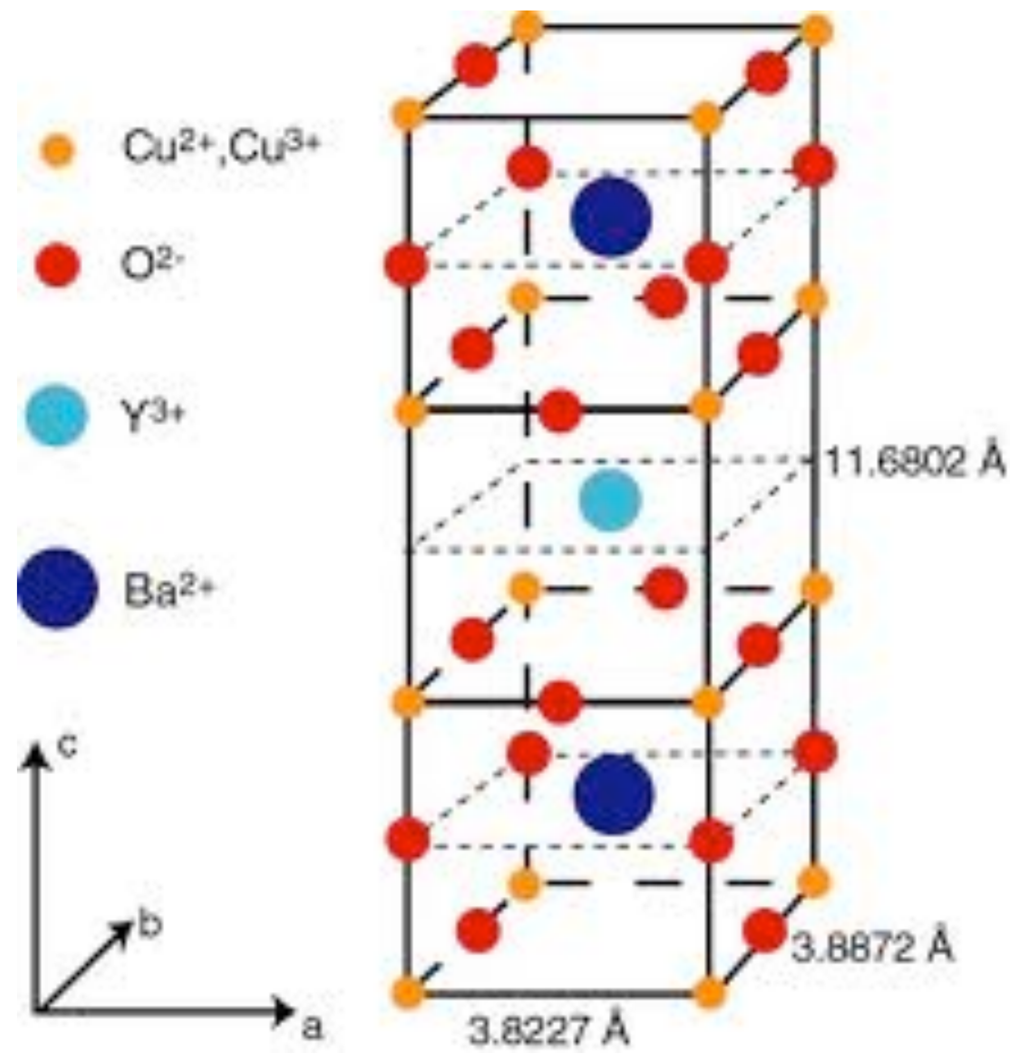
S. Sachdev and R. La Placa, Physical Review Letters **111**, 027202 (2013)
J. D. Sau and S. Sachdev, Physical Review B **89**, 075129 (2014)
A. Allais, J. Bauer, and S. Sachdev, arXiv:1402.4807
A. Allais, J. Bauer, and S. Sachdev, arXiv:1402.6311





Outline

1. Antiferromagnetism in metals and *d*-wave superconductivity

2. Competing order: *d*-wave bond order

3. The pseudogap regime of the hole-doped cuprate superconductors

Angular fluctuations of a multicomponent order

Lauren Hayward, A53.00011, Mile High Ballroom 2C, Monday March 3, 10:00 AM

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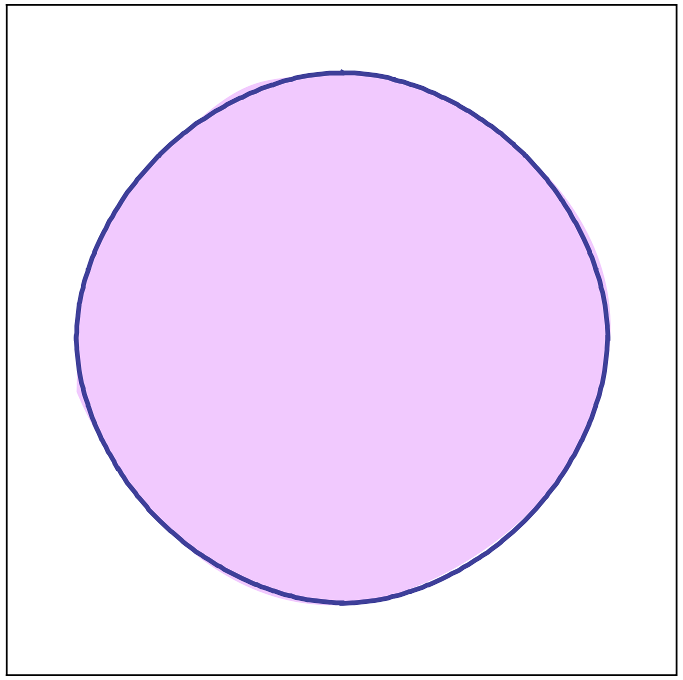
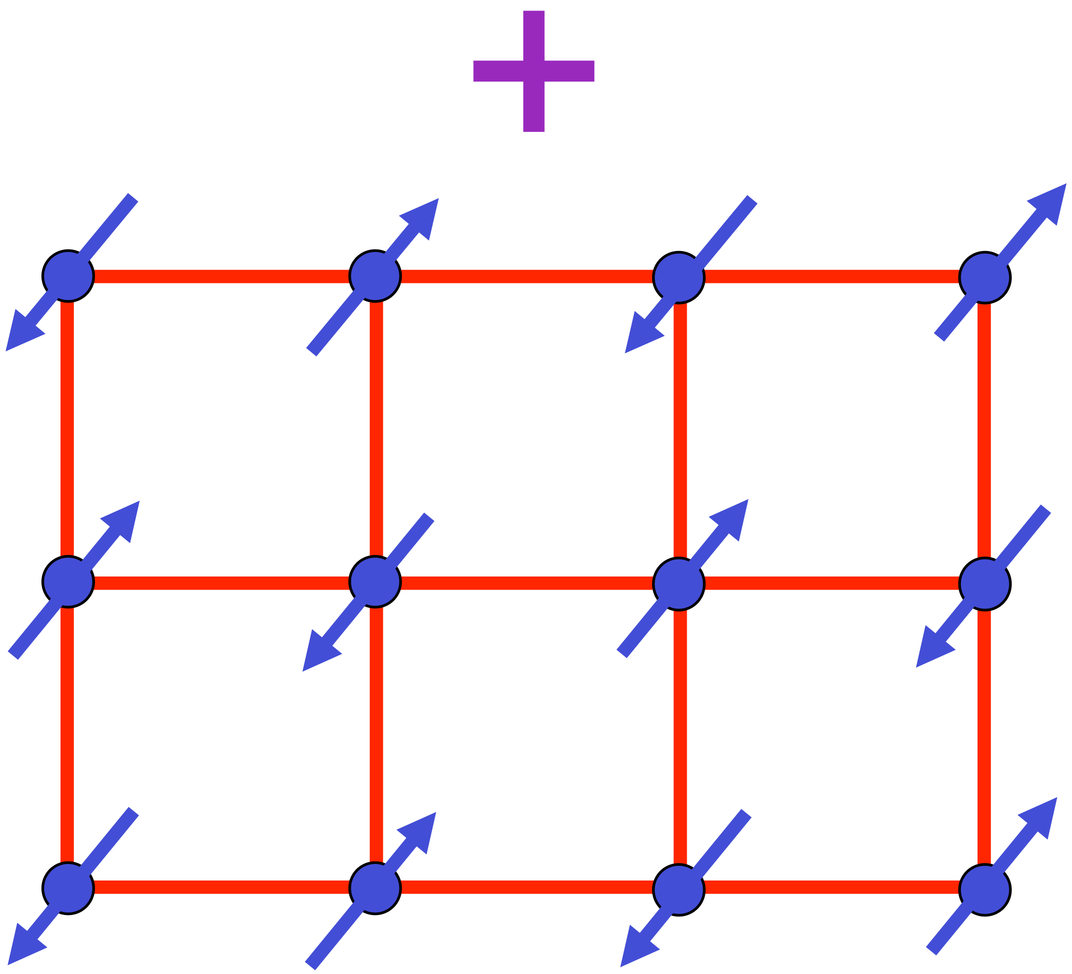
Fermi surface+antiferromagnetism

Metal with "large"
Fermi surface



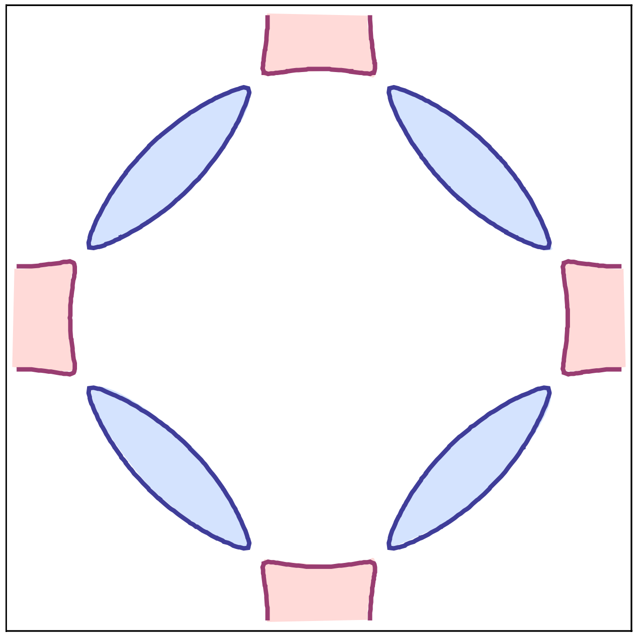


The electron spin polarization obeys

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

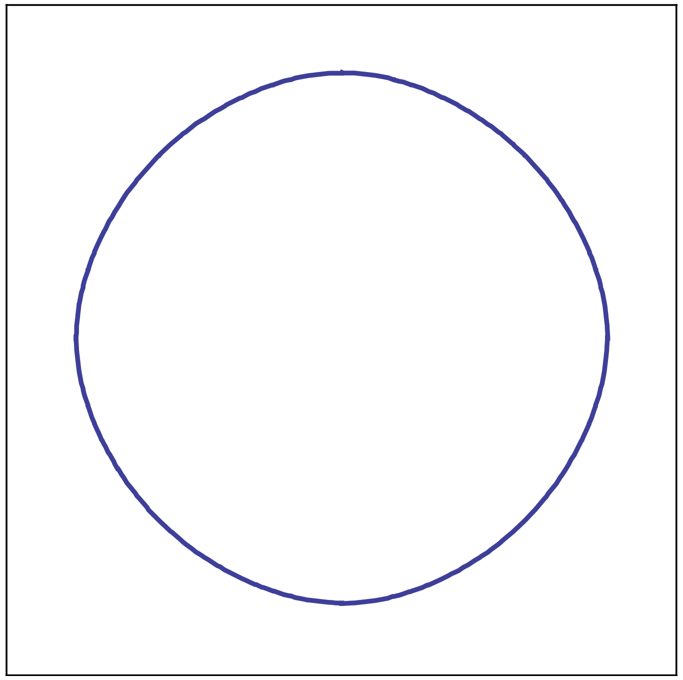
where $\mathbf{K}$ is the ordering wavevector.

Quantum phase transition with onset of antiferromagnetism in a metal



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

Metal with electron and hole pockets



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

Metal with "large" Fermi surface

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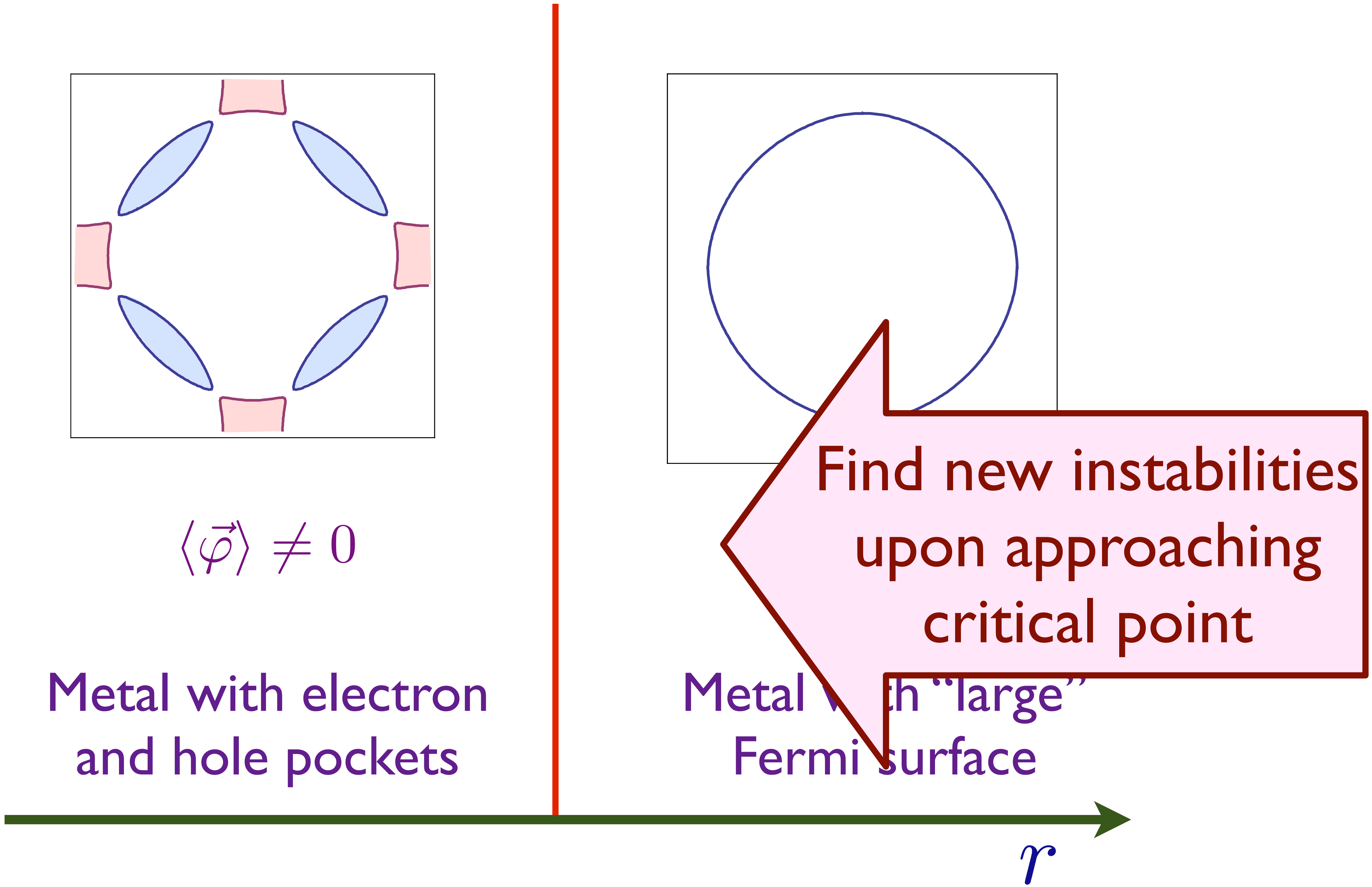
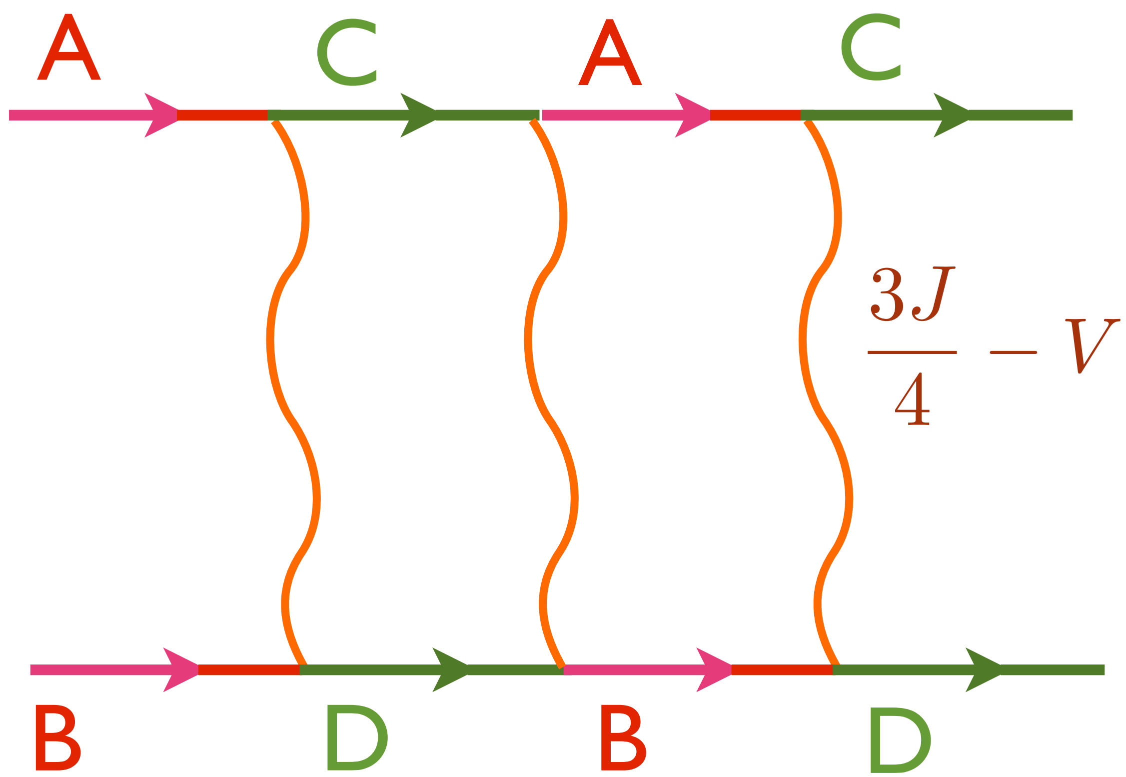
Quantum phase transition with onset of antiferromagnetism in a metal



Pairing "glue" from antiferromagnetic fluctuations

$$H = \sum_{\boldsymbol{x},\boldsymbol{a}} \Big[-t_a c^\dagger_{\boldsymbol{x}+\boldsymbol{a}} c_{\boldsymbol{x}} + \frac{J_a}{8} c^\dagger_{\boldsymbol{x}+\boldsymbol{a}} \vec{\sigma} c_{\boldsymbol{x}+\boldsymbol{a}} \cdot c^\dagger_{\boldsymbol{x}} \vec{\sigma} c_{\boldsymbol{x}} + \frac{V_a}{2} c^\dagger_{\boldsymbol{x}+\boldsymbol{a}} c_{\boldsymbol{x}+\boldsymbol{a}} c^\dagger_{\boldsymbol{x}} c_{\boldsymbol{x}} \Big] + H_U \, ,$$



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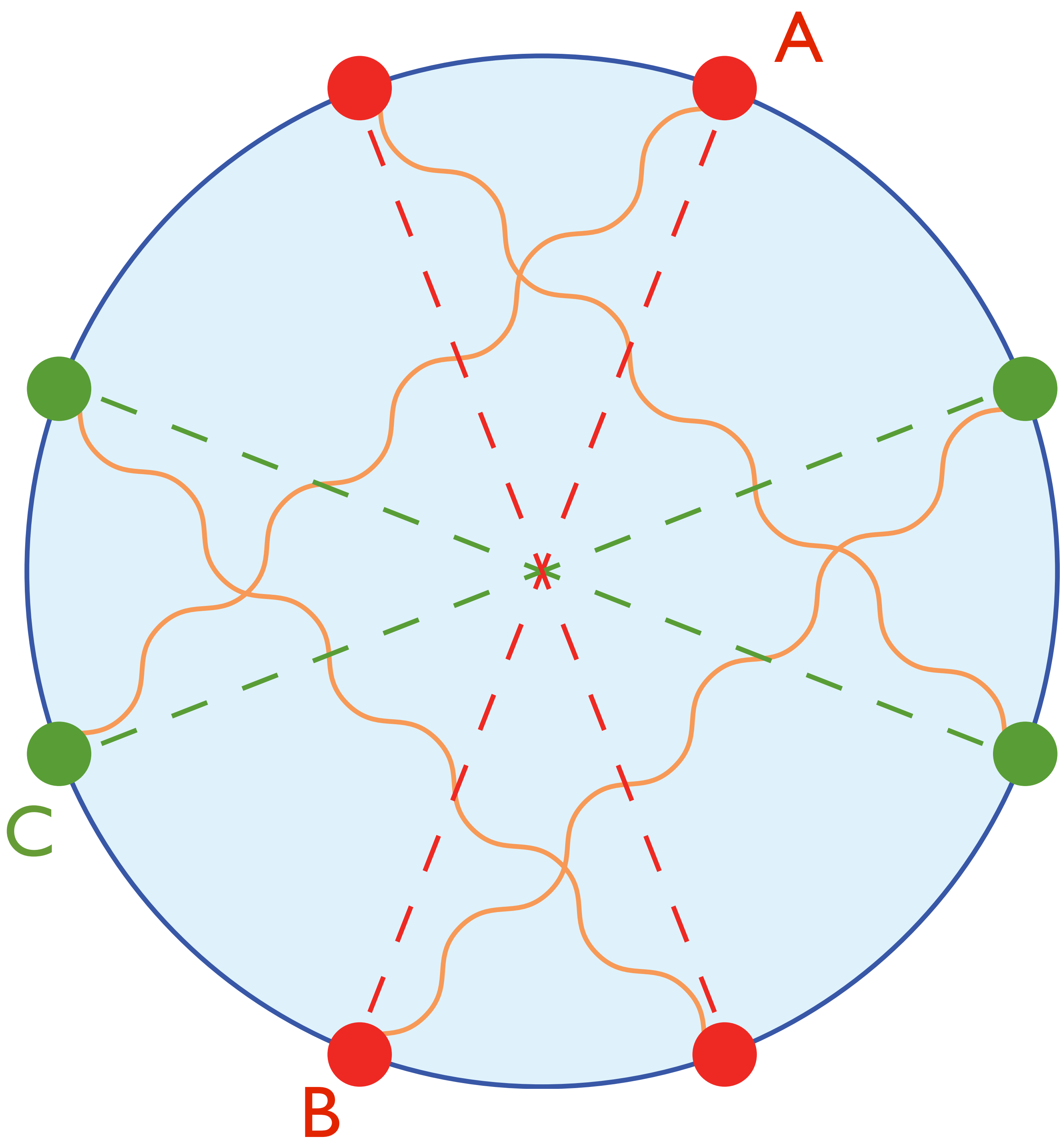

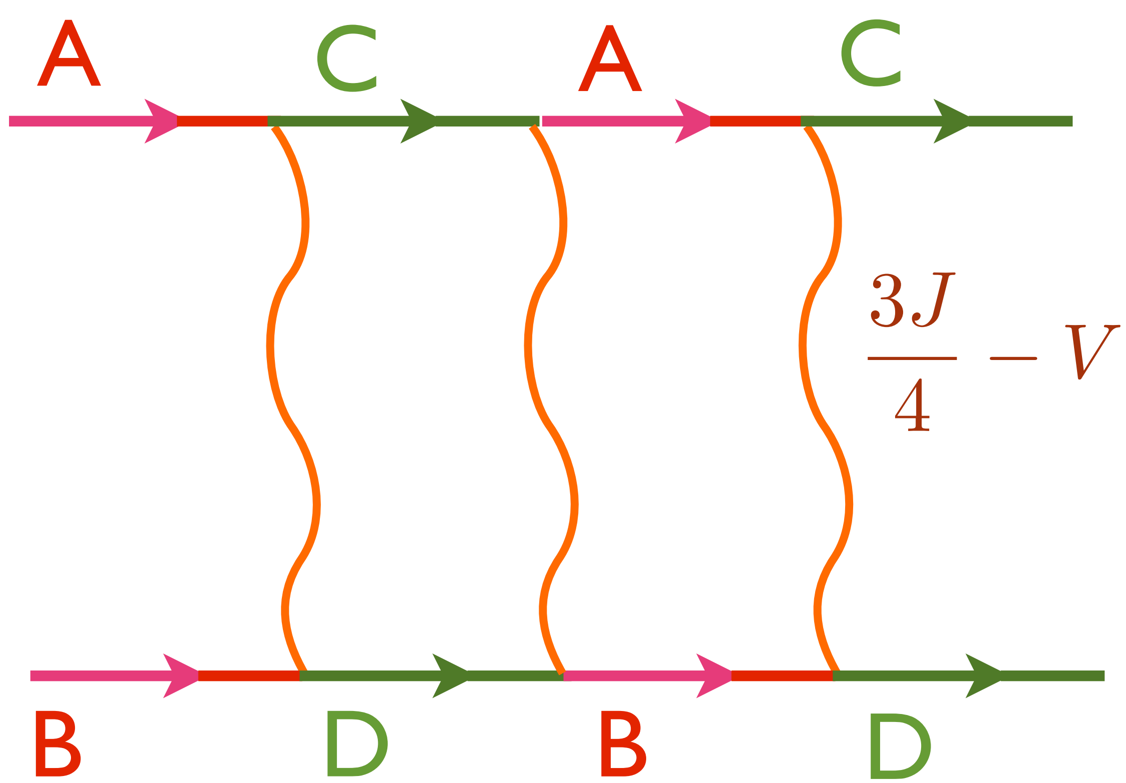

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$$\left\langle c^\dagger_{\mathbf{k}\alpha} c^\dagger_{-\mathbf{k}\beta} \right\rangle = \varepsilon_{\alpha\beta} \Delta_S (\cos k_x - \cos k_y)$$

