Bond order in two-dimensional metals with antiferromagnetic exchange interactions

Gordon Research Conference
Les Diablerets
May 14, 2013

Subir Sachdev

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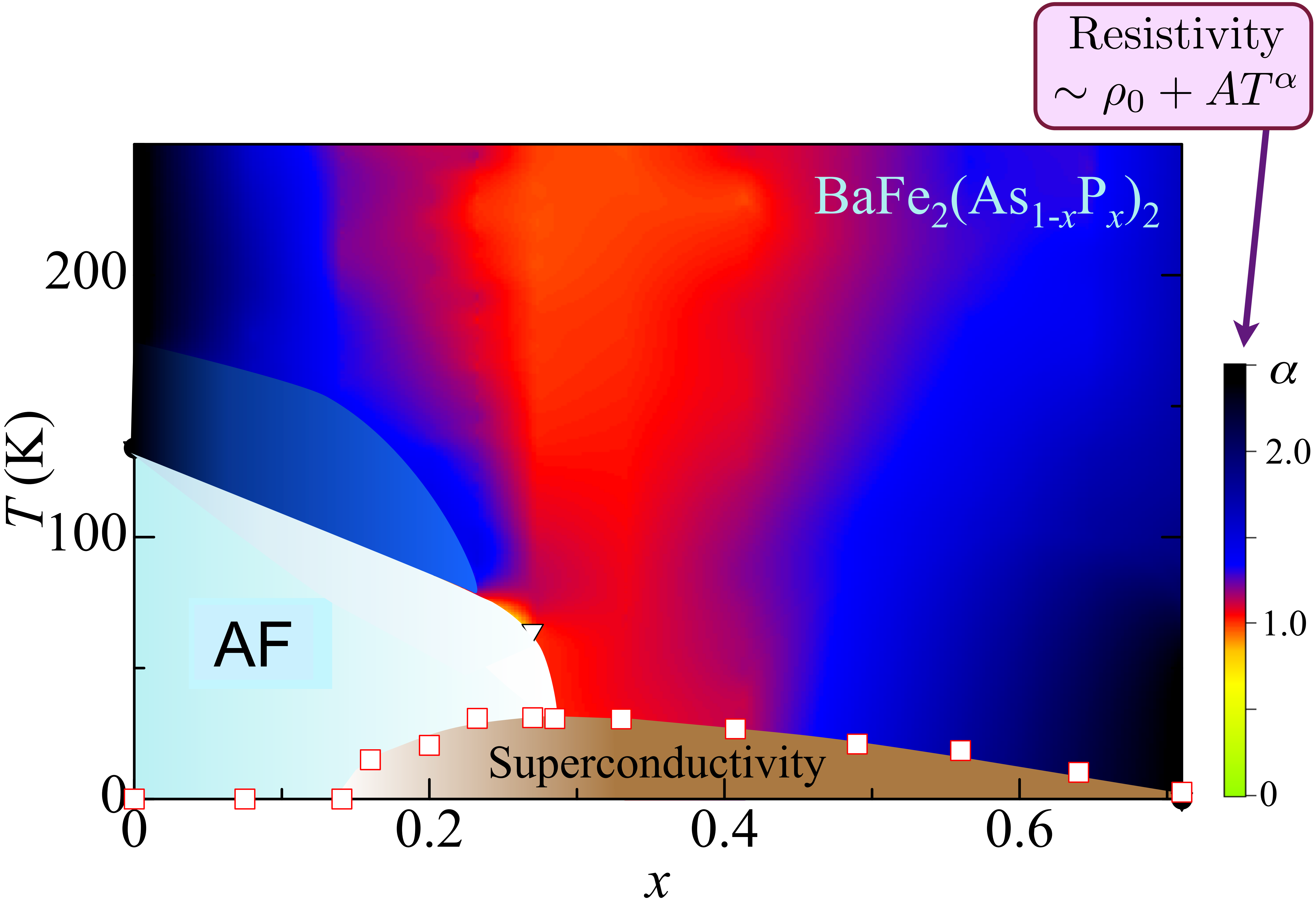
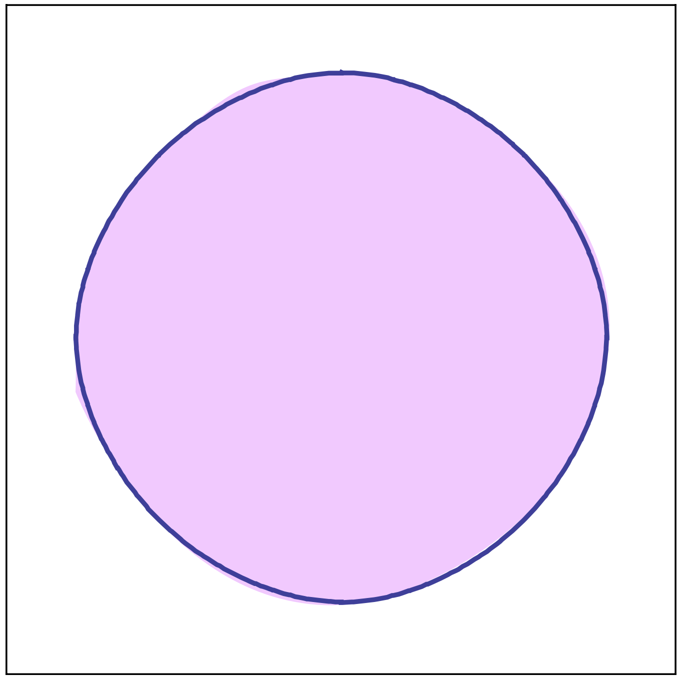