V. J. Emery, *J. Phys. (Paris) Colloq.* **44**, C3-977 (1983)
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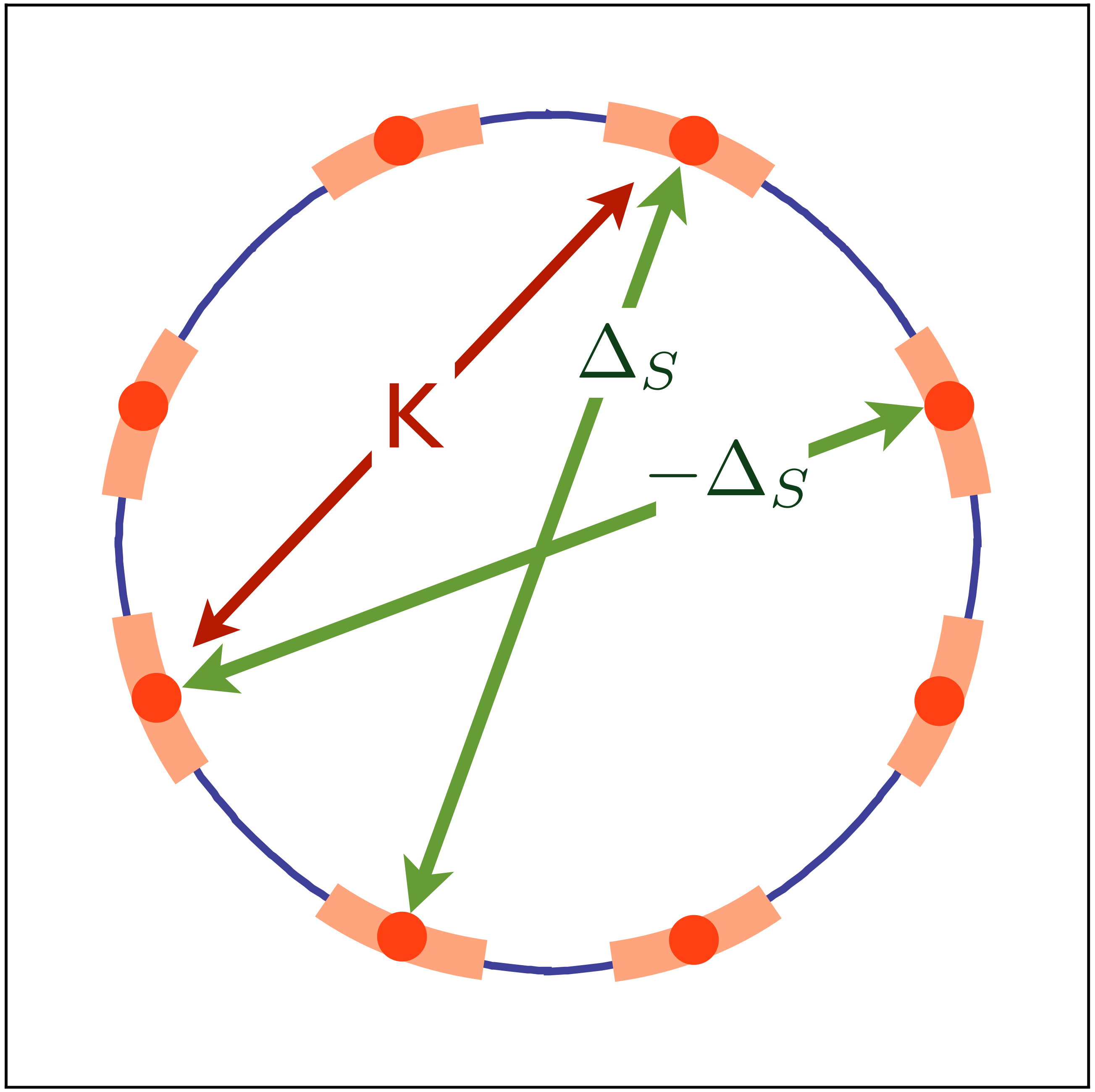

d-wave superconductor: particle-particle pairing at *and near* hot spots, with sign-changing pairing amplitude

Outline

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Angular fluctuations of a multicomponent order

Lauren Hayward, A53.00011, Mile High Ballroom 2C, Monday March 3, 10:00 AM

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

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

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

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

This pseudospin (gauge) symmetry is important in classifying spin liquid ground states of H_J.

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)

Pseudospin symmetry of the exchange interaction

$$H_{tJ} = -\sum_{i,j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \sum_{i<j} J_{ij} \vec{S}_i \cdot \vec{S}_j + V \sum_{\langle ij \rangle} n_i n_j$$

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

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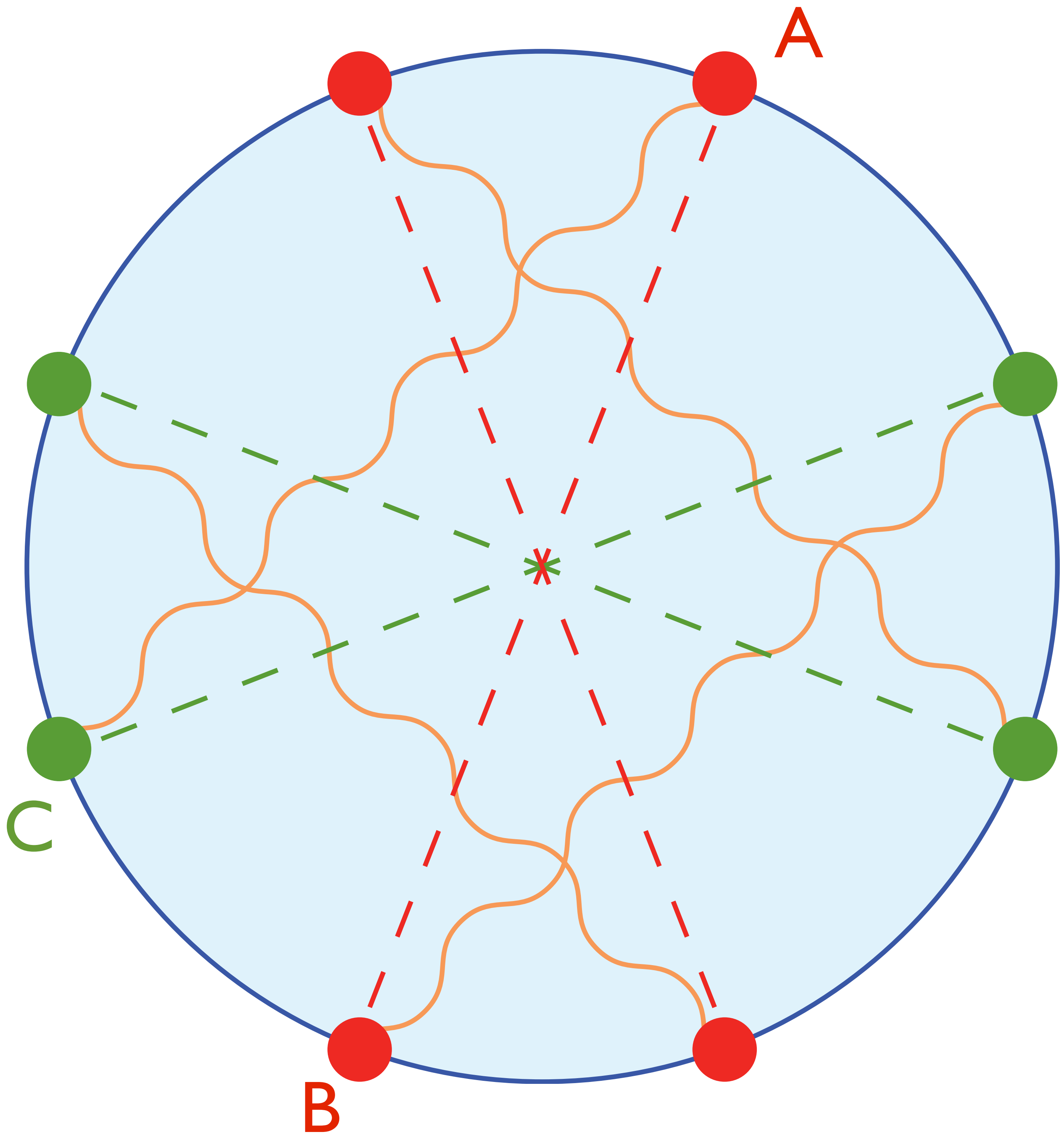
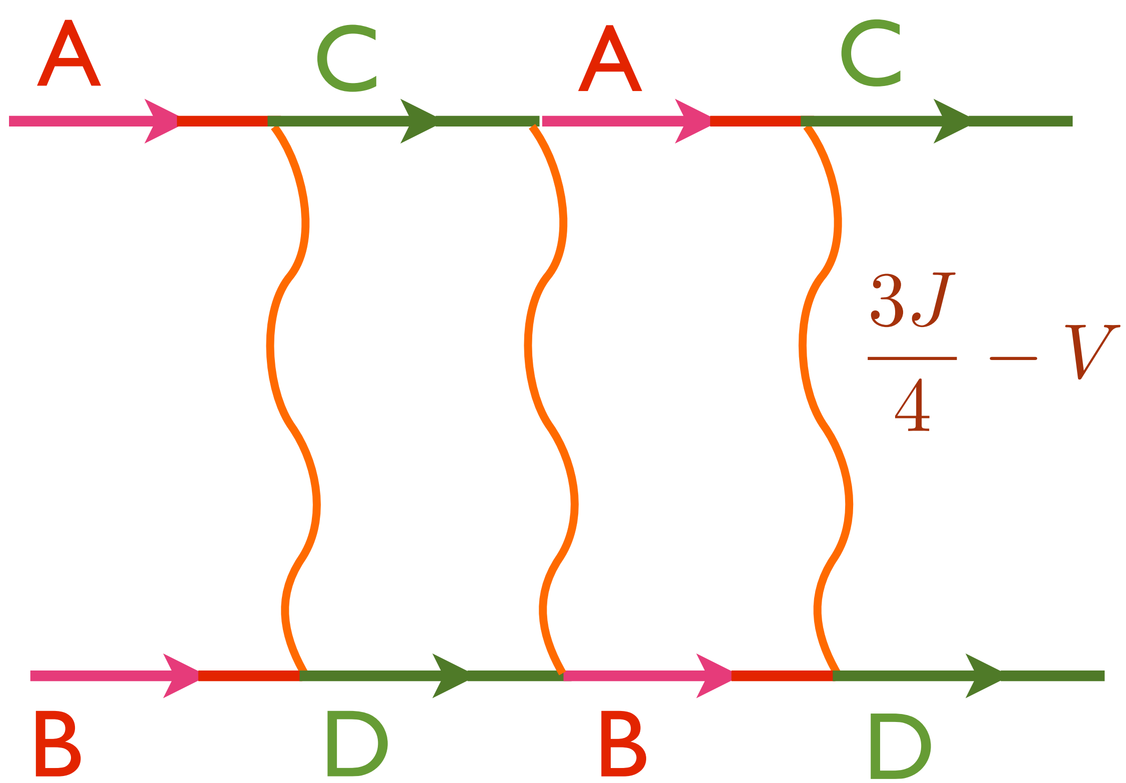
This pseudospin (gauge) symmetry is important in classifying spin liquid ground states of H_J. It is fully broken by t_{ij}, V_{ij}, but we find that it nevertheless has important consequences in ordinary metals with antiferromagnetic interactions.

Pairing "glue" from antiferromagnetic fluctuations





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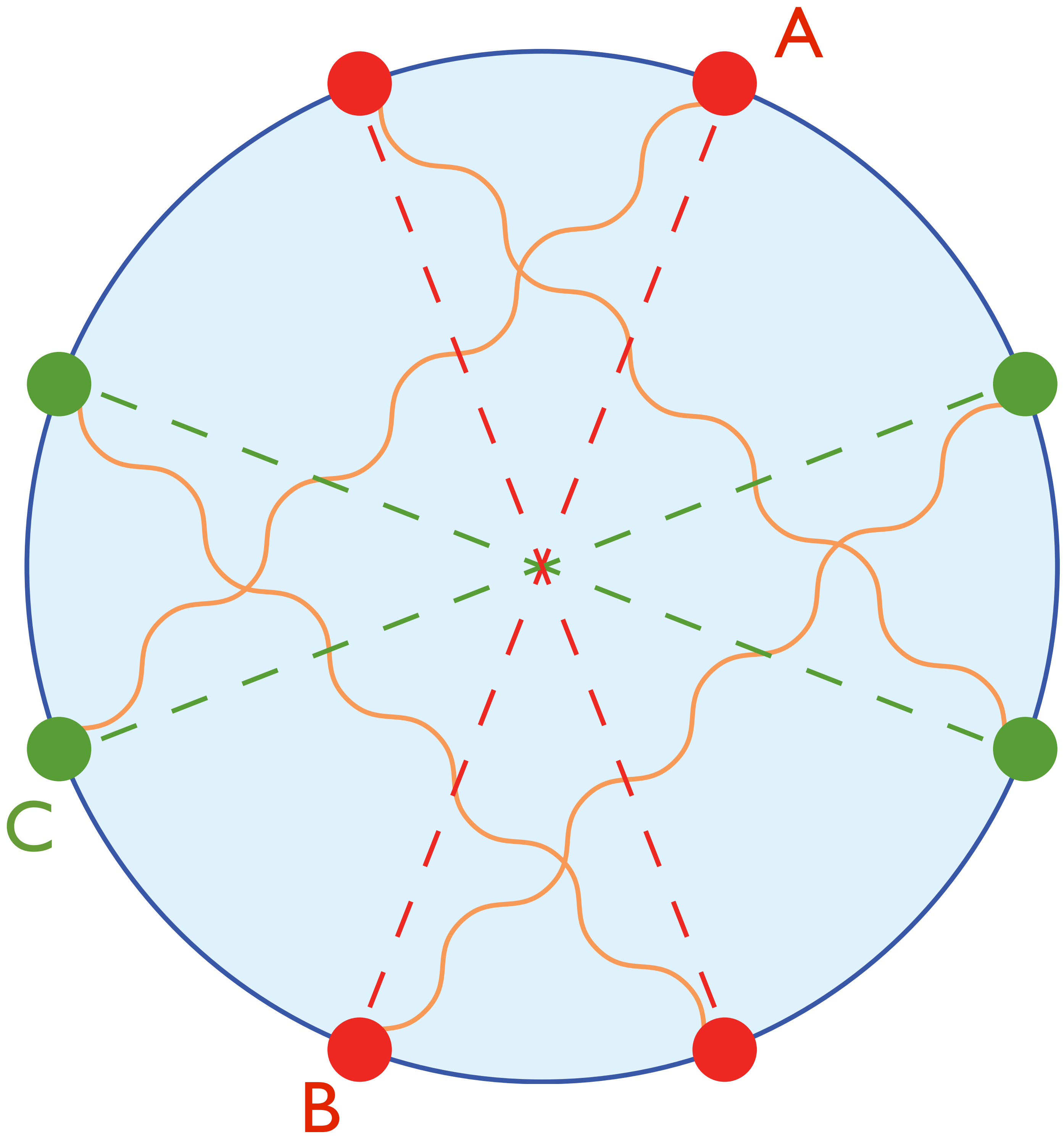
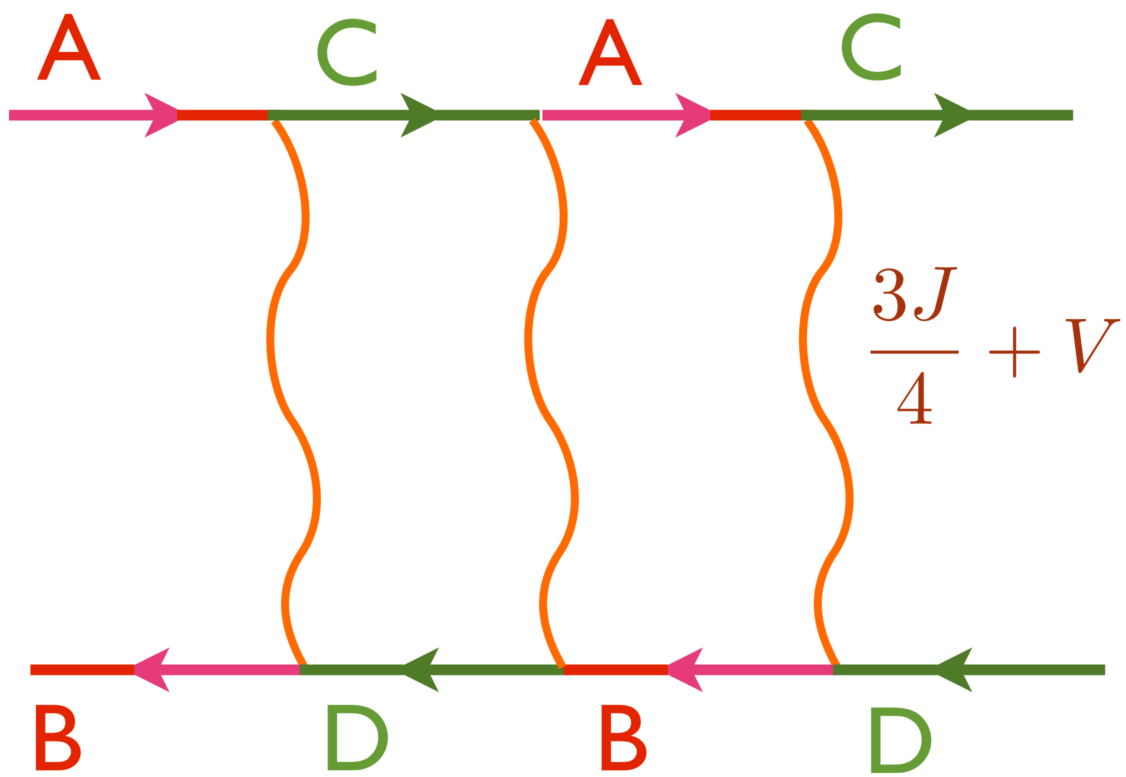
S. Raghu, S.A. Kivelson, and D.J. Scalapino, *Phys. Rev. B* **81**, 224505 (2010)

Same “glue” leads to particle-hole pairing



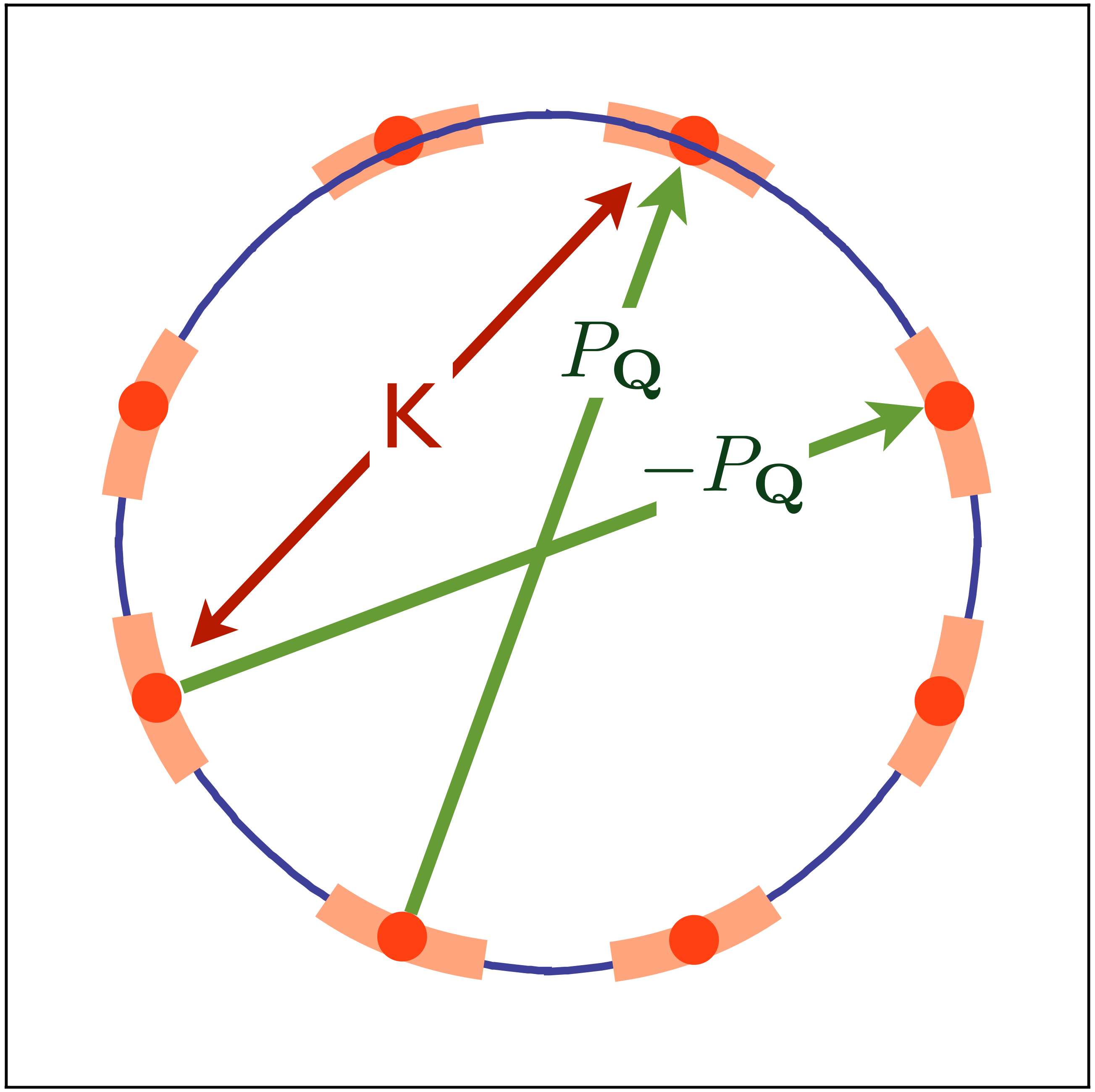


M. A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)
S. Sachdev and R. LaPlaca *Phys. Rev. Lett.* **111**, 027202 (2013)
J. D. Sau and S. Sachdev, *Phys. Rev. B* **89**, 075129 (2014)

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

After pseudospin rotation on *half* the hot-spots

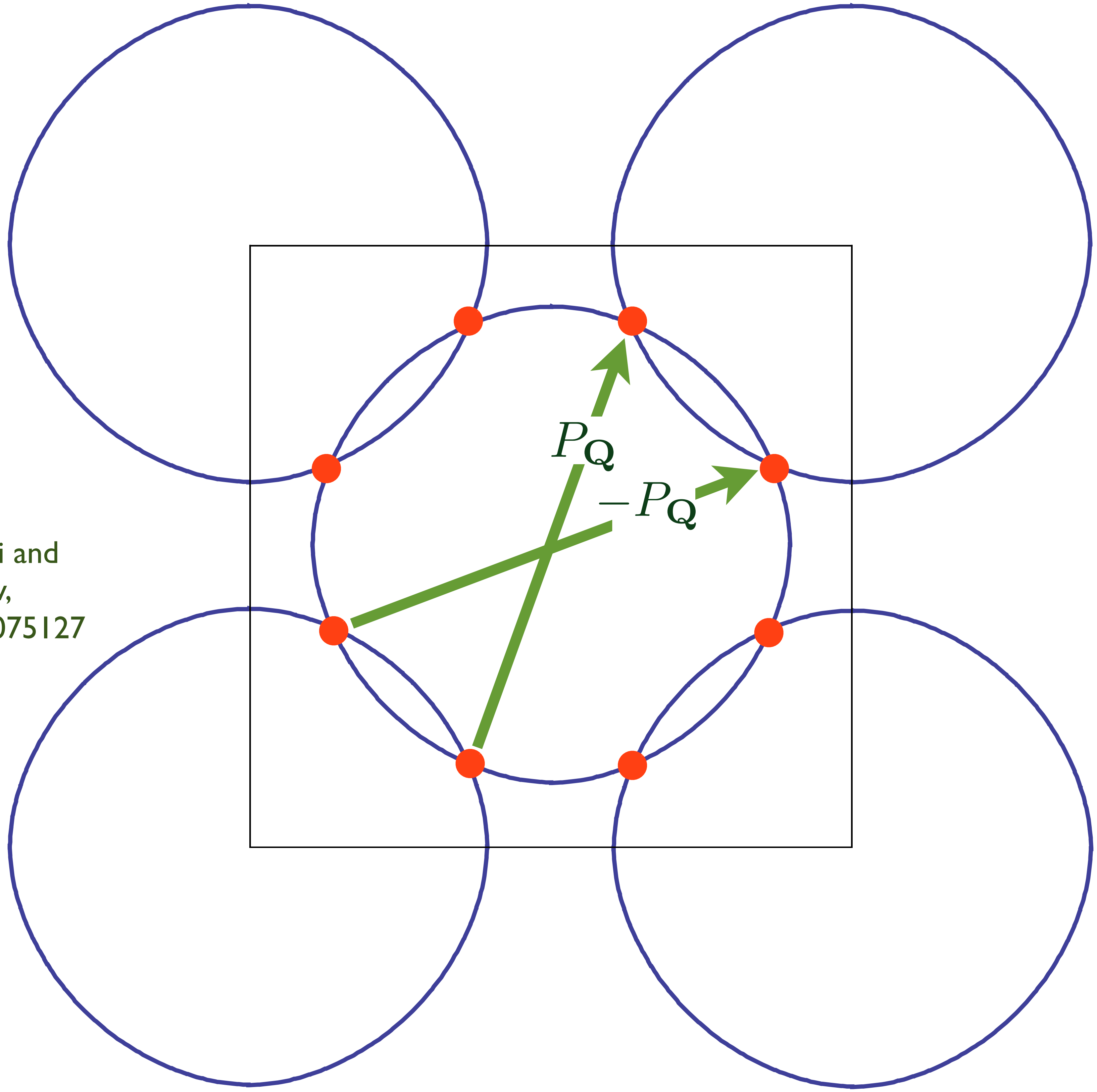
M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)



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

Incommensurate d-wave bond order: particle-hole pairing at <u>*and near*</u> hot spots, with sign-changing pairing amplitude

Incommensurate *d*-wave bond order



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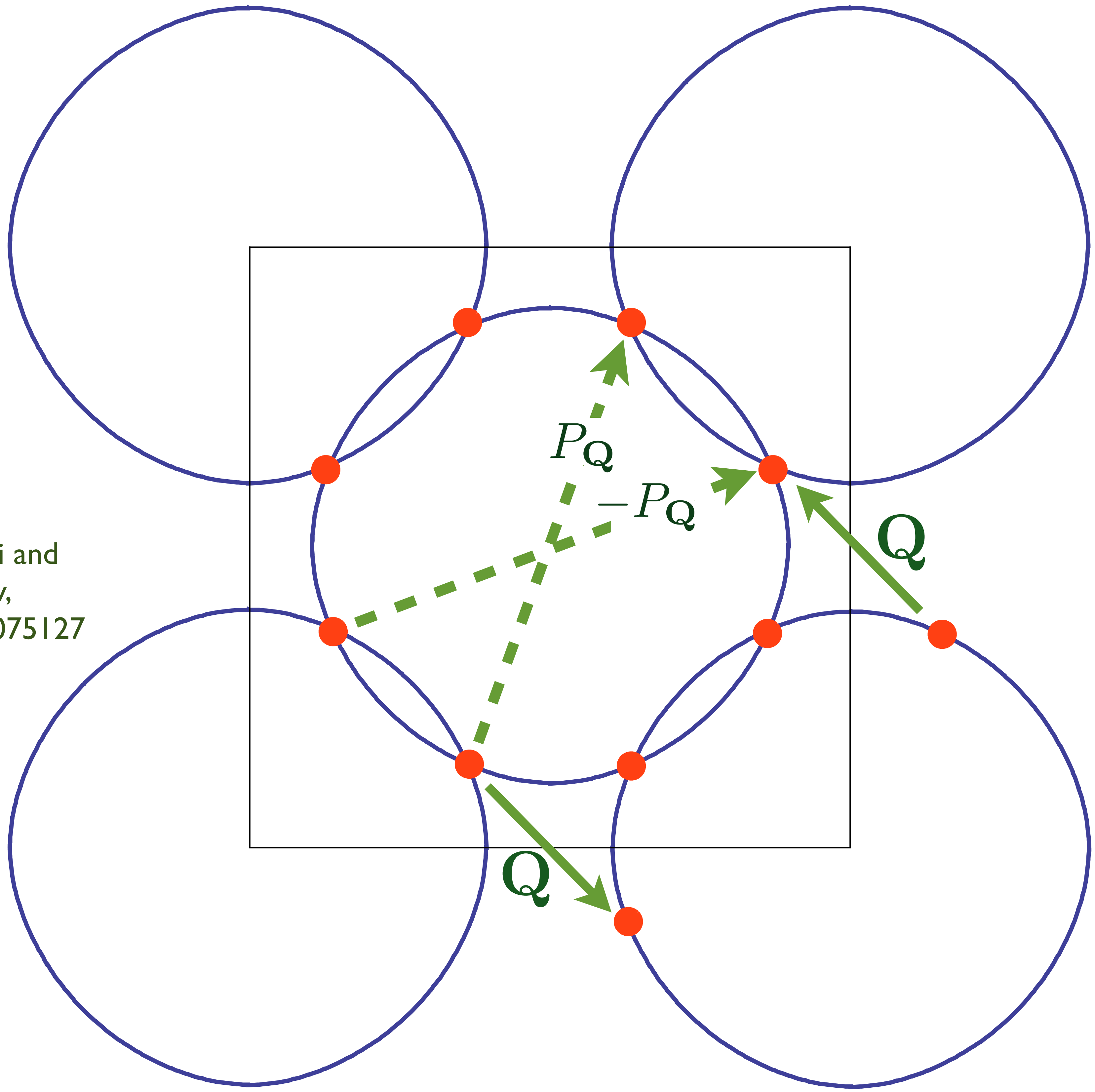

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Phys. Rev. B **85**, 075127
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Bond, charge, and current order

Consider modulation in a bilocal variable at the Cu sites $\mathbf{r}_i$ and $\mathbf{r}_j$

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

relative co-ord.

average co-ord.

The wavevector $\mathbf{Q}$ is associated with a modulation in the *average* co-ordinate $(\mathbf{r}_i + \mathbf{r}_j)/2$: this determines the wavevector of the X-ray scattering peak.

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The interesting part is the dependence on the *relative* co-ordinate $\mathbf{r}_i - \mathbf{r}_j$. The order parameter $P_{\mathbf{Q}}(\mathbf{k})$ can always be expanded as

$$P_{\mathbf{Q}}(\mathbf{k}) = \sum_{\ell} \mathcal{P}_\ell \, \phi_\ell(\mathbf{k})$$

$$\phi_\ell(\mathbf{k}) = \{1, \cos k_x + \cos k_y, \cos k_x - \cos k_y, \sin k_x - \sin k_y, \ldots\}$$

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The usual charge-density-wave has only $\mathcal{P}_s \neq 0$, and so the density wave is non-zero only if $\mathbf{r}_i = \mathbf{r}_j$.

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The bond-ordered state has predominantly $\mathcal{P}_{s'}, \mathcal{P}_d$ non-zero: in this case the density wave is non-zero only if $\mathbf{r}_i$ and $\mathbf{r}_j$ are nearest neighbors.

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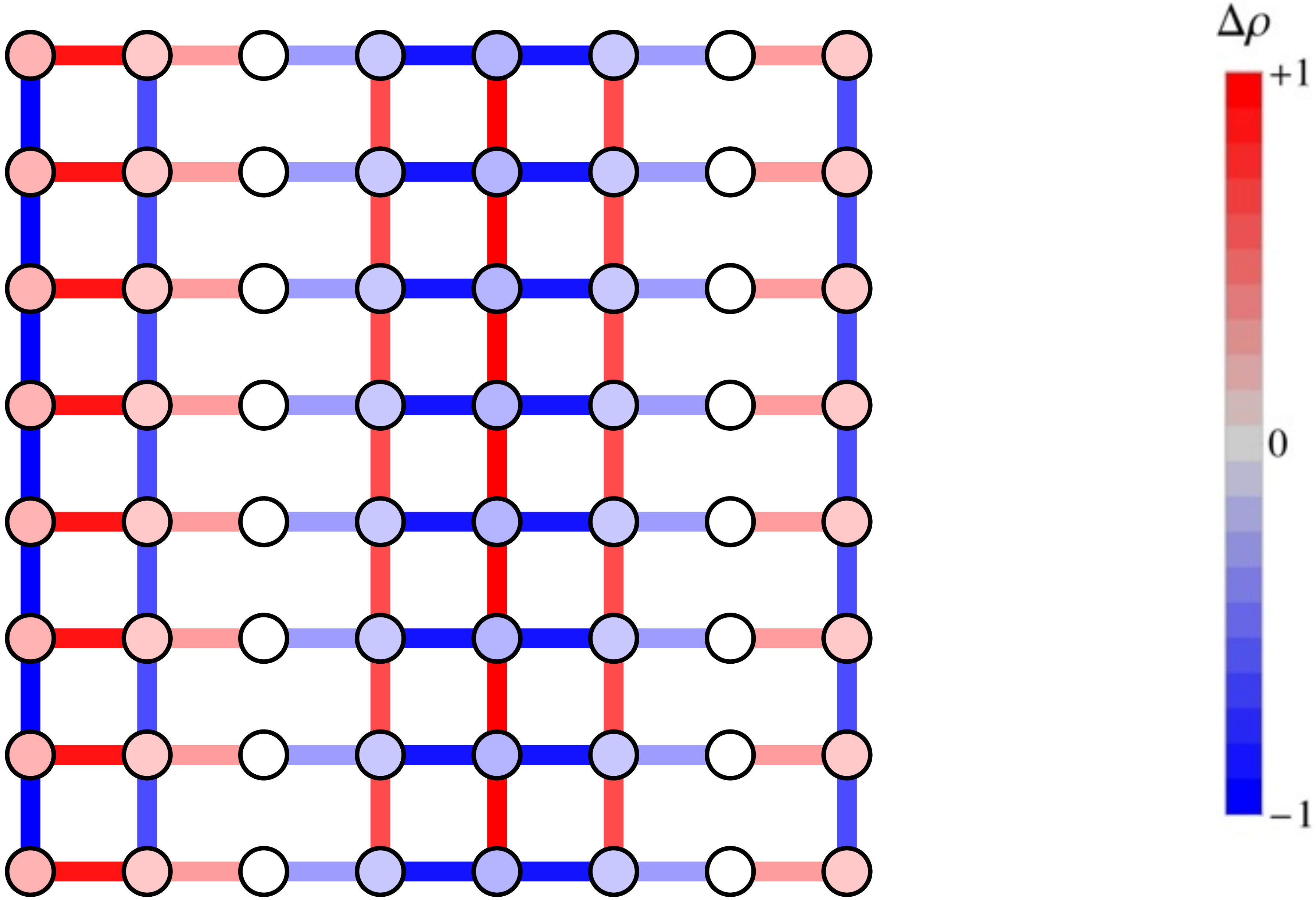
States with spontaneous currents have $\mathcal{P}_p$ non-zero: they break time-reversal

Incommensurate *d*-wave bond order

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

$$P_{ij} = \left[\sum_{\mathbf{k}} P_{\mathbf{Q}}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right] e^{i\mathbf{Q}\cdot(\mathbf{r}_i + \mathbf{r}_j)/2}$$

$$P_{\mathbf{Q}}(\mathbf{k}) = 0.3 + \cos(k_x) - \cos(k_y) \quad \text{and} \quad \mathbf{Q} = (\pi/4, 0)$$



Predominantly *d*-wave bond order.

Bond, charge, and current order

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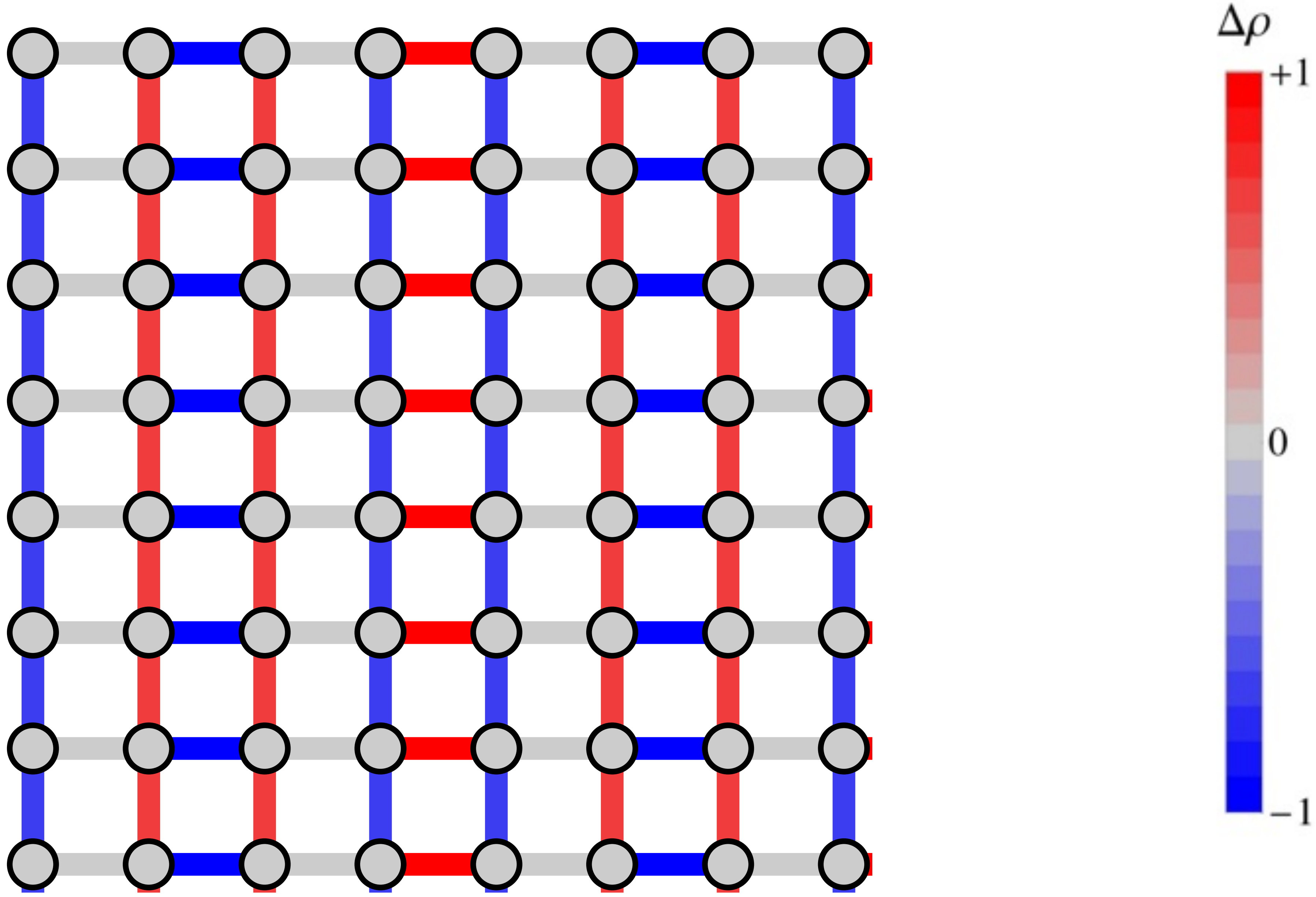
$$P_{\mathbf{Q}}(\mathbf{k}) = \cos(k_x) - \cos(k_y) \quad \text{and} \quad \mathbf{Q} = (\pi/2, 0)$$



d-wave bond order.

Bond, charge, and current order

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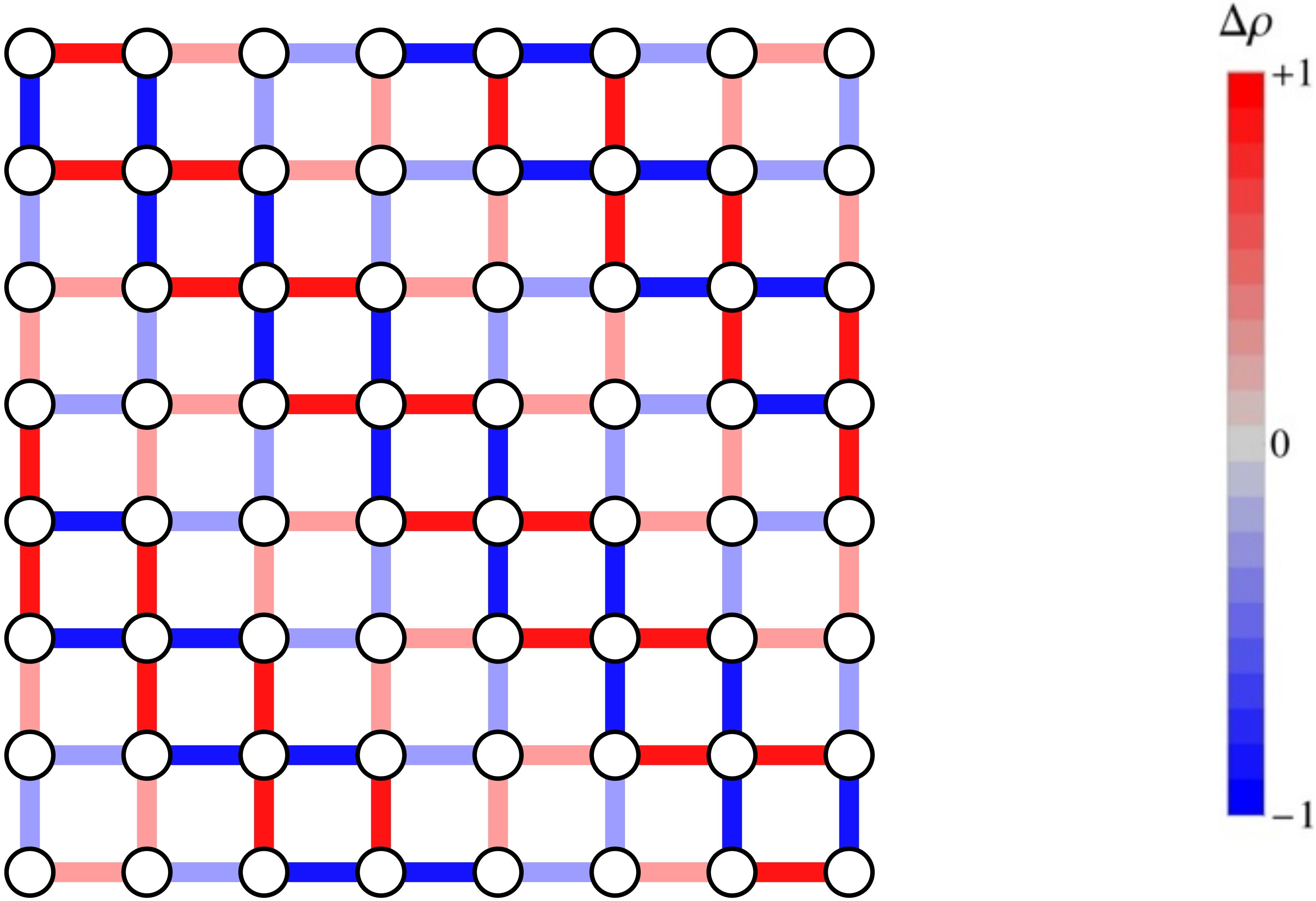
$$P_{\mathbf{Q}}(\mathbf{k}) = \cos(k_x) - \cos(k_y) \quad \text{and} \quad \mathbf{Q} = (\pi/4, \pi/4)$$



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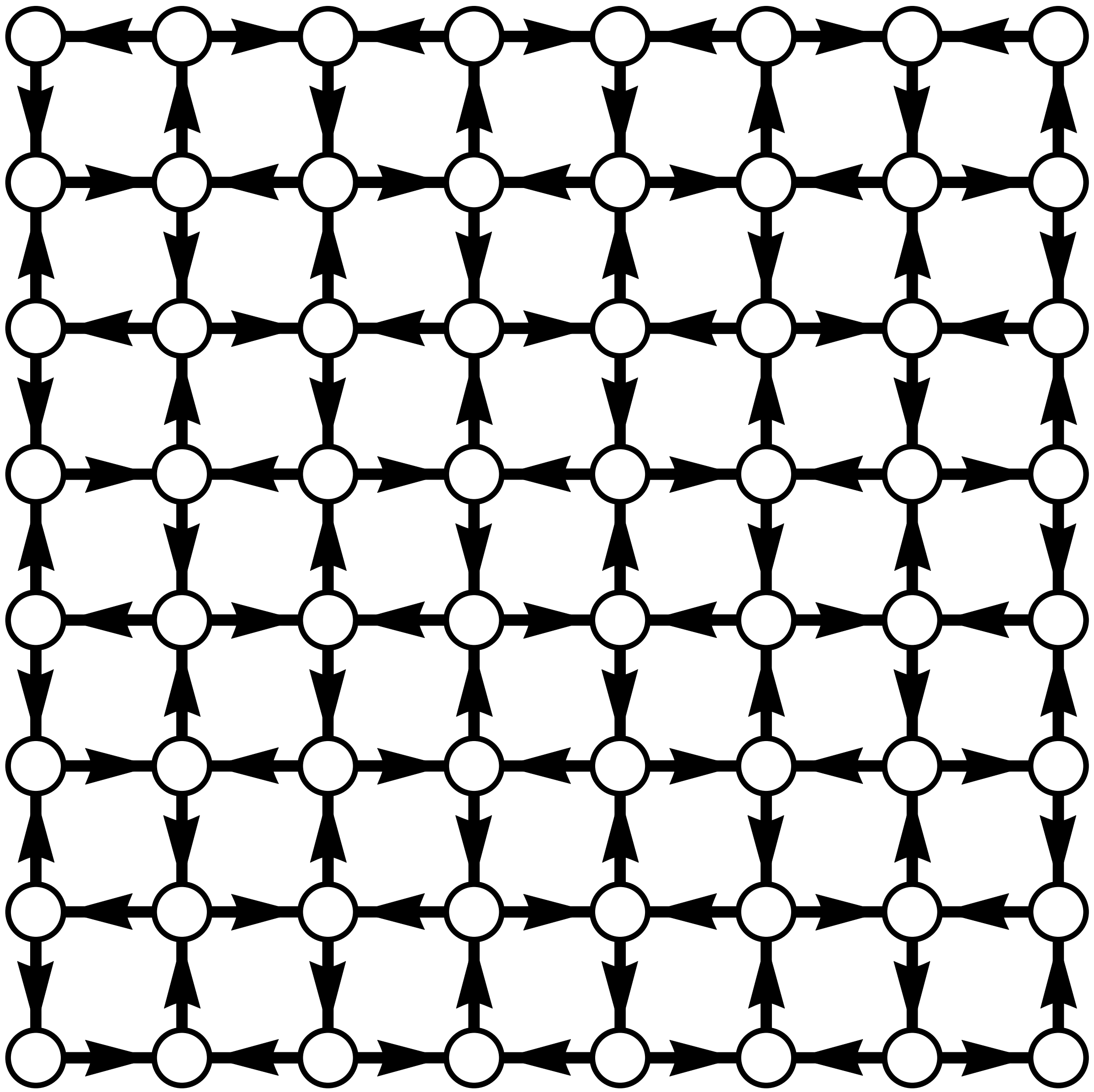


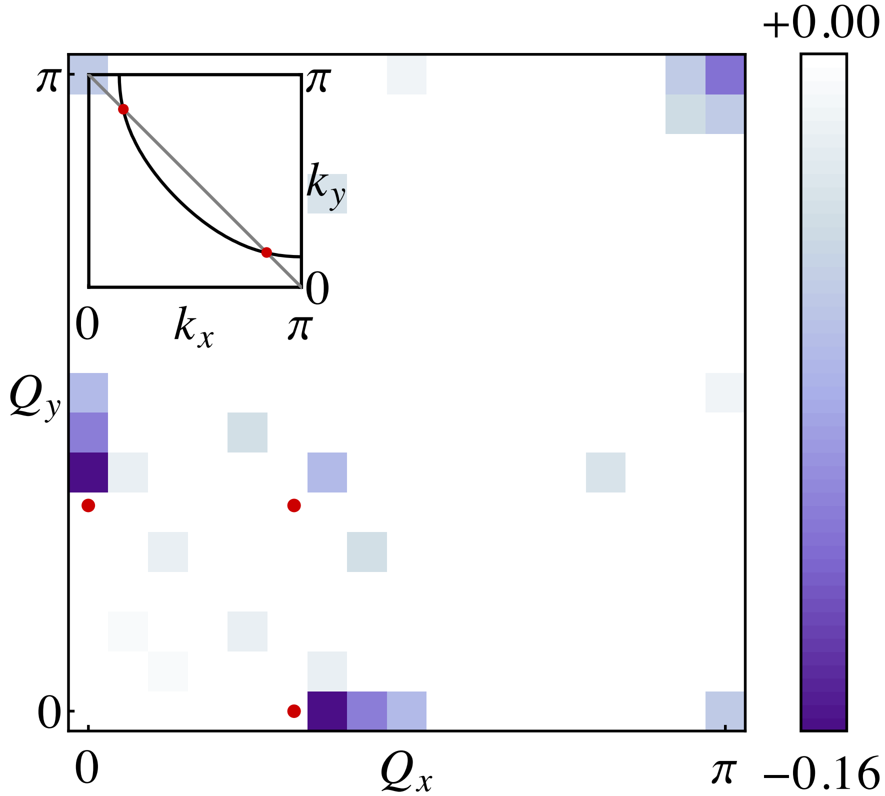
p-wave current order

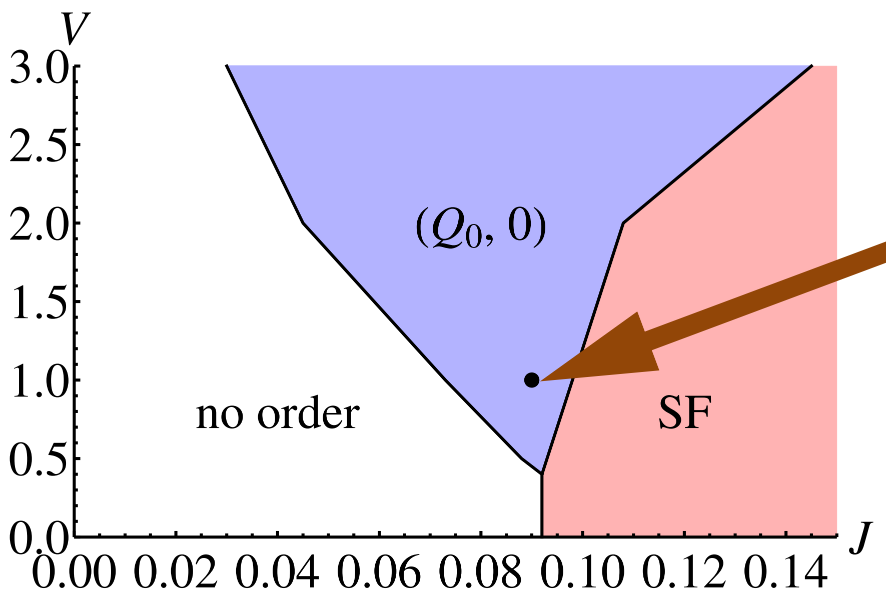
This state breaks time-reversal and is also known as "d-density wave" (*unfortunately*), and "staggered-flux (SF)".

Results of a variational Monte Carlo computation on a wavefunction with double-occupancy projected out.

A. Allais, J. Bauer, and S. Sachdev, arXiv:1402.4807

Q52.00003, Mile High Ballroom 1F, Wednesday March 5, 2:54 PM





Q-plot above at this value of J,V

Andrea Allais

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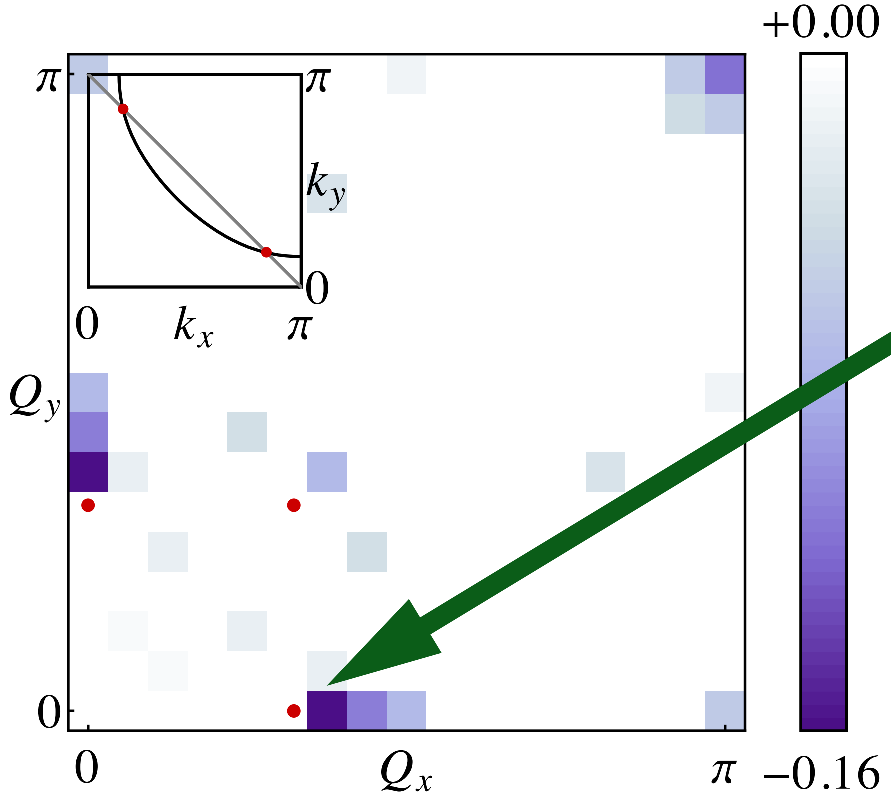
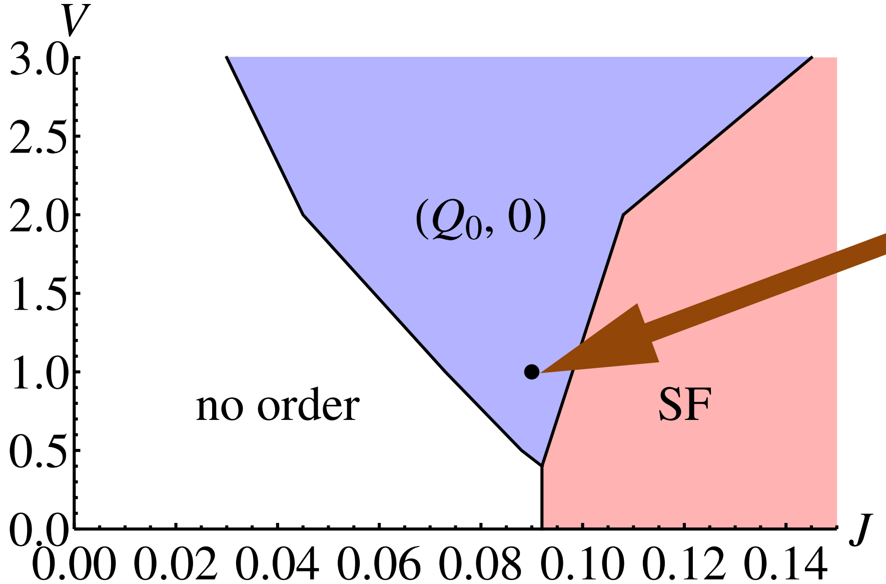


Q of the lowest energy state.
Predominantly d wave



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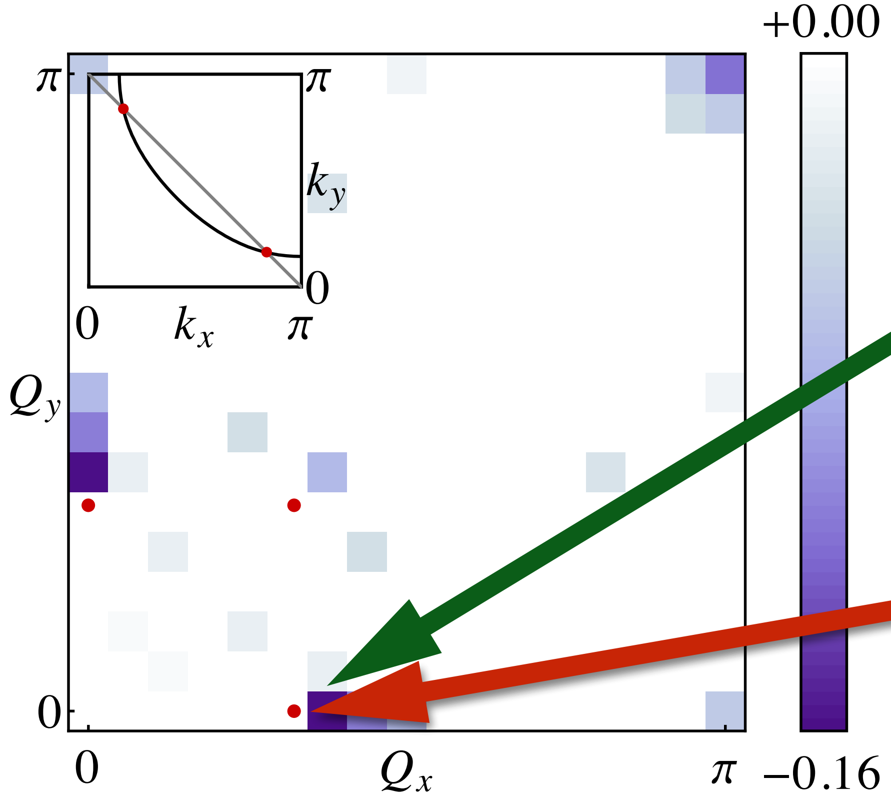
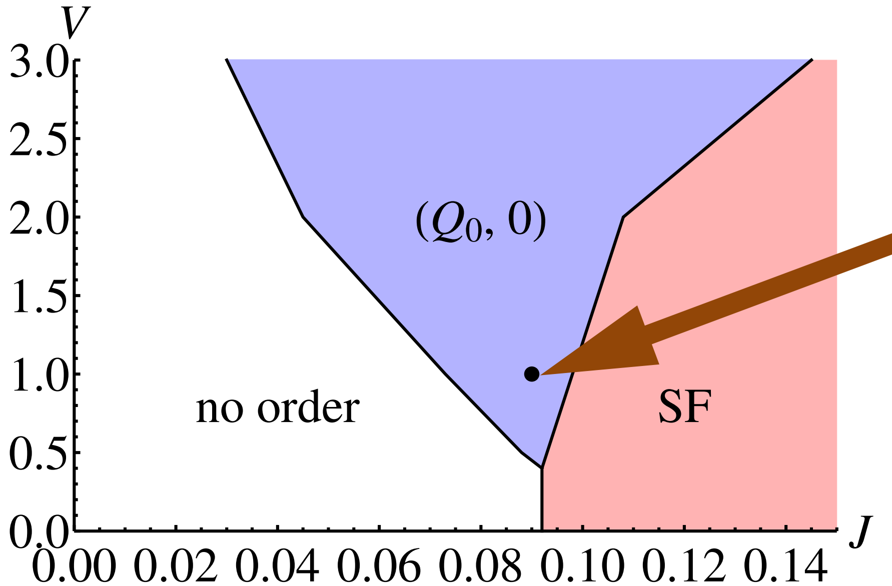


Q of the lowest energy state. Predominantly *d* wave

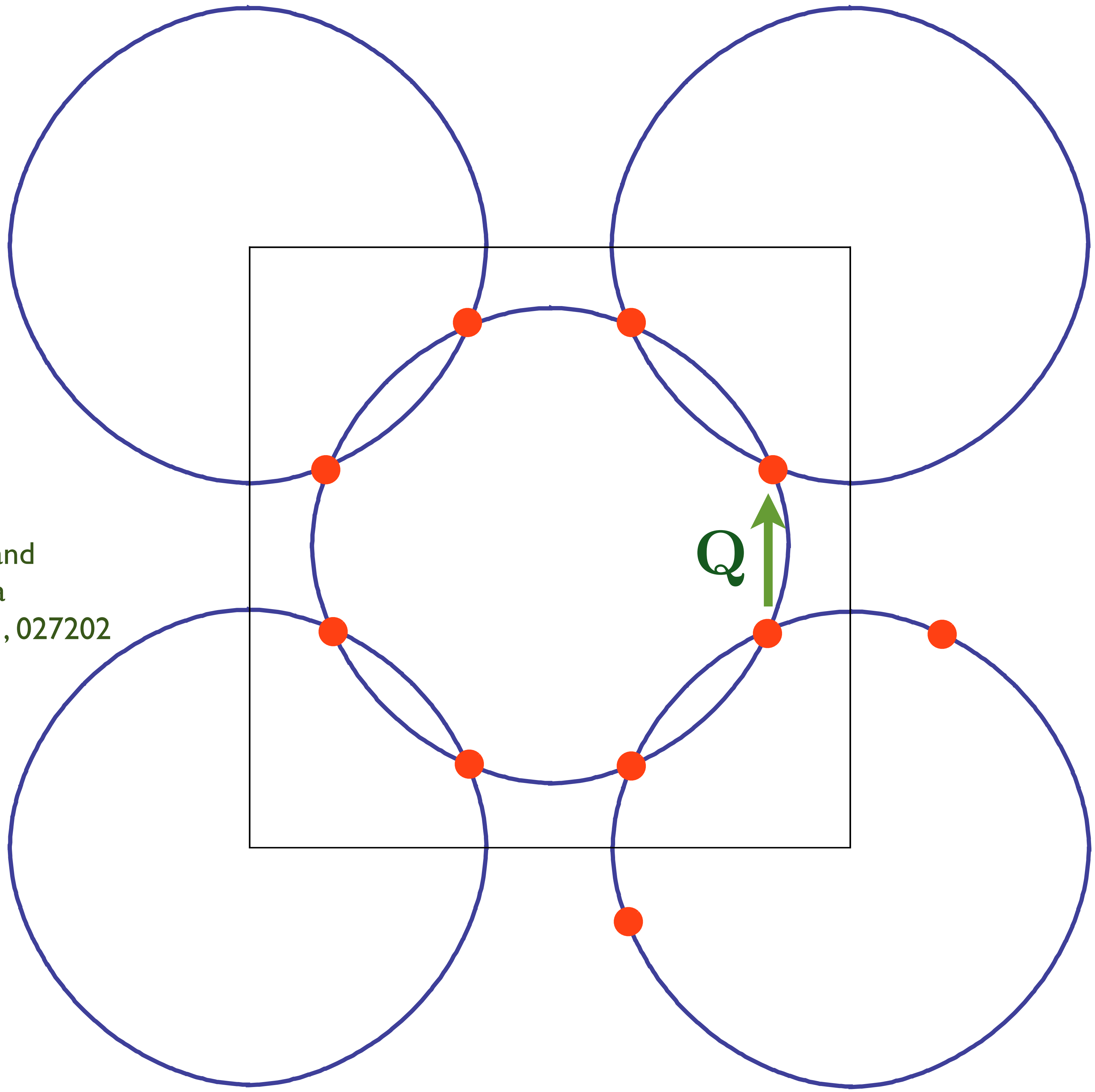
Q as determined by "hotspots"



Q-plot above at this value of J,V

Andrea Allais

Incommensurate *d*-wave bond order



S. Sachdev and
R. LaPlaca
Phys. Rev. Lett. **111**, 027202
(2013)

$$P_{\mathbf{Q}}(\mathbf{k}) = (\cos k_x - \cos k_y) + 0.3 + \ldots$$

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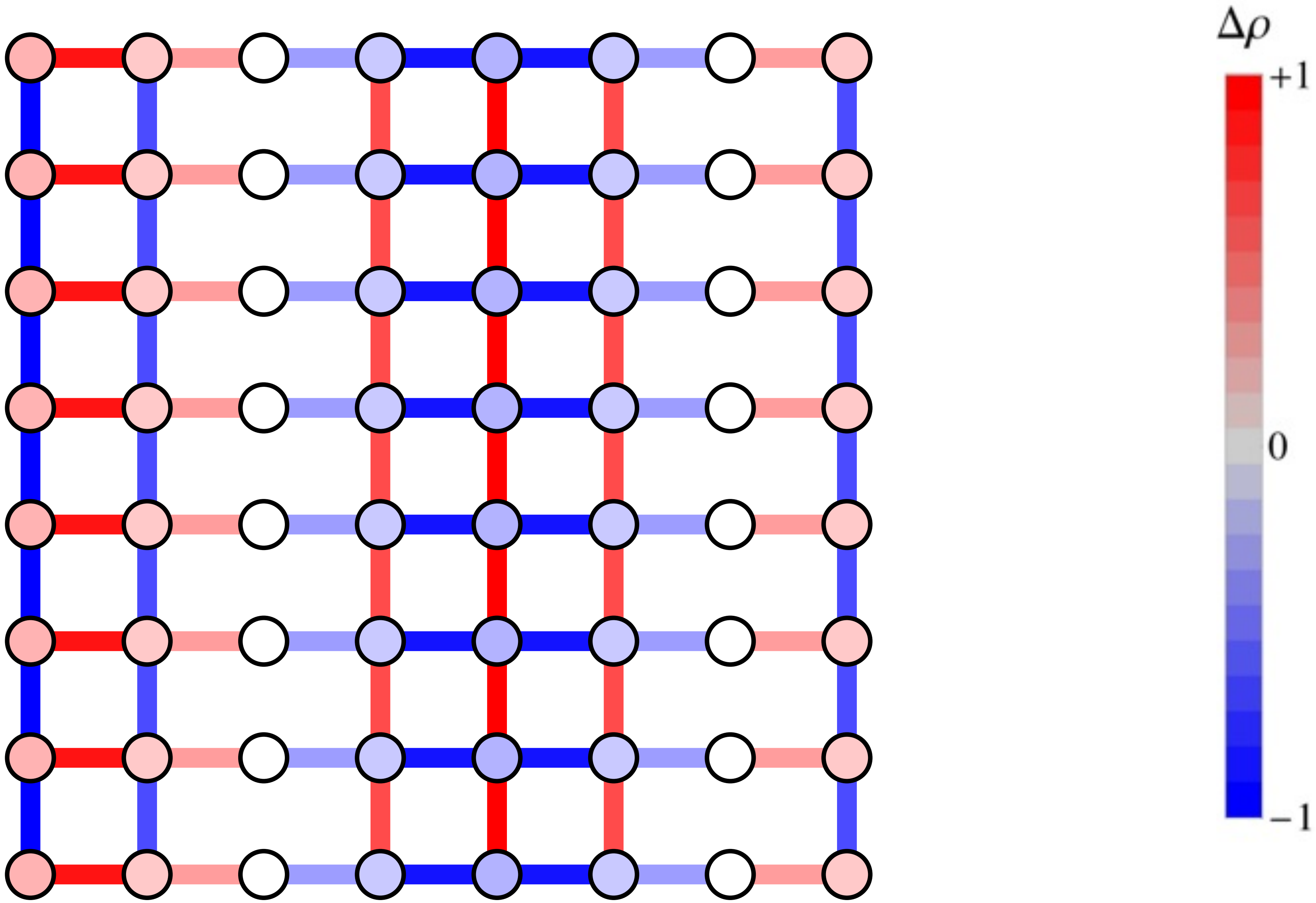
$$P_{\mathbf{Q}}(\mathbf{k}) = 0.3 + \cos(k_x) - \cos(k_y) \quad \text{and} \quad \mathbf{Q} = (\pi/4, 0)$$



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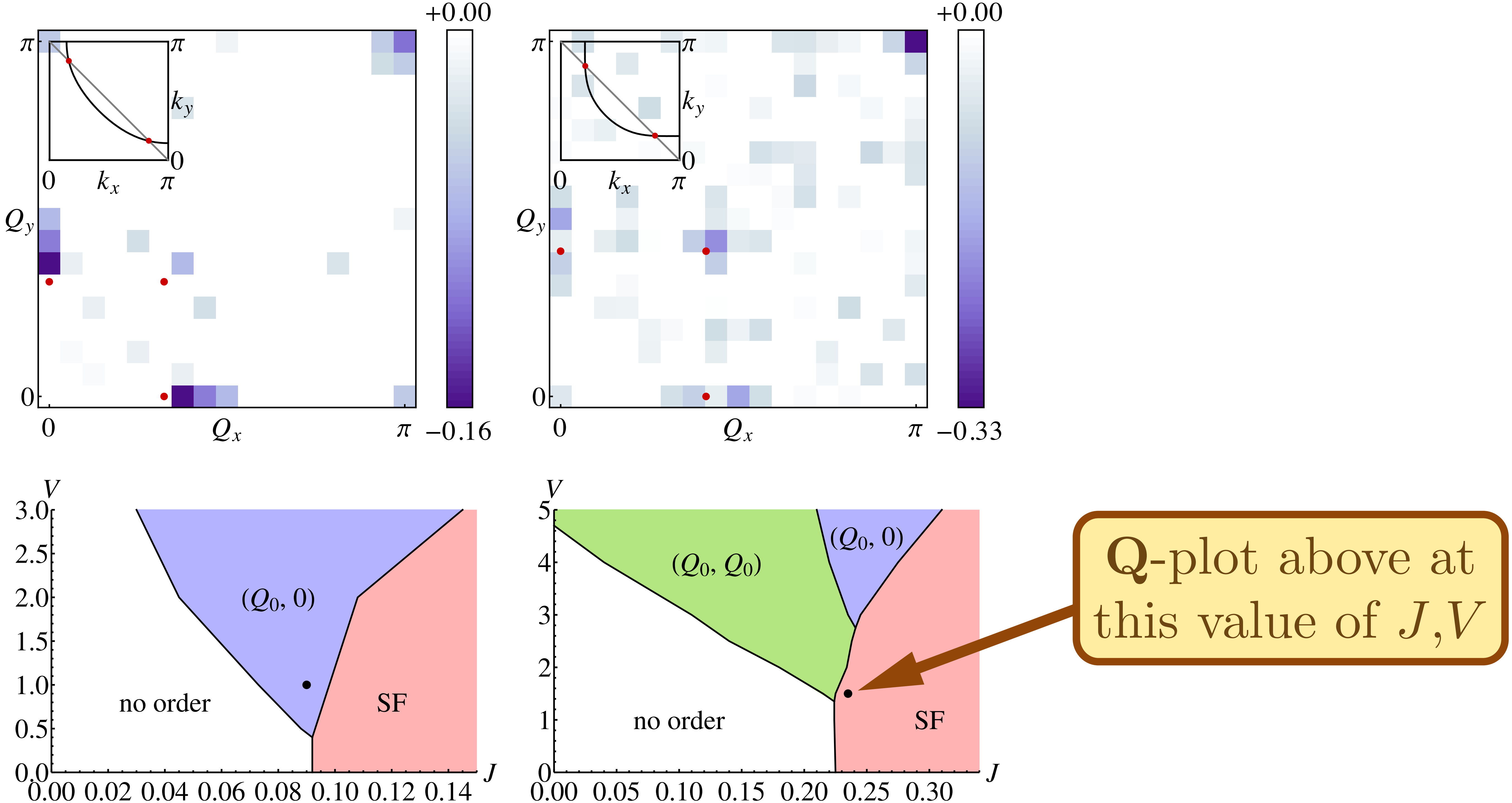

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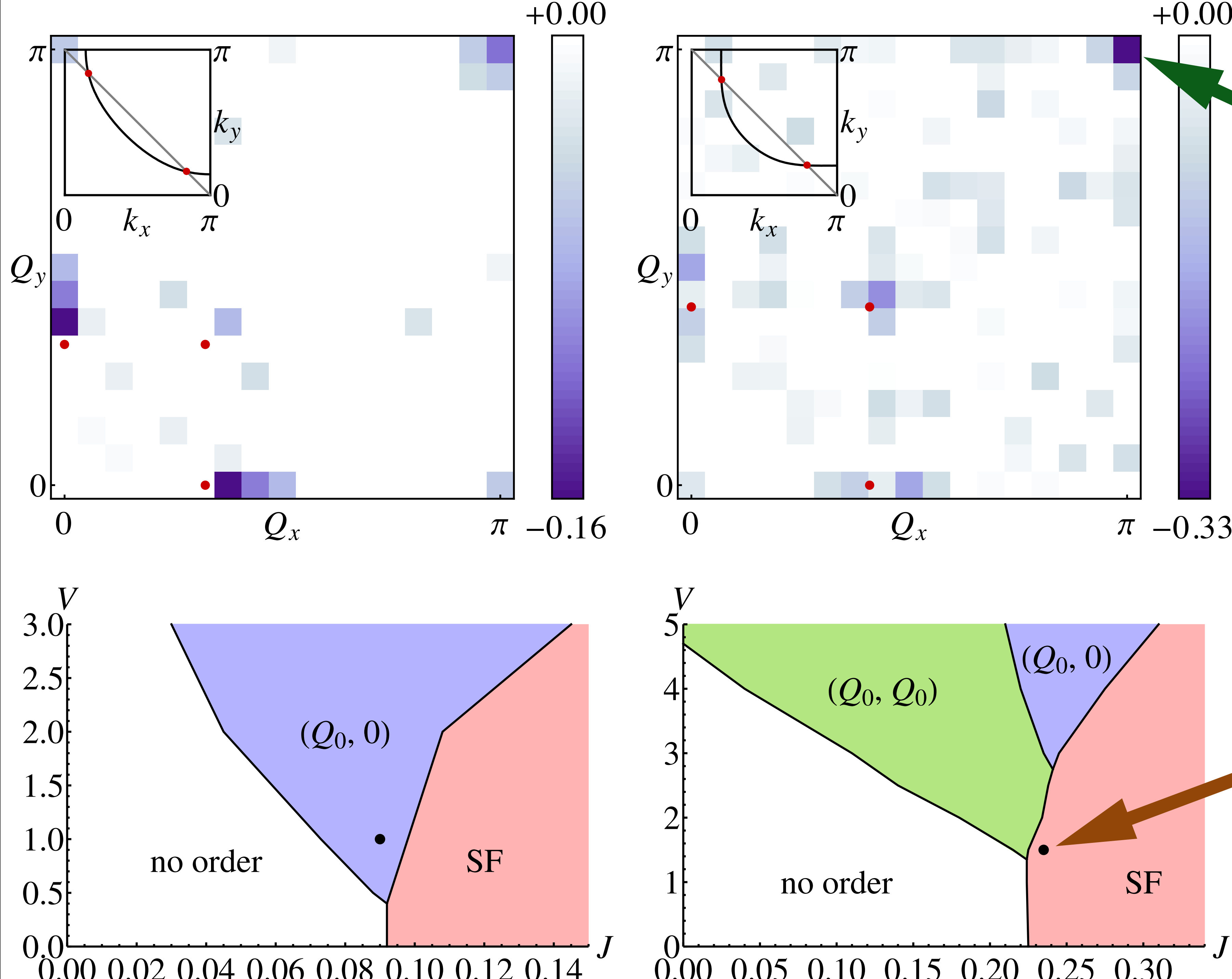

Q of the lowest energy state. p wave (SF), breaks time-reversal

Q-plot above at this value of J,V

Current order

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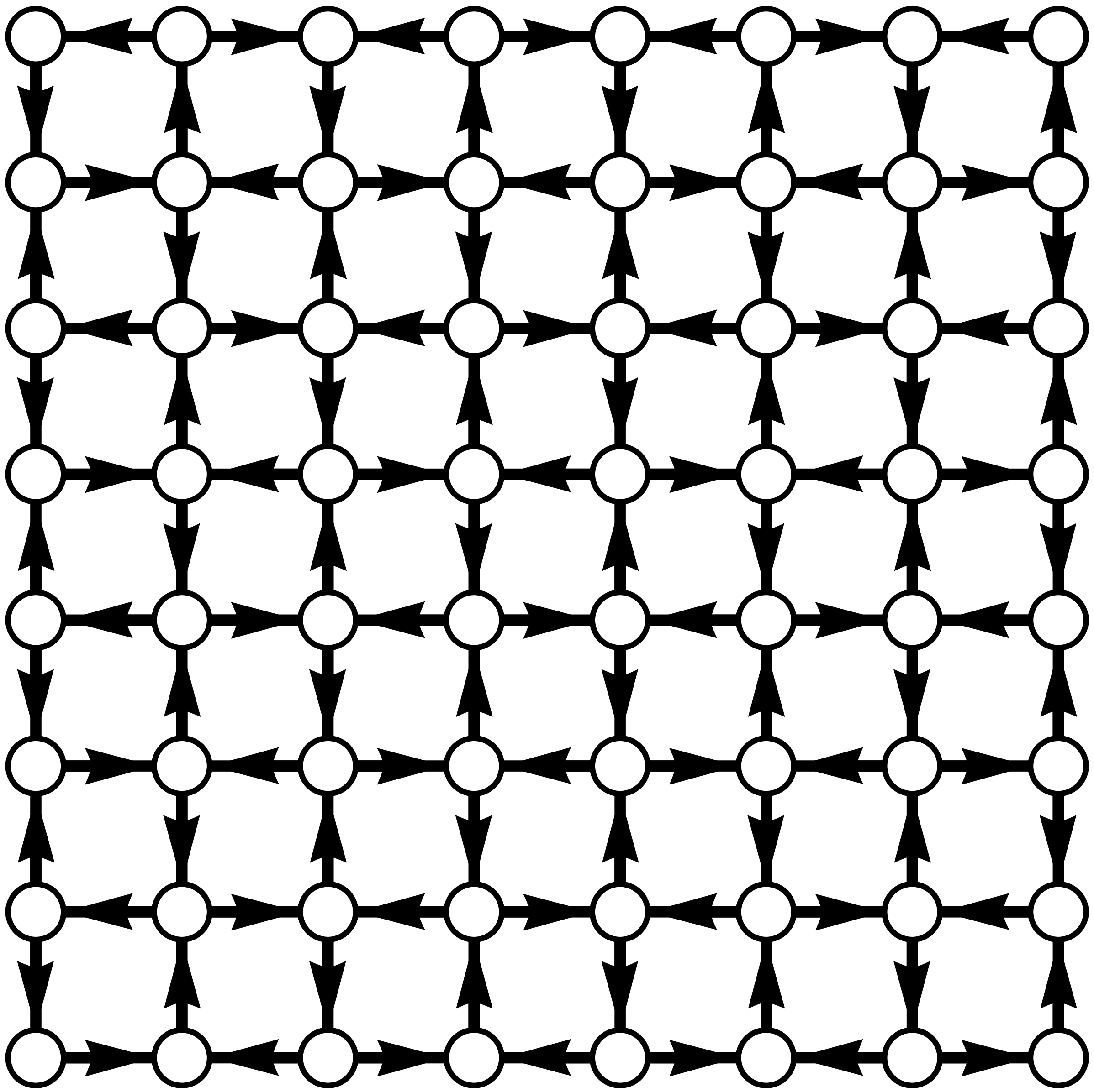

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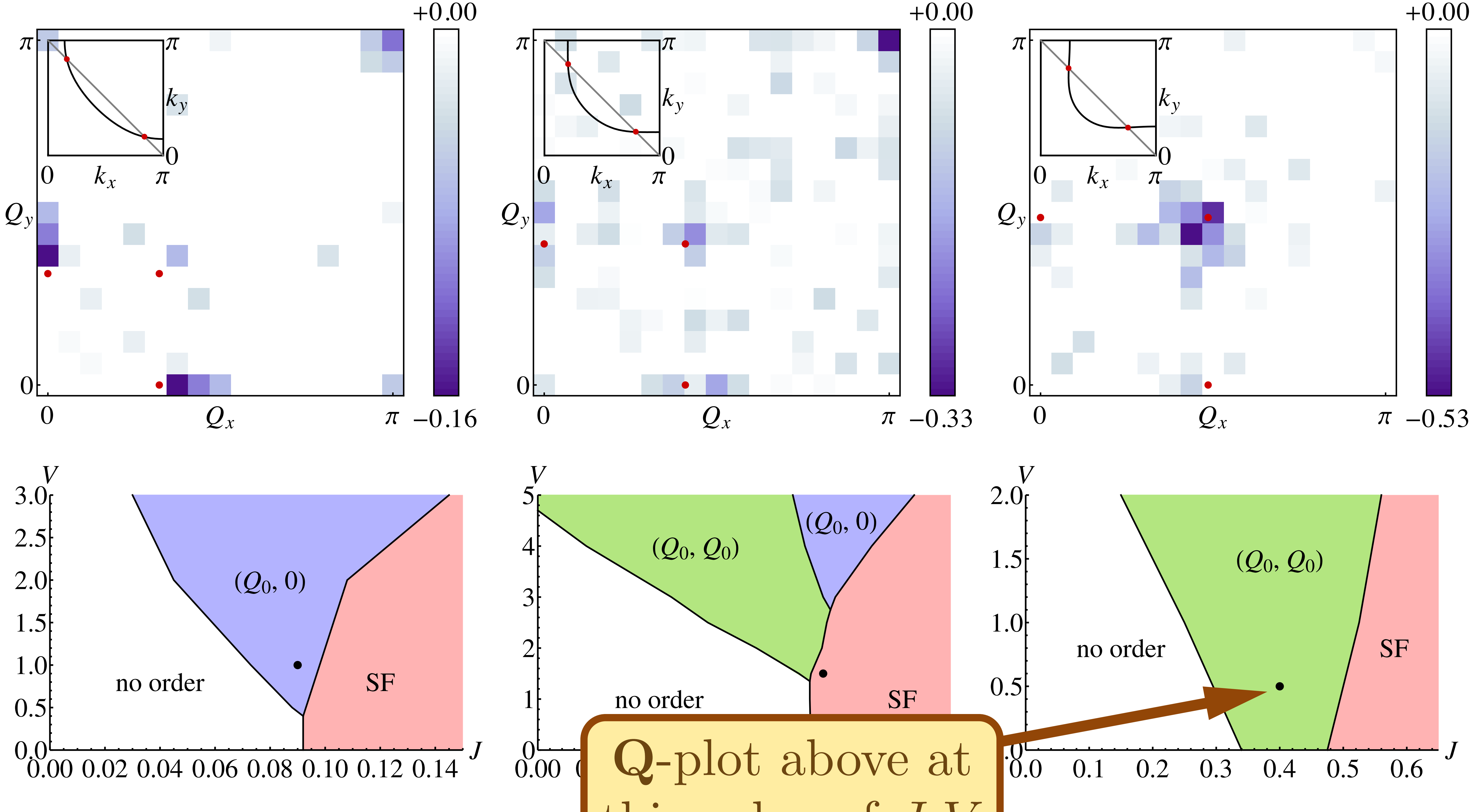

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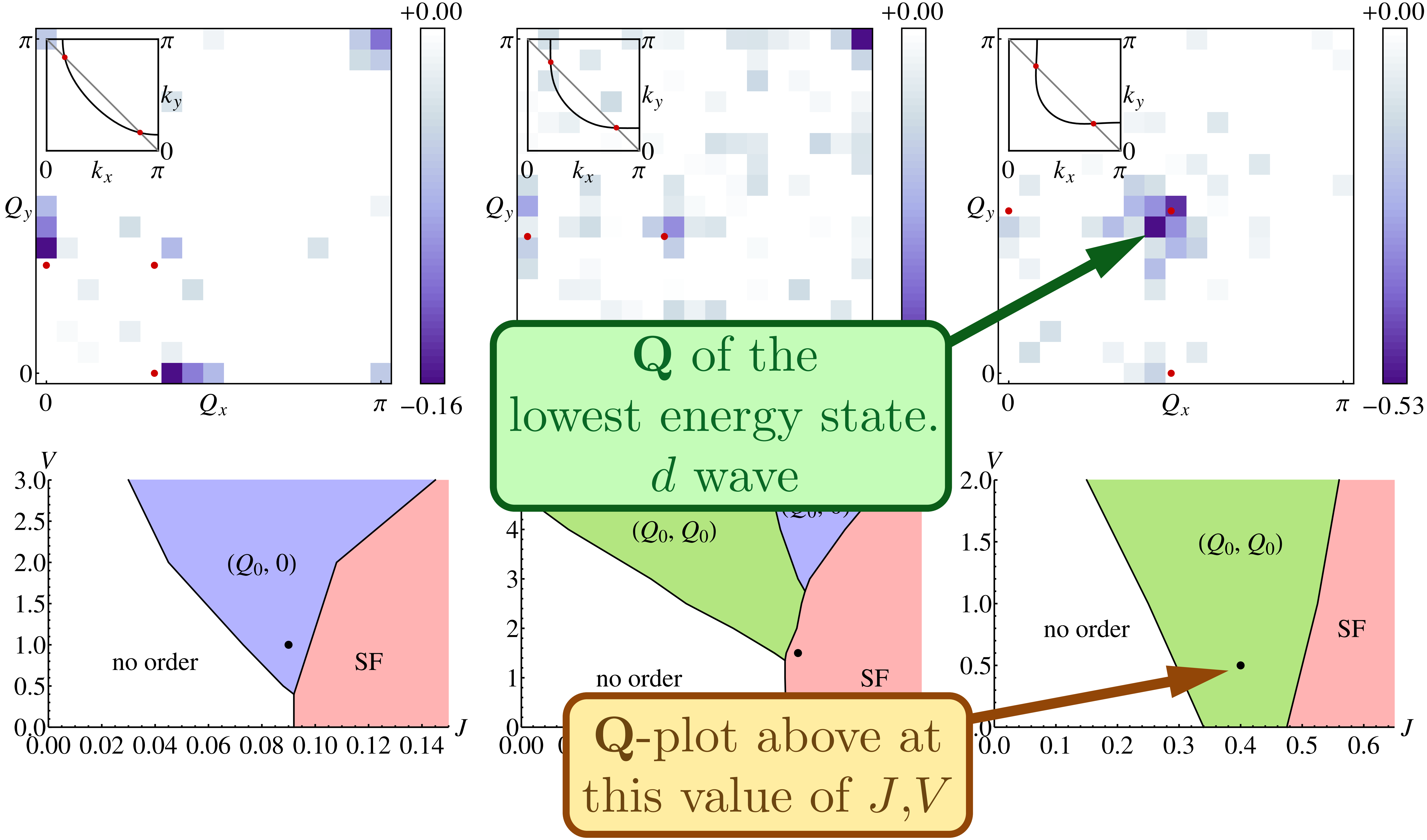

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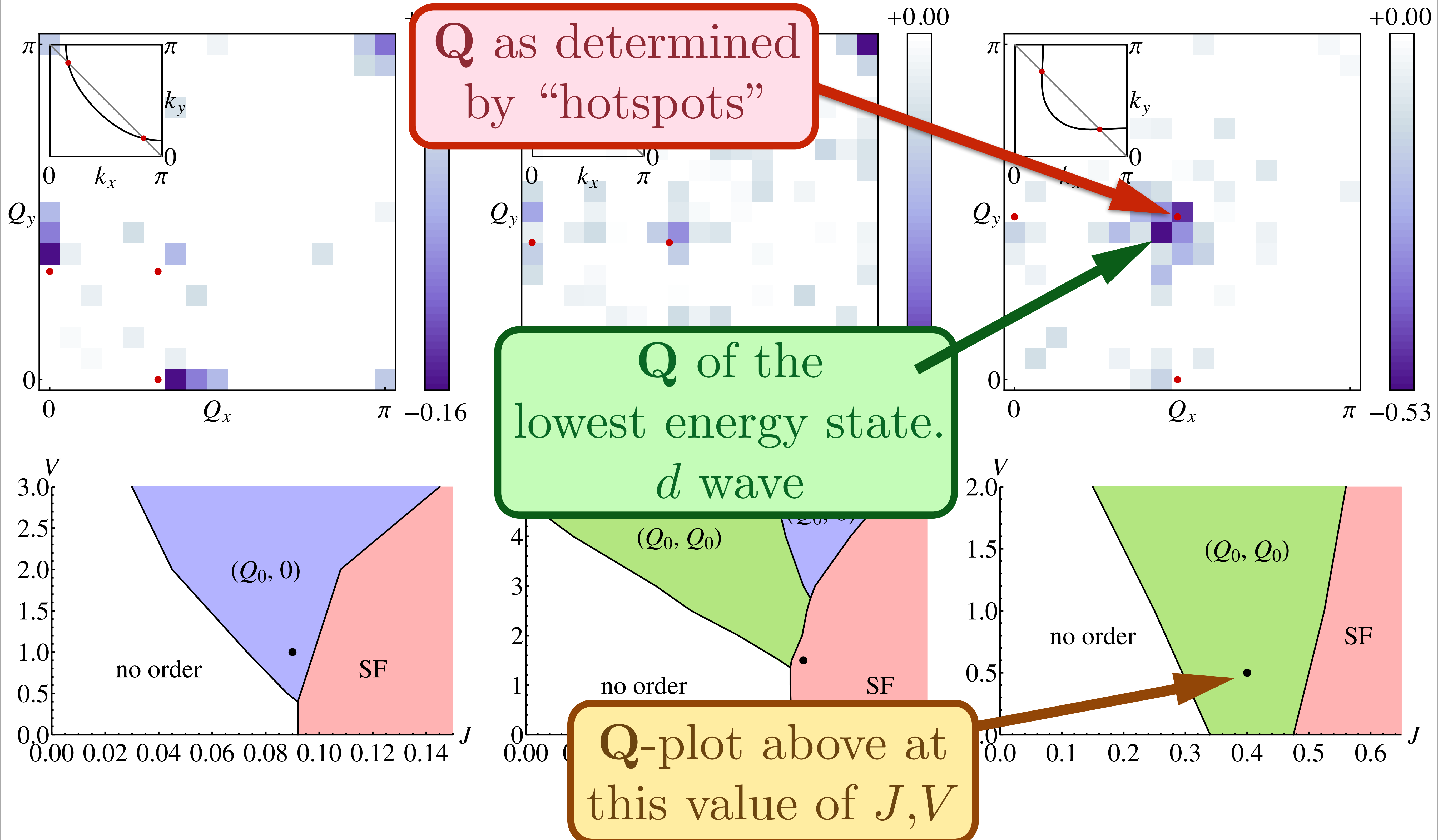
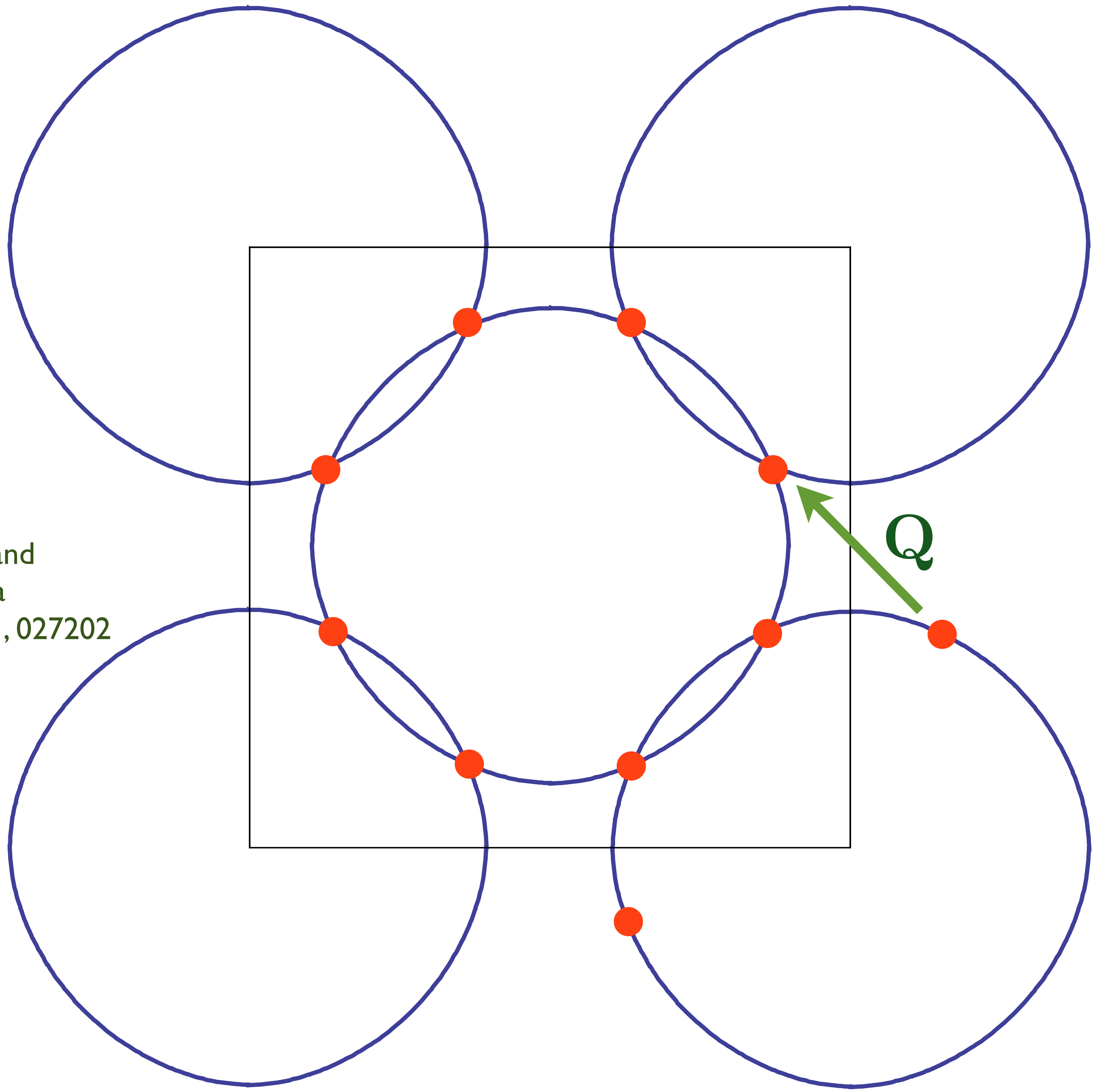


Incommensurate *d*-wave bond order



S. Sachdev and
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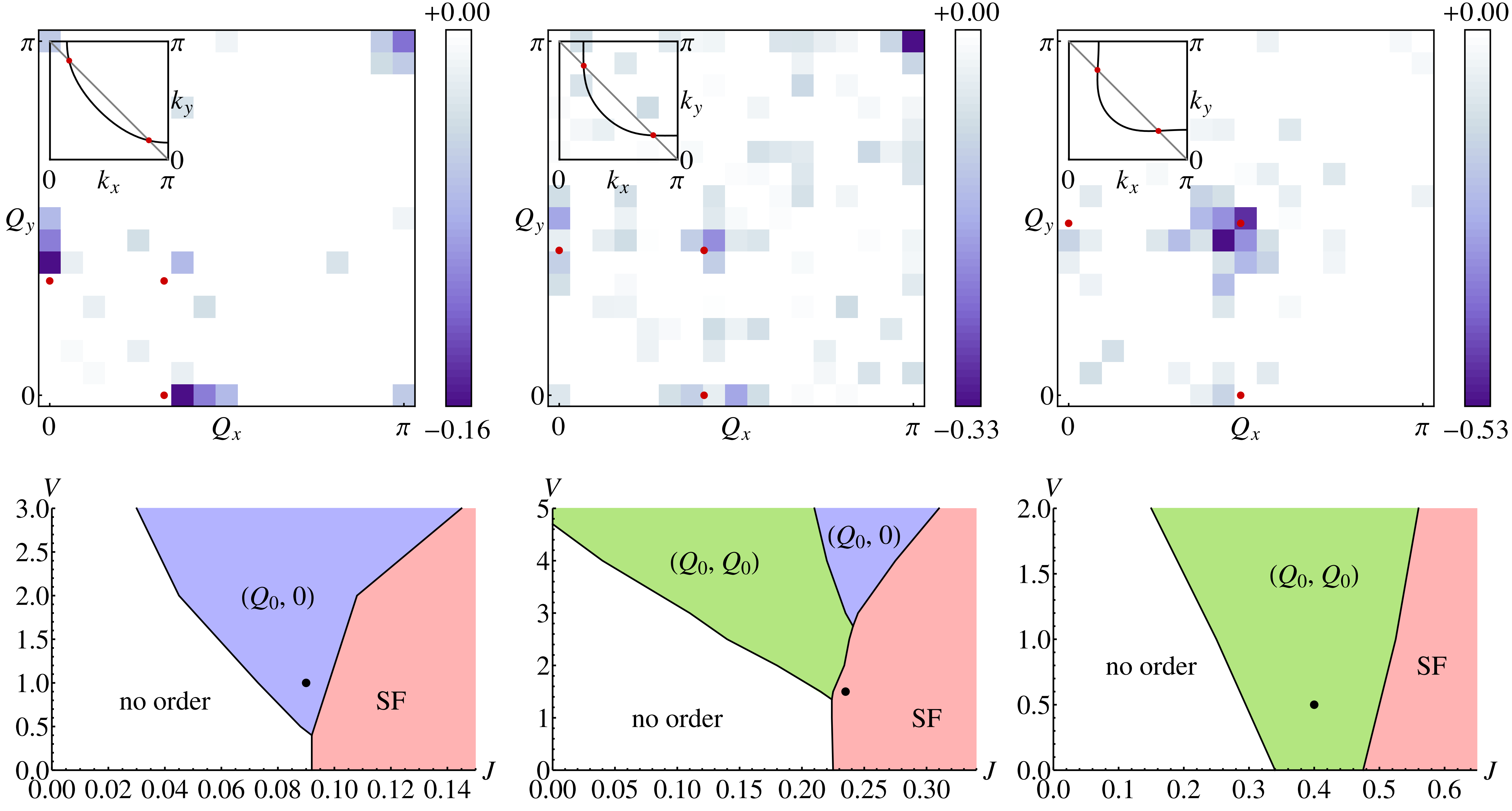
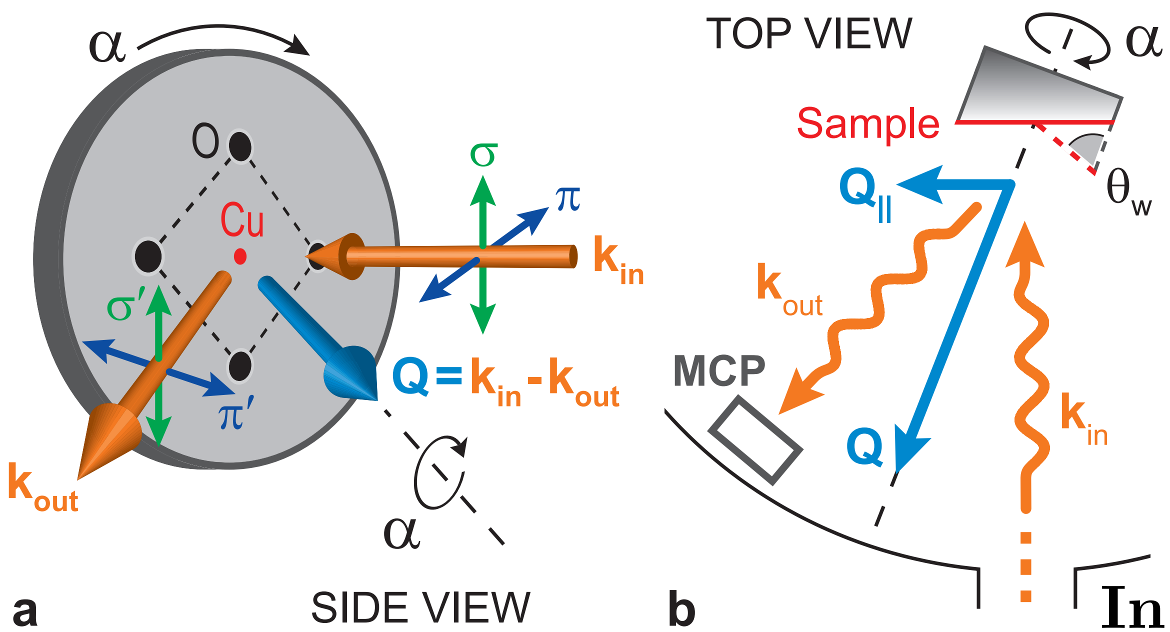


The optimal form-factor for charge order at *both* $(Q_0, 0)$ and (Q_0, Q_0) is predominantly d-wave.

See also talk by
Debanjan Chowdhury
(Y52.00015, Friday 10:48 AM, Mile High Ballroom 1F)
on the issue of the wavevector of the bond order
and on implications for photoemission.

The symmetry of charge order in the cuprates

R. Comin, R. Sutarto, F. He, E. da Silva Neto, L. Chauviere, A. Frano, R. Liang, W.N. Hardy, D.A. Bonn, Y. Yoshida, H. Eisaki, J. E. Hoffman, B. Keimer, G.A. Sawatzky, and A. Damascelli, arXiv:1402.5415



Polarization and angular analysis of X-ray scattering at $\mathbf{Q} = (Q_0, 0)$ in Bi2201 and YBCO

In addition, by adopting a special experimental geometry, we also resolve the *intra-unit-cell* symmetry of the charge ordered state, which is revealed to be a *d*-wave bond-order. These results represent a fundamental advancement in our microscopic description of charge order in cuprates, and provide crucial insights for the understanding of its origin and interplay with superconductivity and magnetism.

This type of predominantly *d*-wave bond order at $\mathbf{Q} = (Q_0, 0)$ was first predicted in S. Sachdev and R. LaPlaca, Phys. Rev. Lett. **111**, 027202 (2013).

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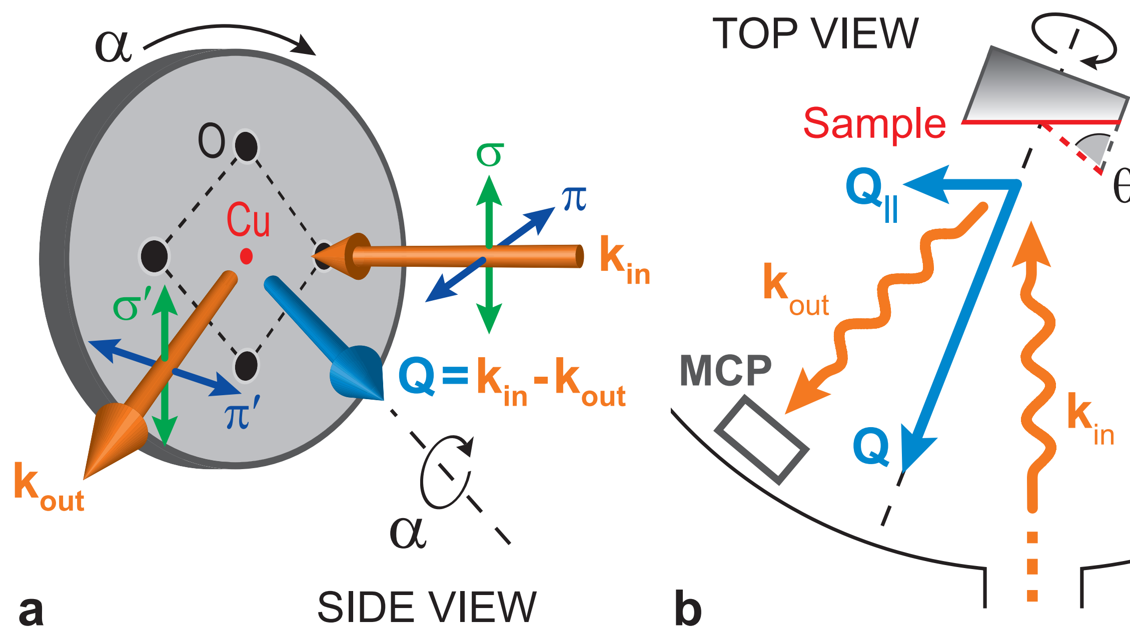

Δ_{CDW}	Probability levels P (%)	
	Bidirectional	Unidirectional
Δ_s	30.3	38.8
$\Delta_{s'}(\cos k_x + \cos k_y)$	12.0	6.0
$\Delta_d\ (\cos k_x - \cos k_y)$	**81.8**	**87.6**

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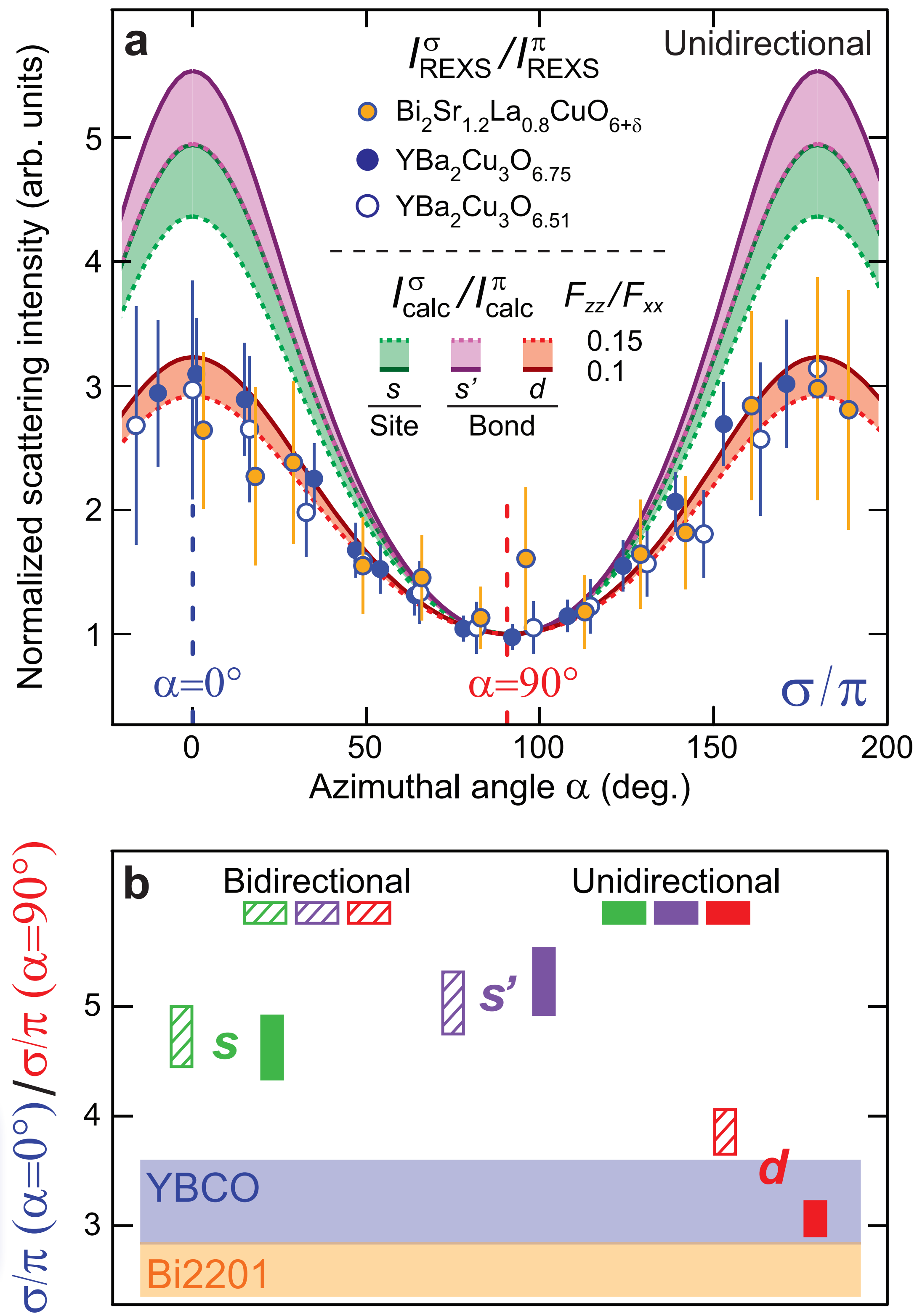


Outline

1. Antiferromagnetism in metals and *d*-wave superconductivity

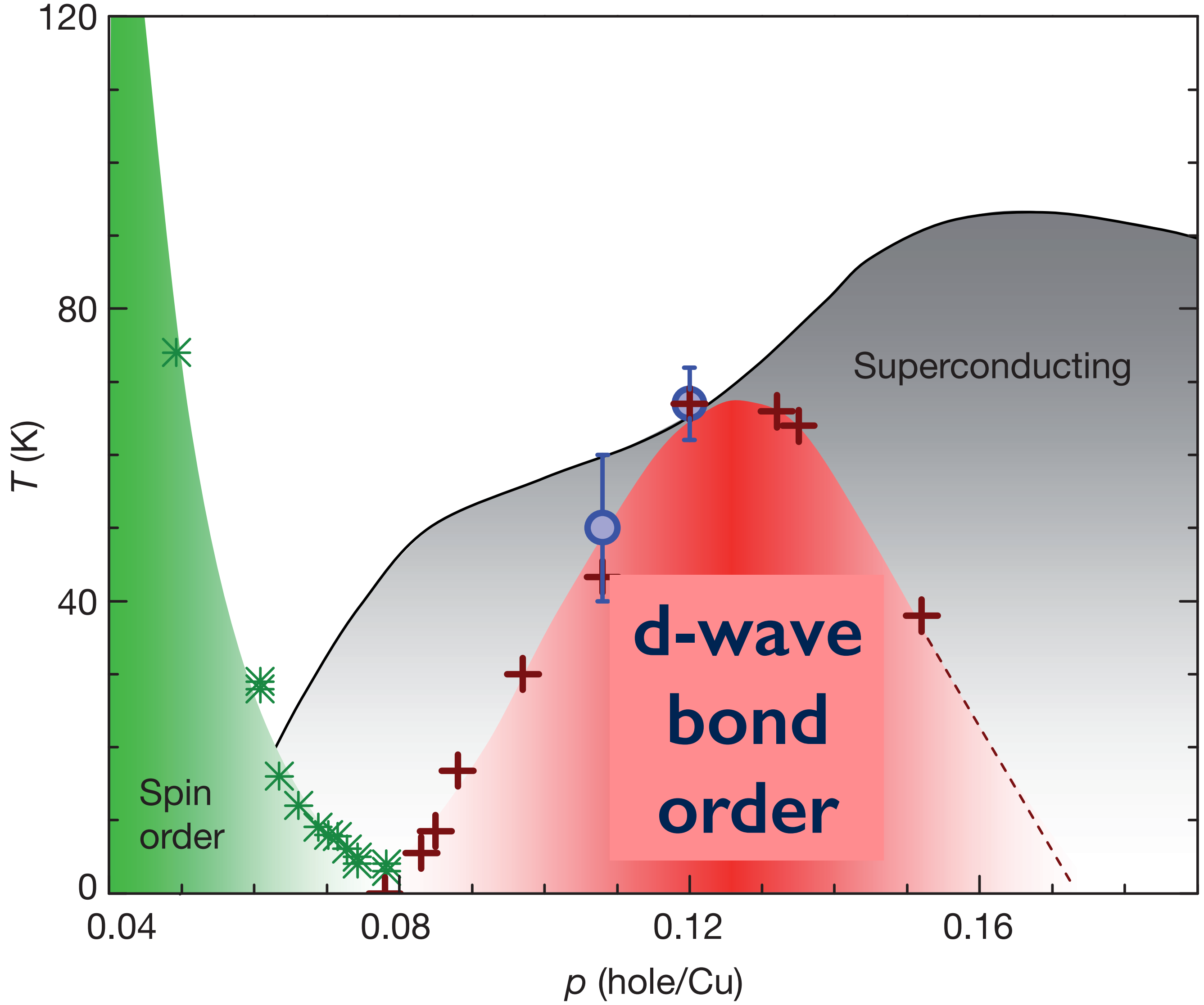
2. Competing order: *d*-wave bond order

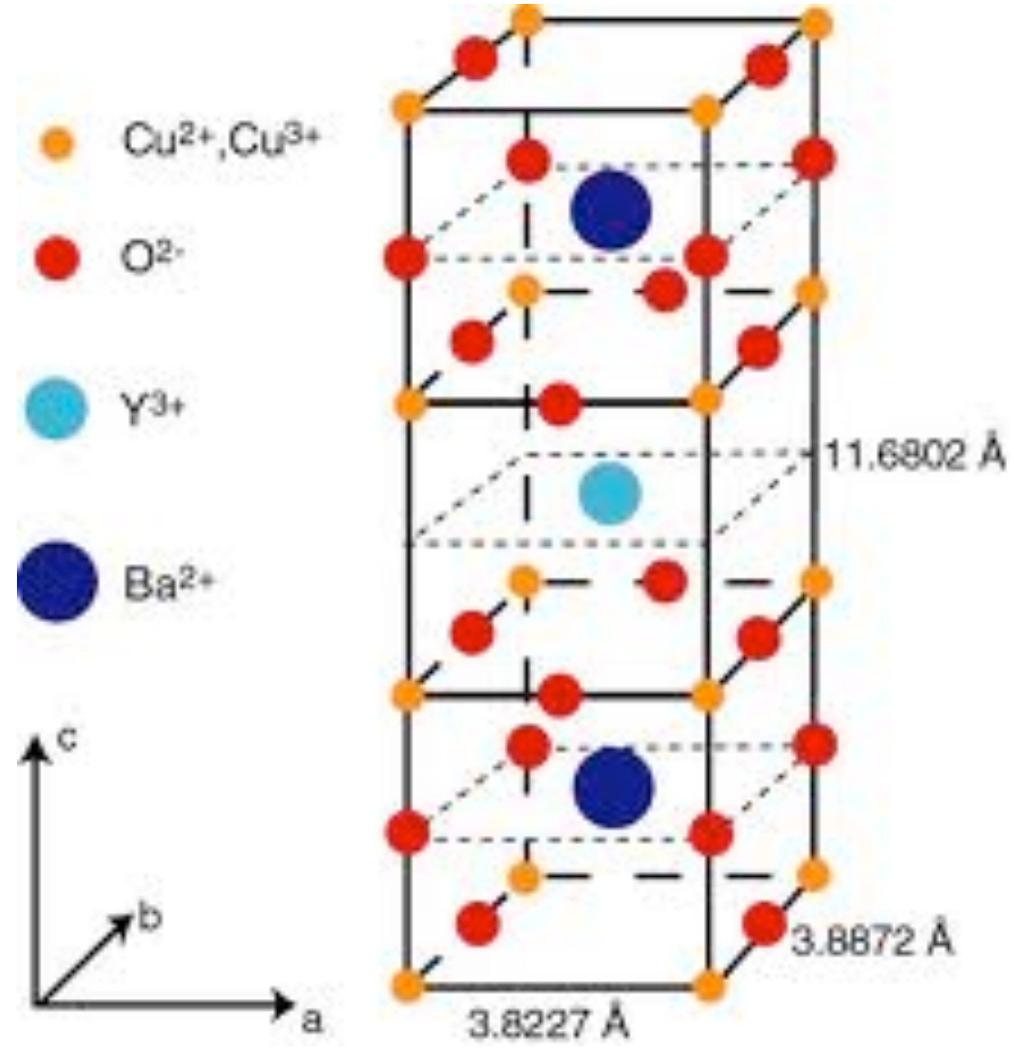
3. The pseudogap regime of the hole-doped cuprate superconductors

   Angular fluctuations of a multicomponent order

   Lauren Hayward, A53.00011, Mile High Ballroom 2C, Monday March 3, 10:00 AM

M. Vojta and S. Sachdev, Physical Review Letters **83**, 3916 (1999)
M. Vojta and O. Rosch, Physical Review B **77**, 094504 (2008)
M. Metlitski and S. Sachdev, Physical Review B **82**, 075128 (2010)
S. Sachdev and R. La Placa, Physical Review Letters **111**, 027202 (2013)
J. D. Sau and S. Sachdev, Physical Review B **89**, 075129 (2014)
A. Allais, J. Bauer, and S. Sachdev, arXiv:1402.4807
A. Allais, J. Bauer, and S. Sachdev, arXiv:1402.6311





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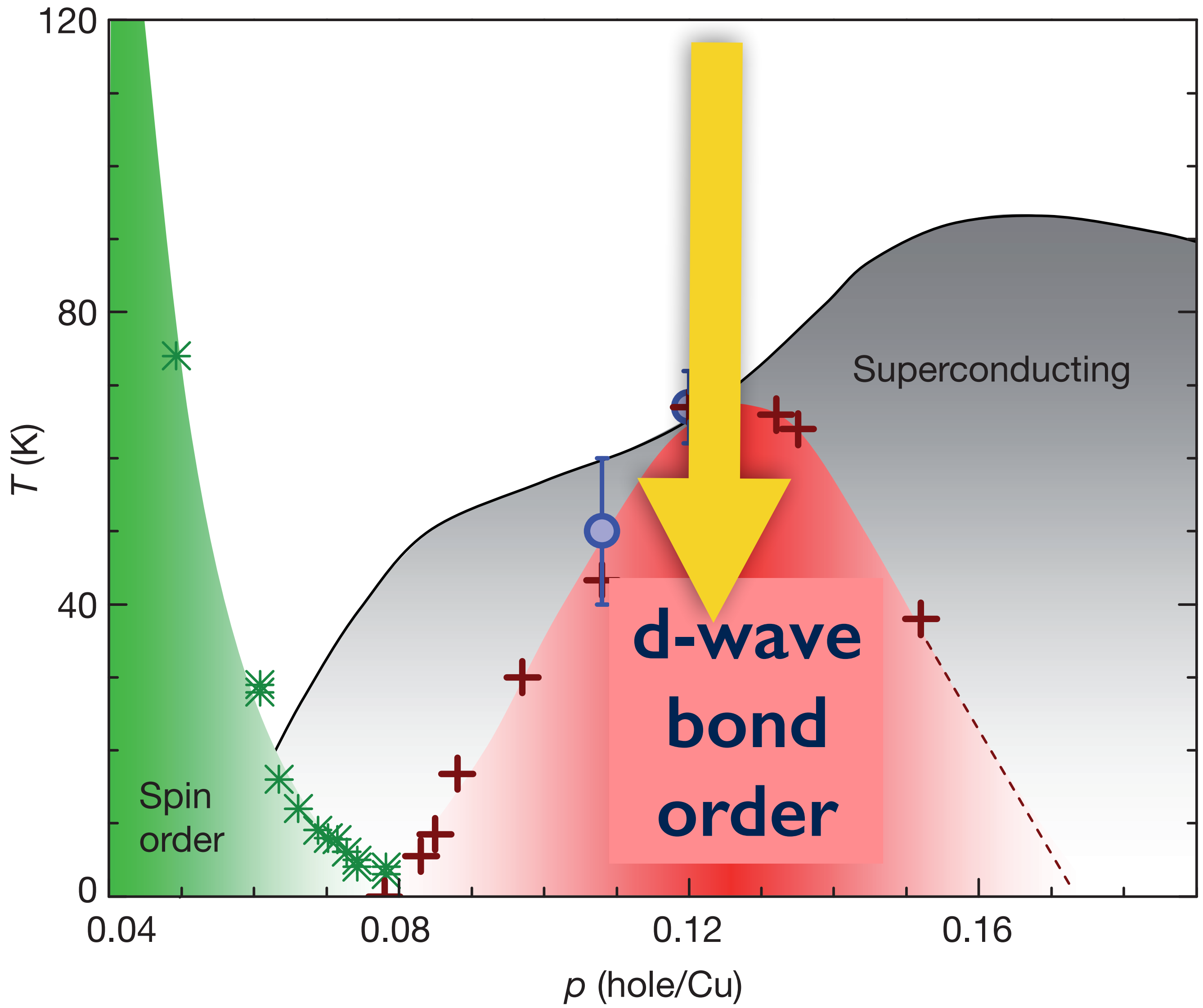
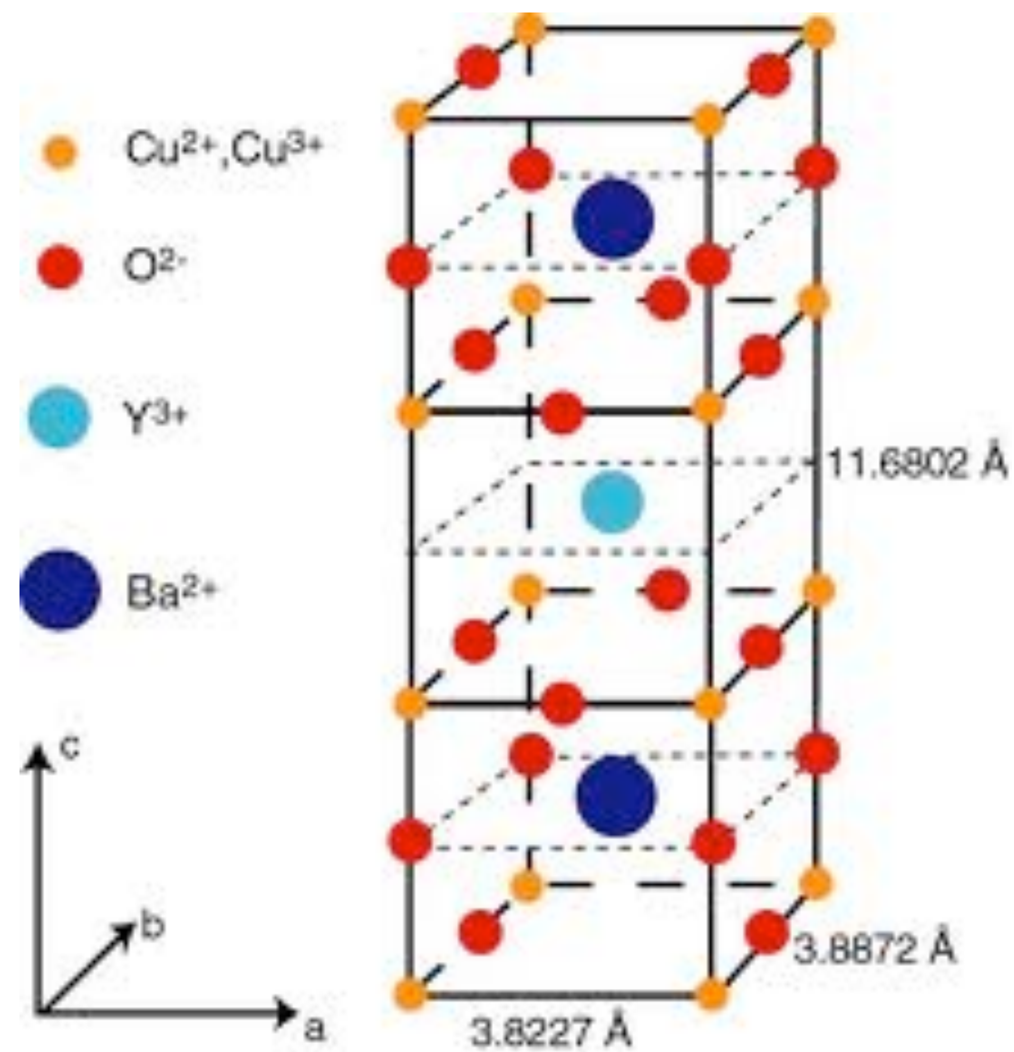
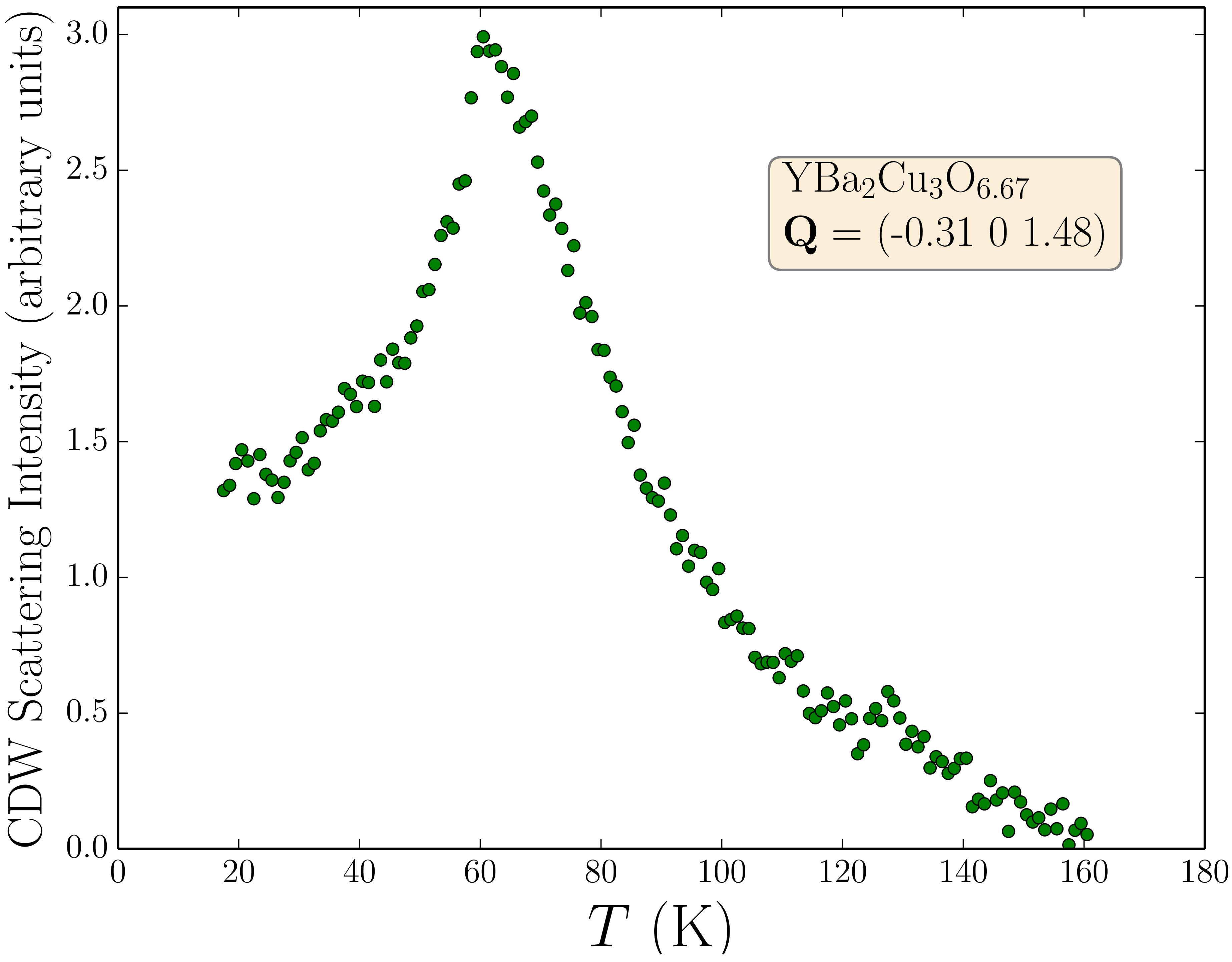




A. J. Achkar, X. Mao, Christopher McMahon, R. Sutarto, F. He, Ruixing Liang, D. A. Bonn, W. N. Hardy, D. G. Hawthorn, arXiv:1312.6630.



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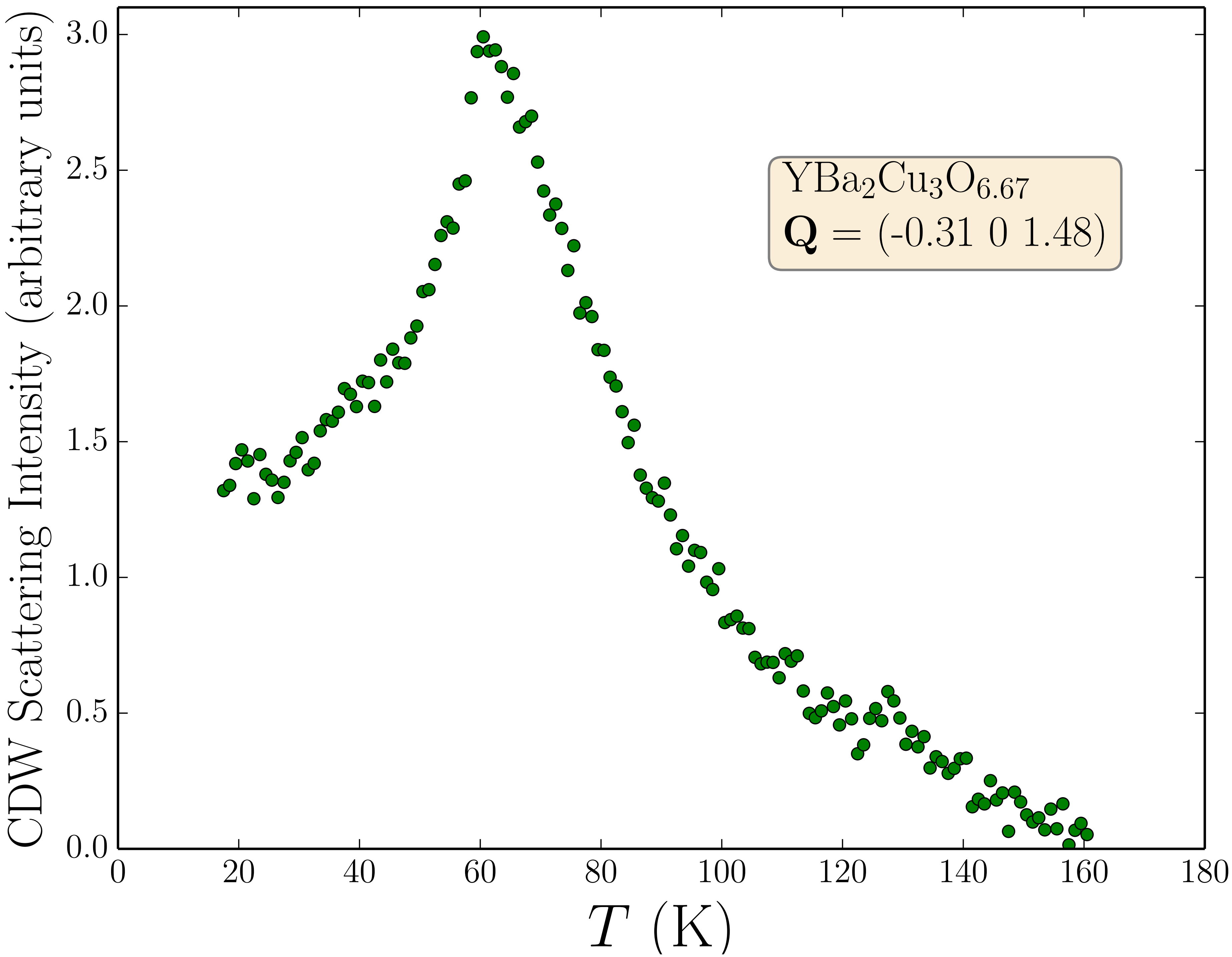


Onset is unlike an arrested ordering transition, or precursor critical fluctuations

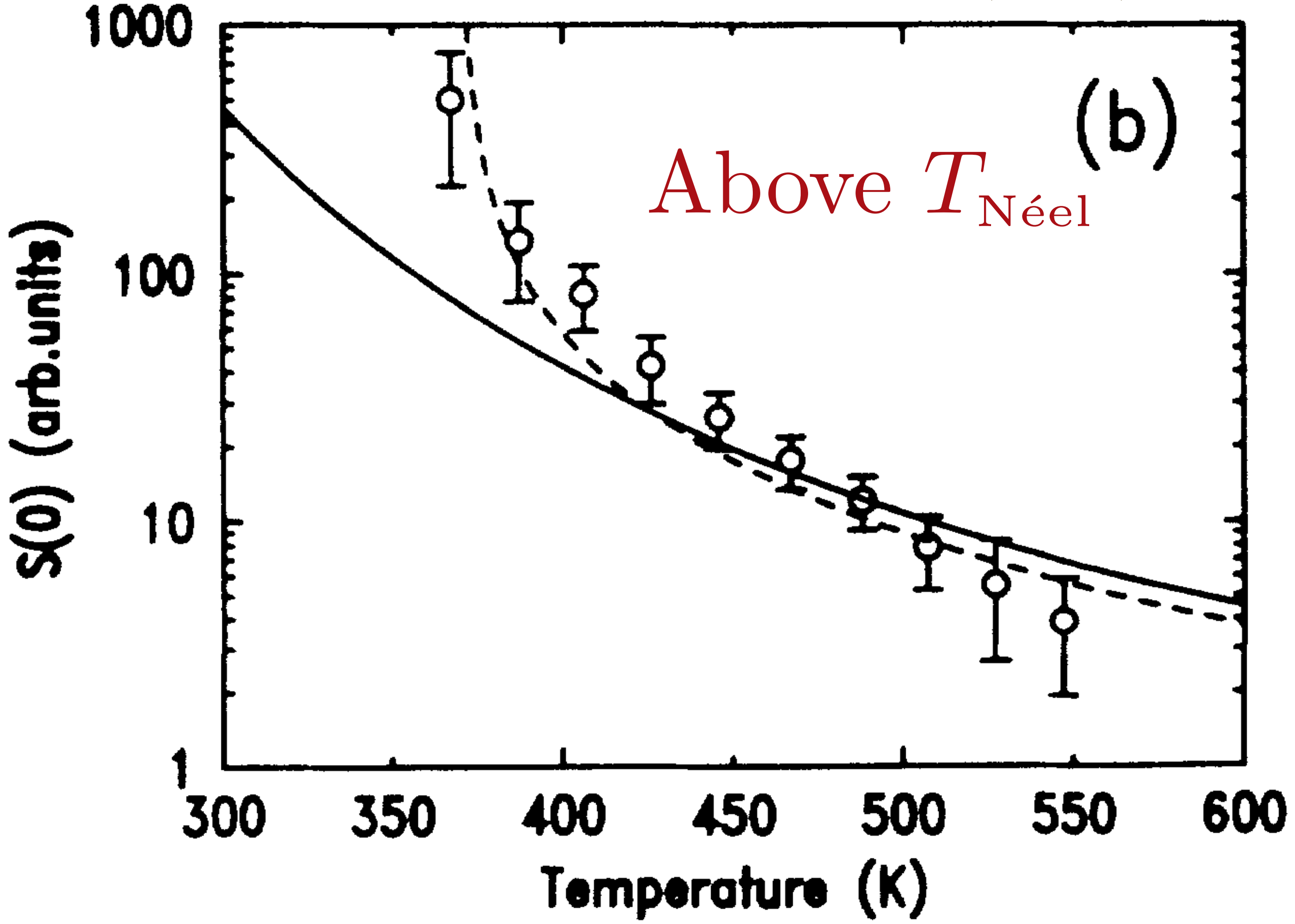
Key idea: analogy with the onset of antiferromagnetism in the *insulator* La_2CuO_4

Gradual onset of intensity over a wide range of T is a consequence of *angular thermal* fluctuations of an order parameter with 3 or more components in 2 spatial dimensions

Polyakov, 1975
Chakravarty, Halperin, Nelson 1989

$$T_{\text{Néel}} = 325\text{K}$$

B. Keimer *et al.*,
Phys. Rev. B **46**, 14034 (1992).



Multi-component order parameter for the pseudogap

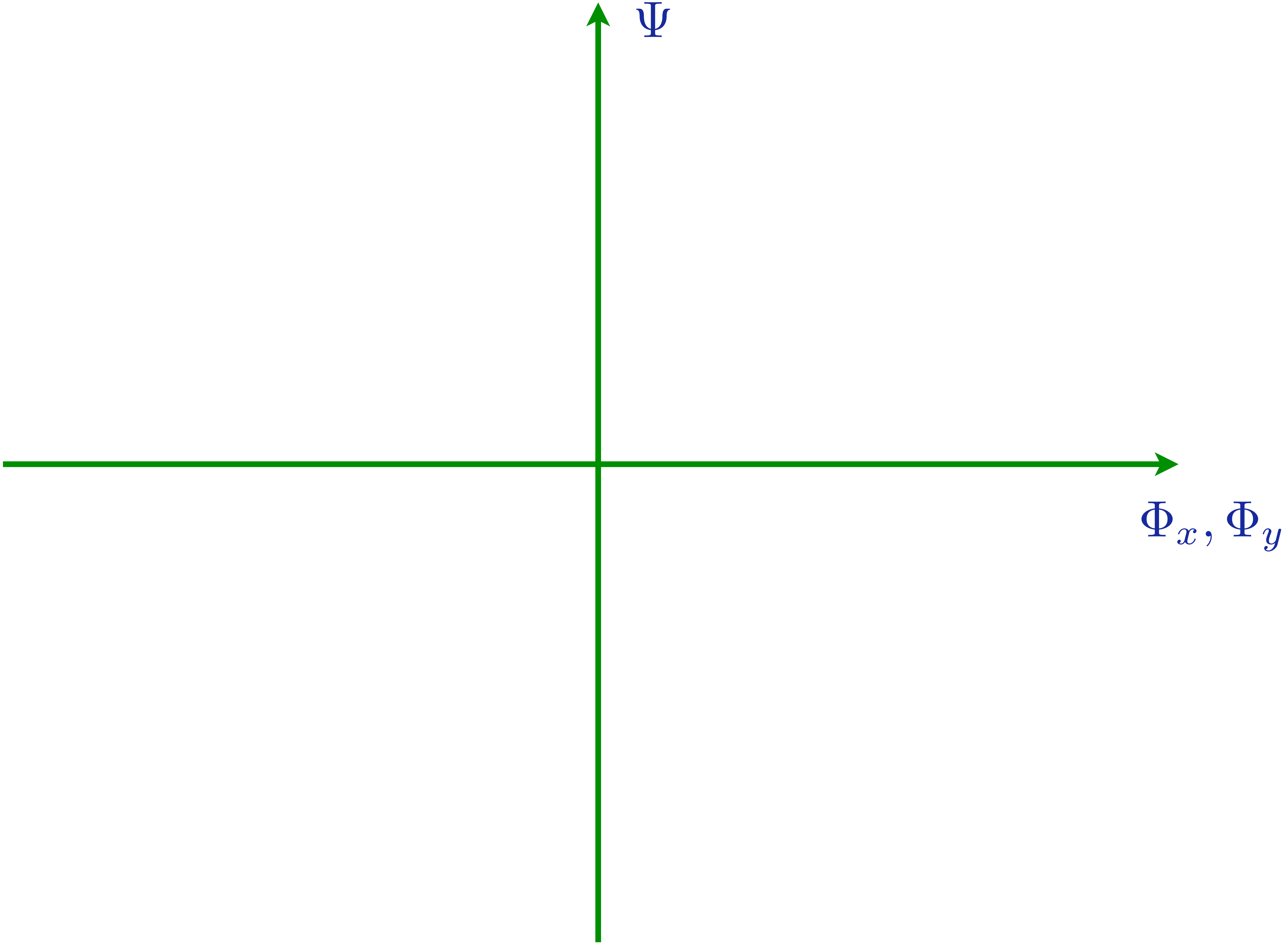
Superconducting order $\Psi(\mathbf{r})$:

$$\left\langle c_{i\alpha}^\dagger c_{j\beta}^\dagger \right\rangle = \varepsilon_{\alpha\beta} \left[\sum_{\mathbf{k}} \Delta_S(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right] \Psi\left((\mathbf{r}_i + \mathbf{r}_j)/2 \right)$$

Charge/bond order $\Phi_{x,y}(\mathbf{r})$ at wavevectors $\mathbf{Q}_{x,y}$:

$$\begin{aligned} \left\langle c_{i\alpha}^\dagger c_{j\beta} \right\rangle = {} & \delta_{\alpha\beta} \left[\sum_{\mathbf{k}} P_{\mathbf{Q}_x}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right] e^{i\mathbf{Q}_x\cdot(\mathbf{r}_i + \mathbf{r}_j)/2} \Phi_x\left((\mathbf{r}_i + \mathbf{r}_j)/2 \right) \\ & + \delta_{\alpha\beta} \left[\sum_{\mathbf{k}} P_{\mathbf{Q}_y}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right] e^{i\mathbf{Q}_y\cdot(\mathbf{r}_i + \mathbf{r}_j)/2} \Phi_y\left((\mathbf{r}_i + \mathbf{r}_j)/2 \right) \end{aligned}$$

Multi-component order parameter



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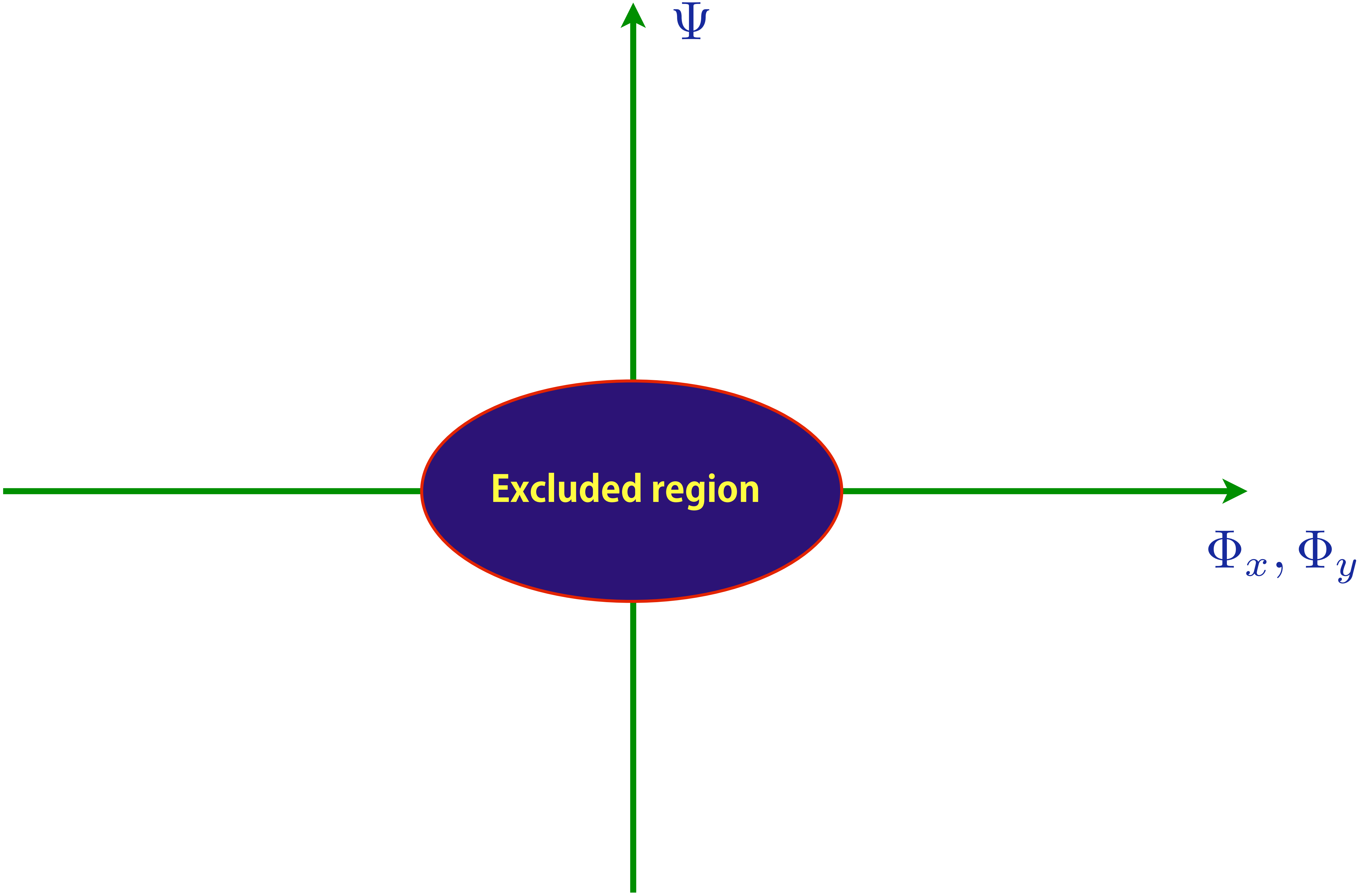

Support from theory of antiferromagnetic quantum criticality

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

K. B. Efetov, H. Meier, and C. Pepin, *Nature Physics* **9**, 442 (2013)

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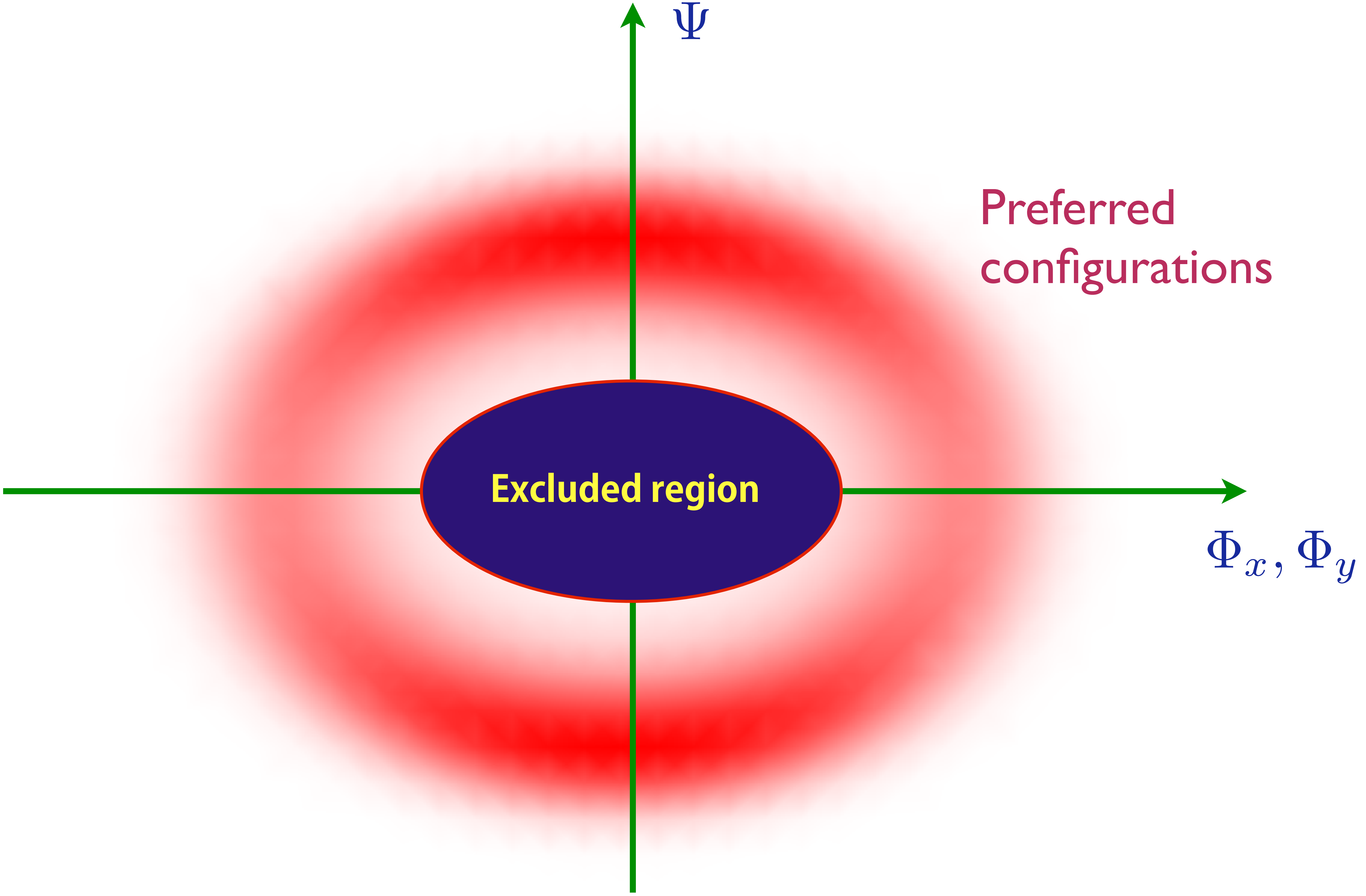

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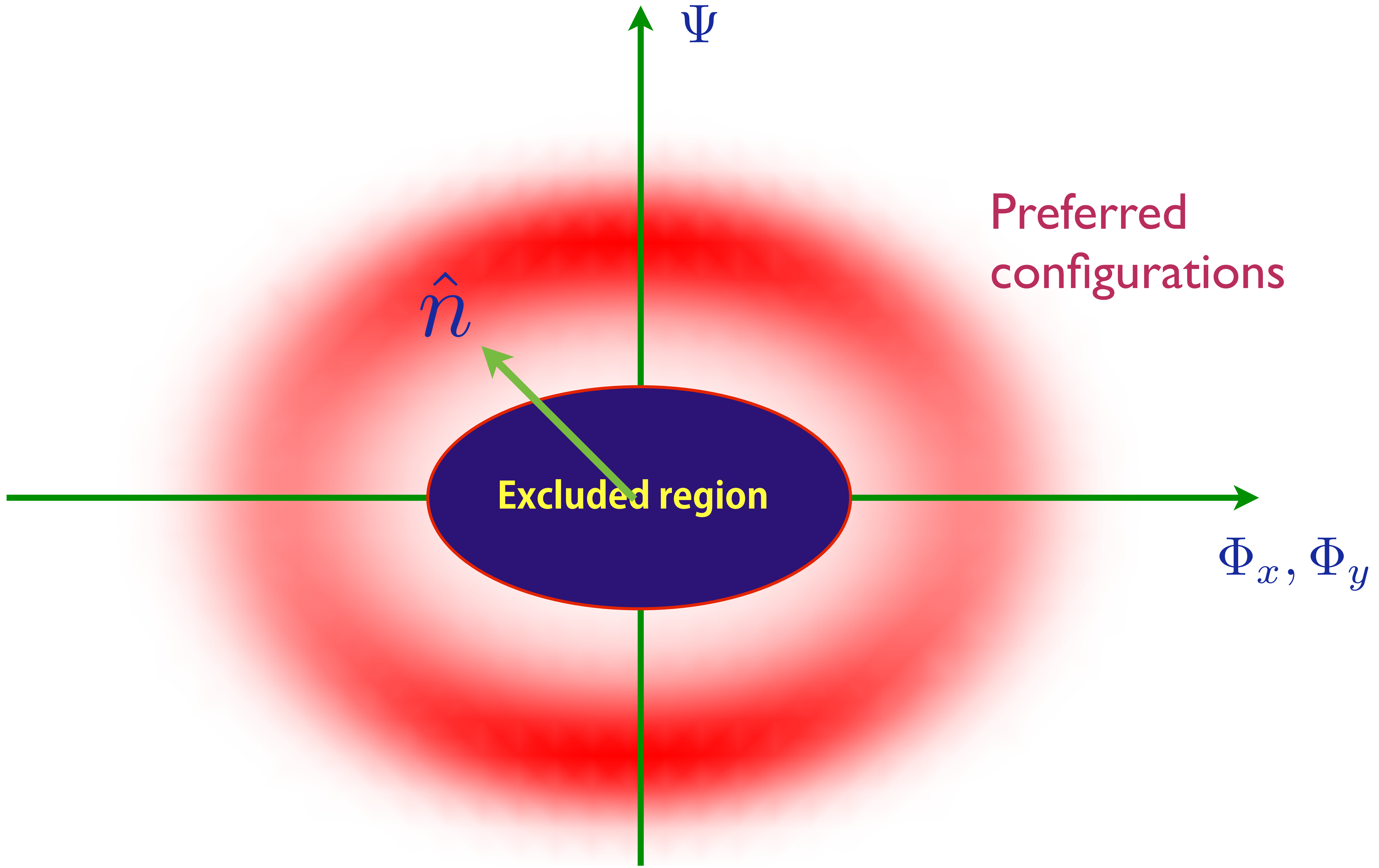

Label order parameter by a
6-component unit vector n_α with $\sum_\alpha n_\alpha^2 = 1$

O(6) non-linear sigma model

$$\mathcal{Z} = \int \mathcal{D}n_\alpha(\mathbf{r})\,\delta\left(\sum_{\alpha=1}^{6} n_\alpha^2(\mathbf{r}) - 1\right) \exp\left(- \frac{\rho_s}{2T} \int d^2 r \left[\sum_{\alpha=1}^{2} (\nabla n_\alpha)^2 + \lambda \sum_{\alpha=3}^{6} (\nabla n_\alpha)^2 + g \sum_{\alpha=3}^{6} n_\alpha^2 + w \left[\left(n_3^2 + n_4^2\right)^2 + \left(n_5^2 + n_6^2\right)^2 \right] \right] \right).$$

where $\Psi \propto n_1 + i n_2$, $\Phi_x \propto n_3 + i n_4$, $\Phi_y \propto n_5 + i n_6$.

Describes $\mathrm{O}(6) \Rightarrow \mathrm{O}(2)\times\mathrm{O}(2)\times\mathrm{O}(2)\rtimes\mathbb{Z}_2$. The coupling g determines the anisotropy between superconductivity and charge order.

Solve by cluster Monte Carlo and $1/N$ expansion.

L. E. Hayward, D. G. Hawthorn, R. G. Melko, and S. Sachdev, *Science*, in press, arXiv:1309.6639

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Only source of T-dependence; strongly constraints theoretical predictions

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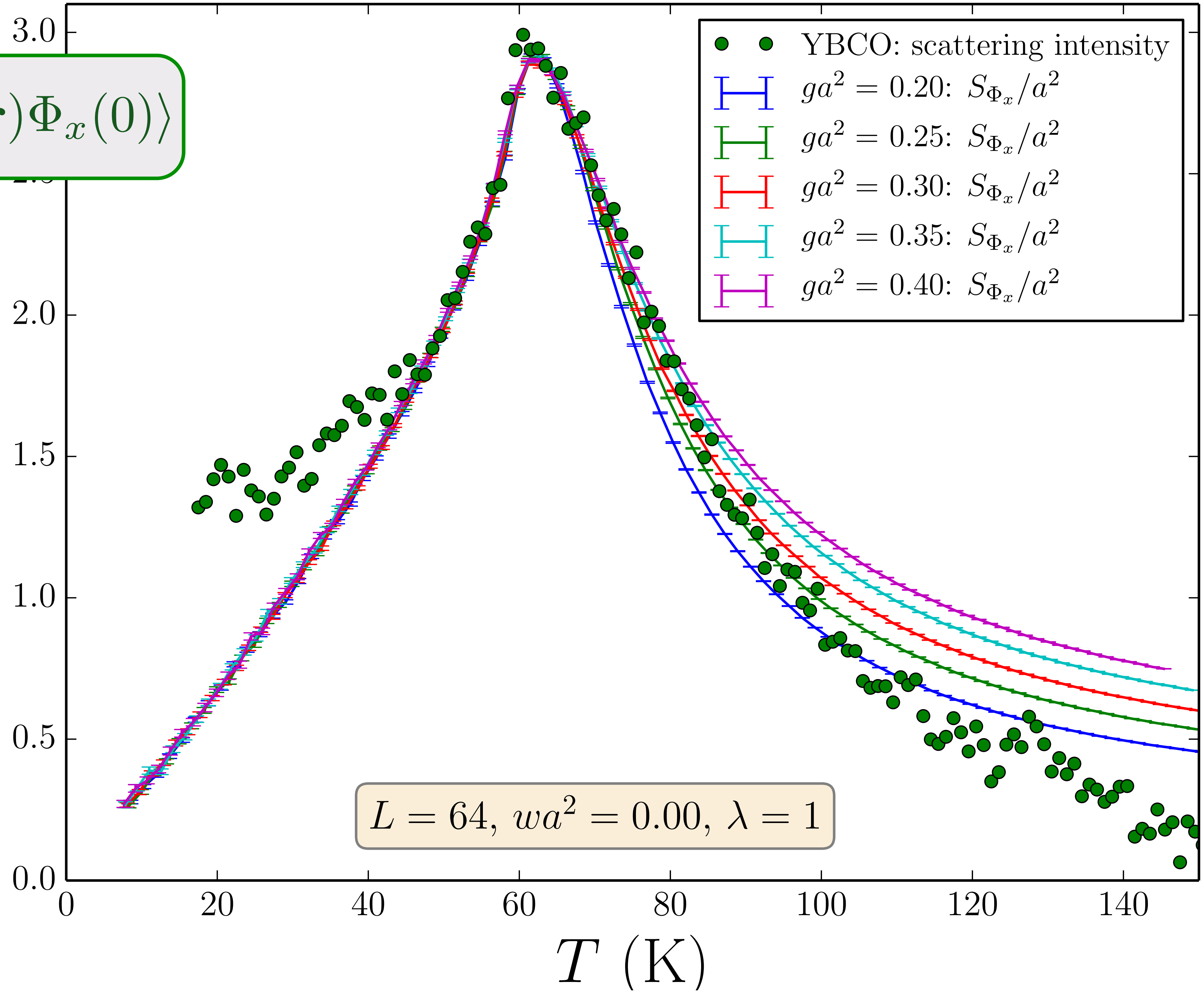
Comparison of Monte Carlo with experiments

$$S_{\Phi_x} = \int d^2 r \, \langle \Phi_x(\mathbf{r}) \Phi_x(0) \rangle$$

Charge order structure factor S_{Φ_x}



Lauren Hayward

For $ga^2 = 0.30$ and $wa^2 = 0.0$ we have $\rho_s = 160$K.
The height was also rescaled to make the peak heights match.

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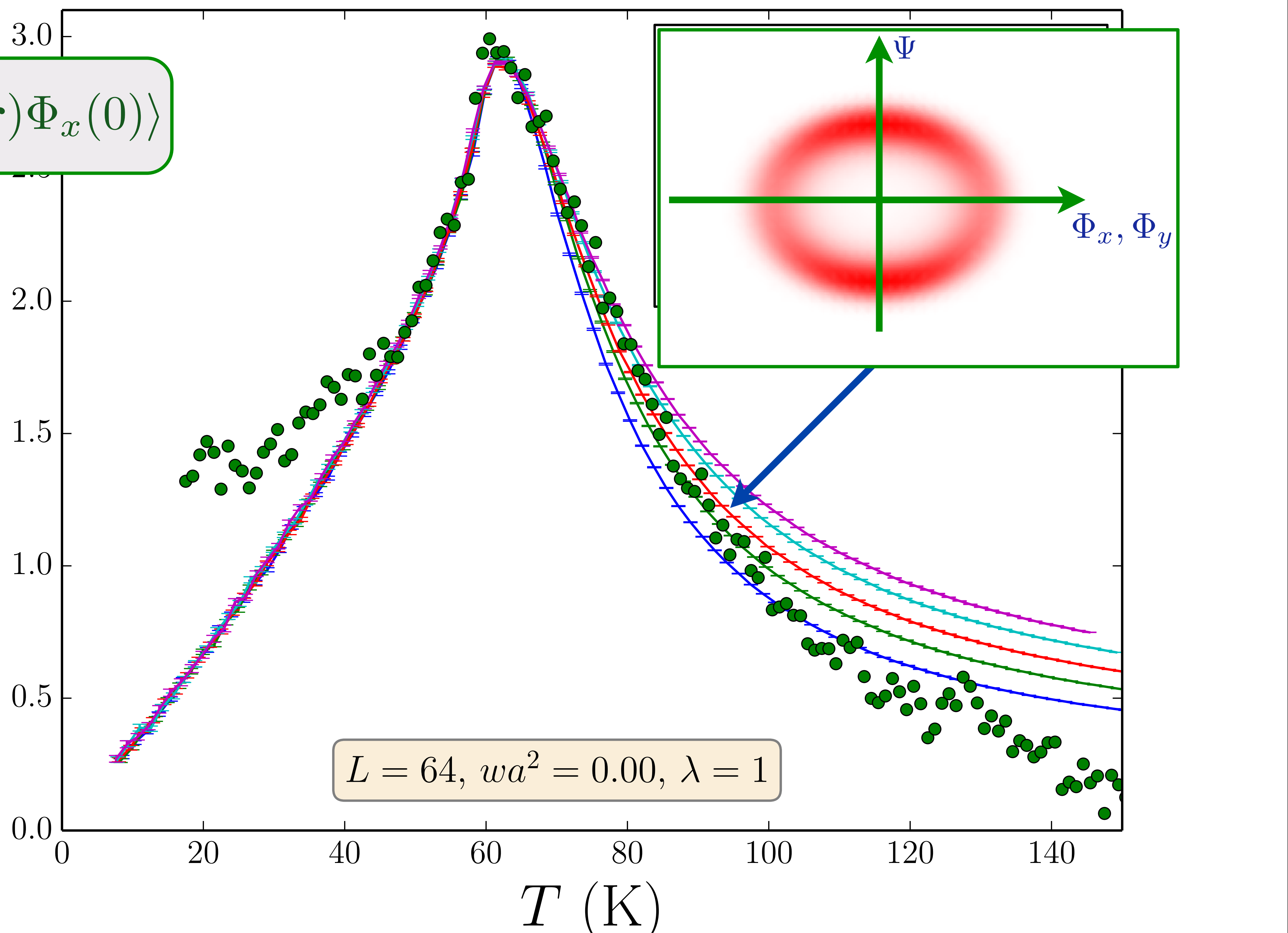

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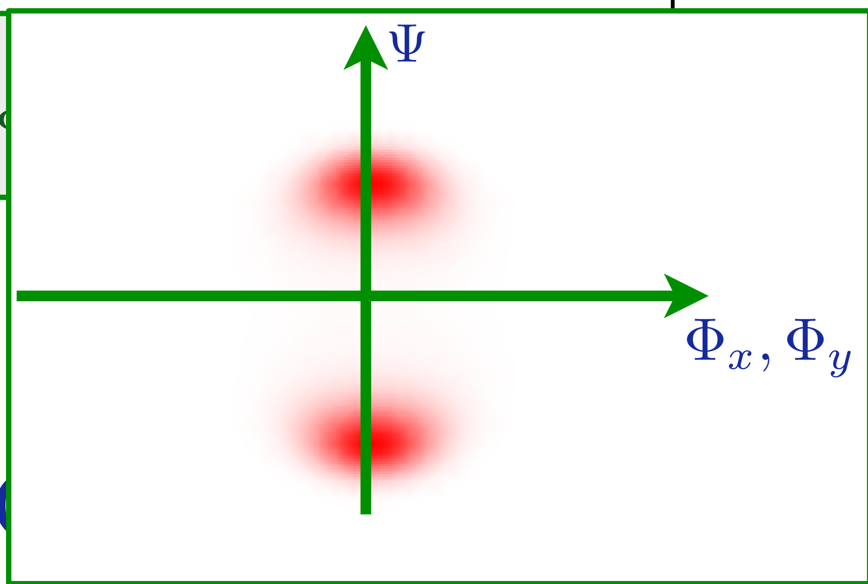

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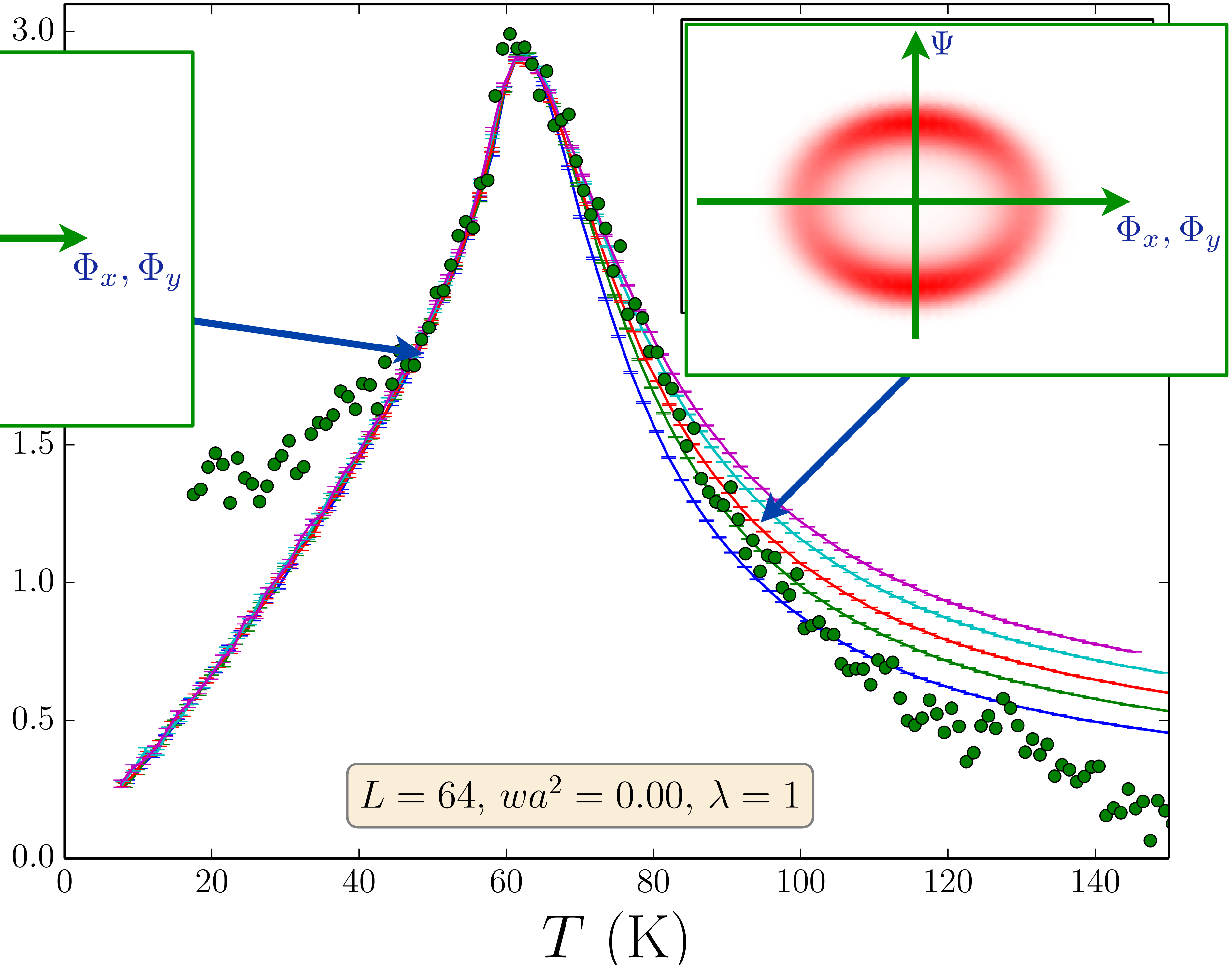
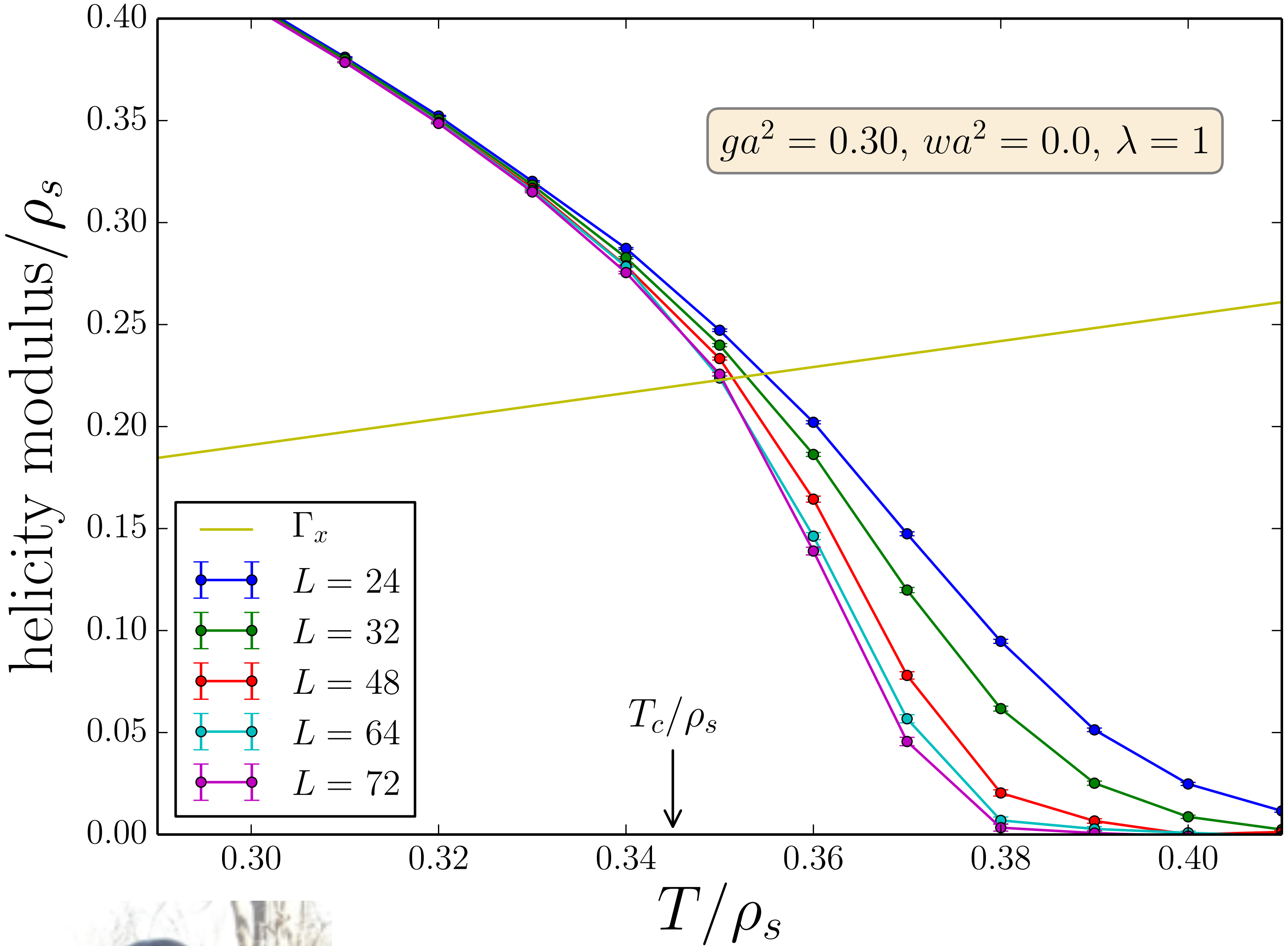


Lauren Hayward

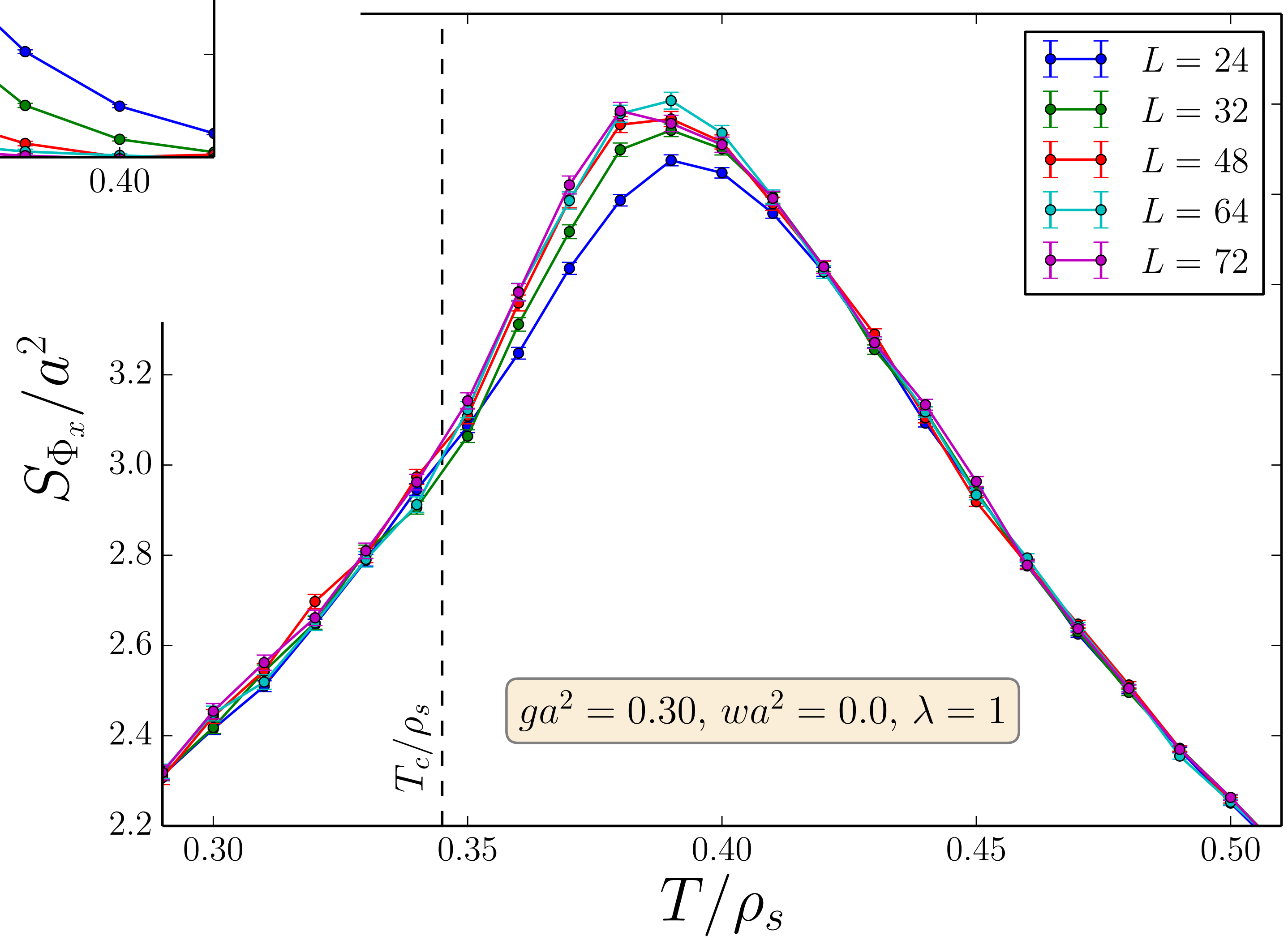
For $ga^2 = 0.30$ and $wa^2 = 0.0$ we have $\rho_s = 160\text{K}$.
The height was also rescaled to make the peak heights match.

L. E. Hayward, D. G. Hawthorn, R. G. Melko, and S. Sachdev, *Science*, in press, arXiv:1309.6639

Onset of superconductivity in Monte Carlo



Lauren Hayward



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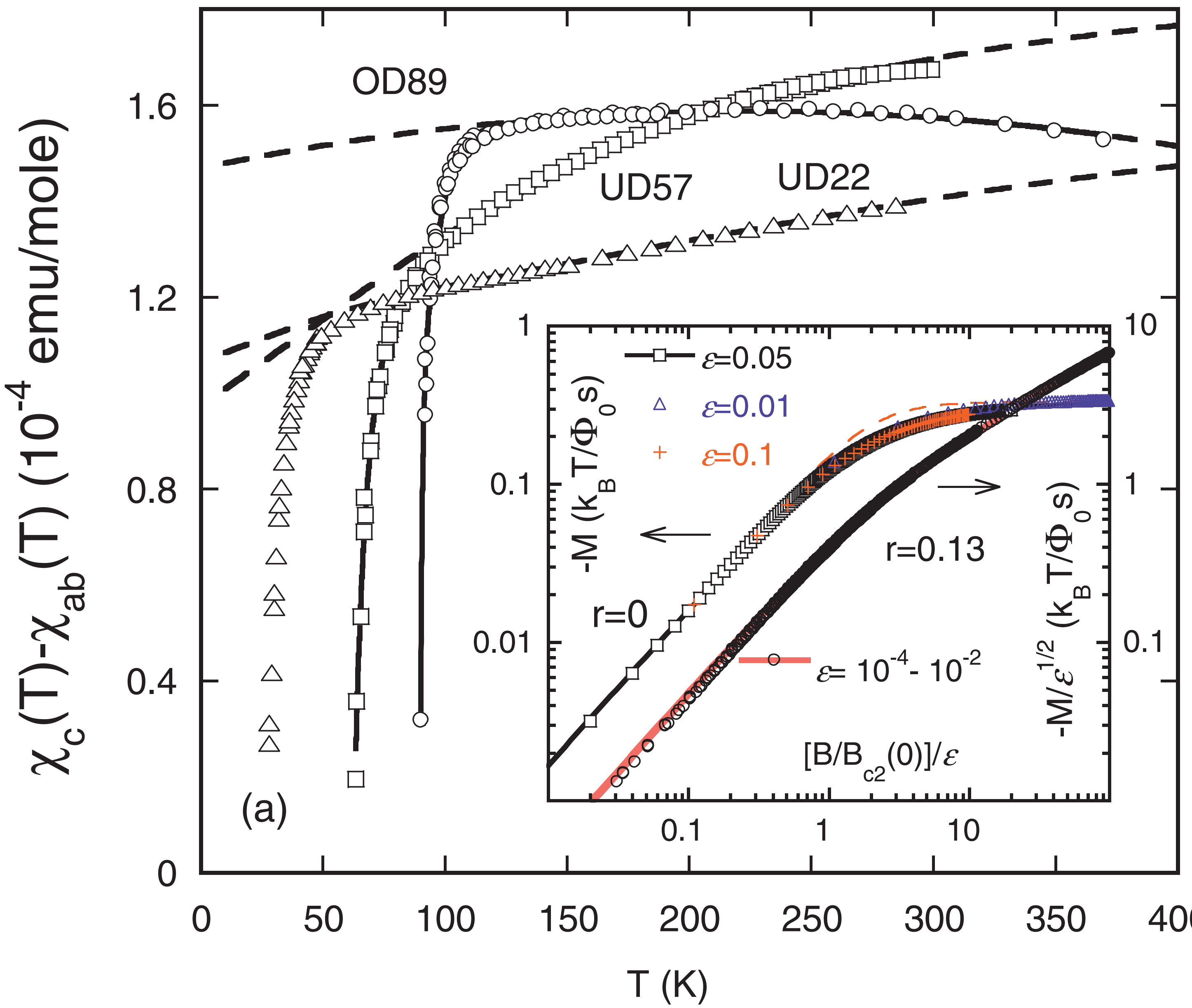
Diamagnetism in the pseudogap

Diamagnetism of $YBa_2Cu_3O_{6+x}$ crystals above T_c: Evidence for Gaussian fluctuations

I. Kokanović,[1,2,*] D. J. Hills,[1] M. L. Sutherland,[1] R. Liang,[3] and J. R. Cooper[1]

PHYSICAL REVIEW B **88**, 060505(R) (2013)



Diamagnetism in the pseudogap

- The *same* set of parameters used to describe X-ray scattering, also predict the strength of superconducting fluctuations above T_c. We characterize the diamagnetism by computing a dimensionless ratio, $R(T)$, between the diamagnetic susceptibility, χ_d, and the charge order correlation length:

$$R(T) \equiv \frac{12\pi \, \chi_d(T)}{k_B T \xi_{\rm cdw}^2}$$

L. E. Hayward, D. G. Hawthorn, R. G. Melko, and S. Sachdev, *to appear*

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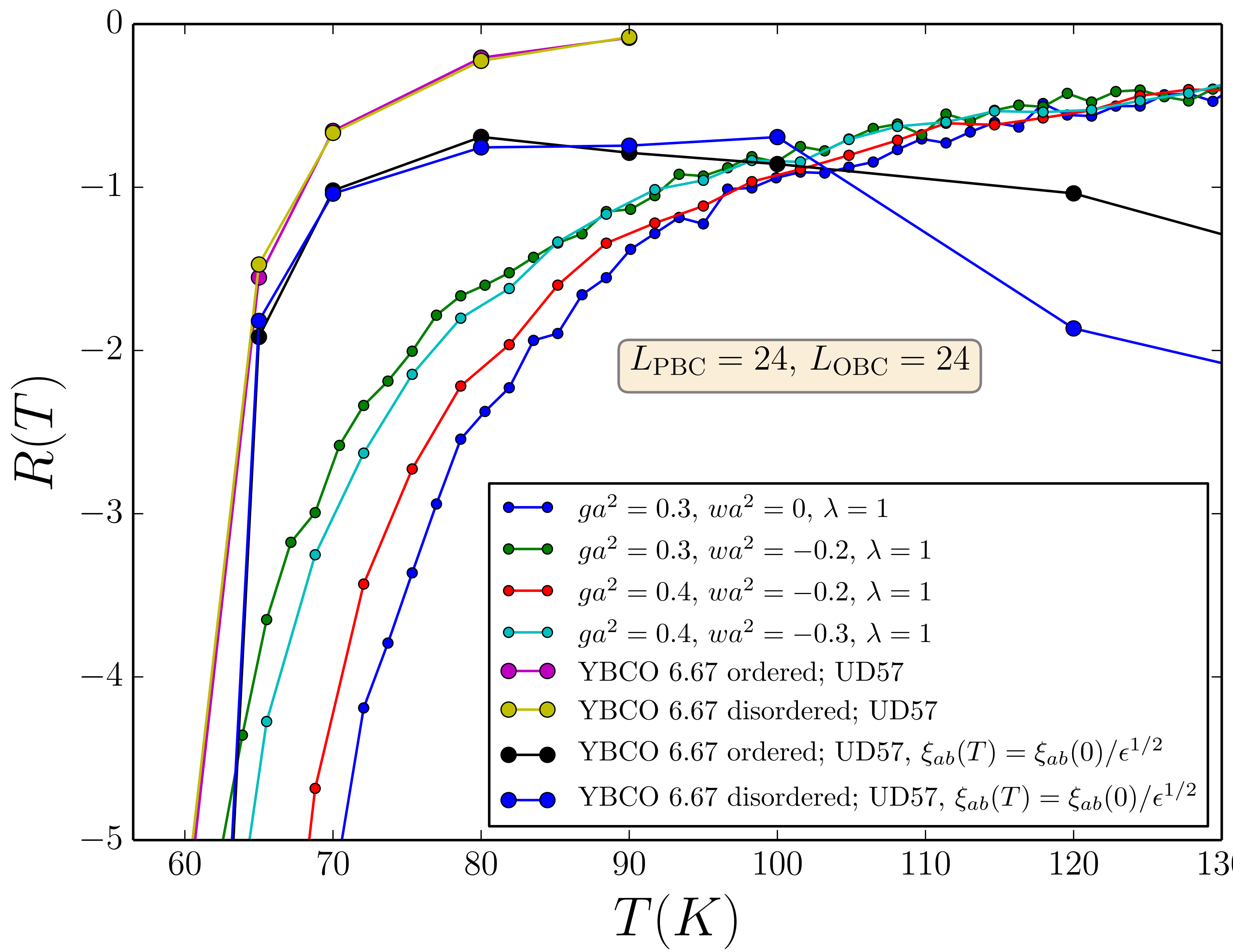

Lauren Hayward

L. E. Hayward, D. G. Hawthorn, R. G. Melko, and S. Sachdev, *to appear*

- The charge order of the cuprates was argued to be predominantly *d*-wave bond order by S. Sachdev and R. LaPlaca (*Phys. Rev. Lett.* **111**, 027202 (2013)). This predicted order appears to have been observed in recent X-ray scattering experiments by Comin *et al.* (arXiv:1402.5415)

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- Angular, classical, thermal fluctuations of a multi-component order parameter, involving charge order and superconductivity, describe the pseudogap regime in YBCO.