S. Kasahara, T. Shibauchi, K. Hashimoto, K. Ikada, S. Tonegawa, R. Okazaki, H. Shishido, H. Ikeda, H. Takeya, K. Hirata, T. Terashima, and Y. Matsuda, *Physical Review B* **81**, 184519 (2010)

Fermi surface+antiferromagnetism

Metal with "large" Fermi surface



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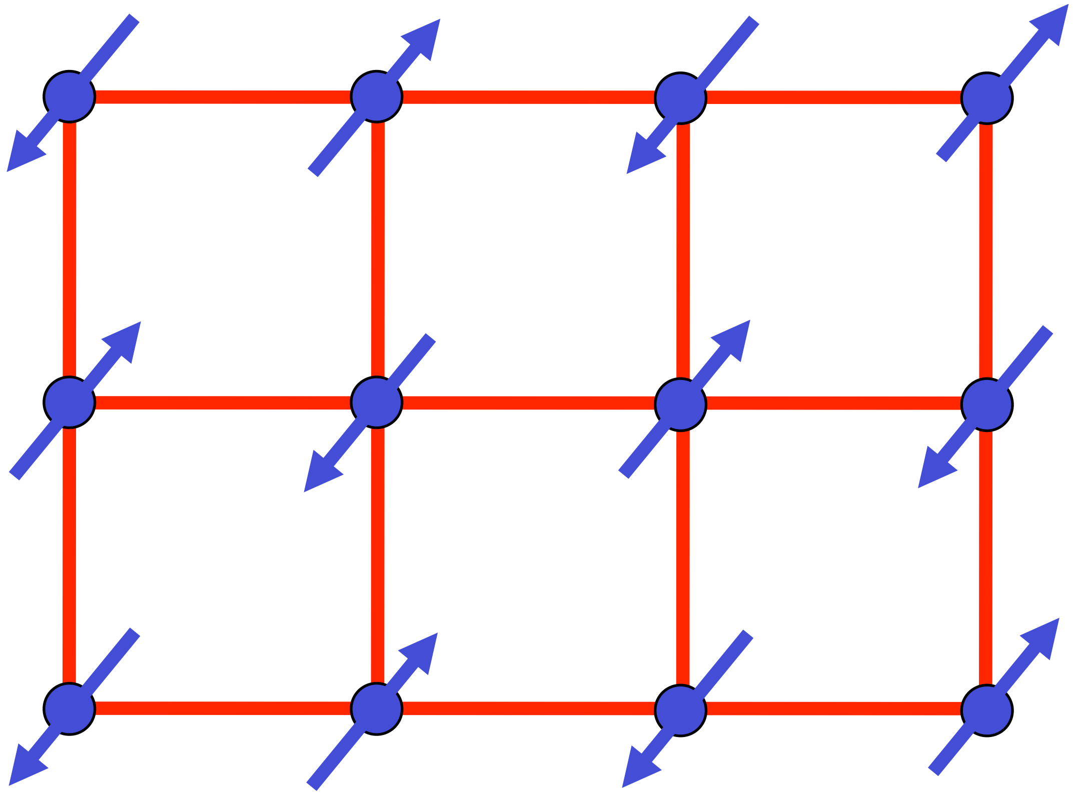
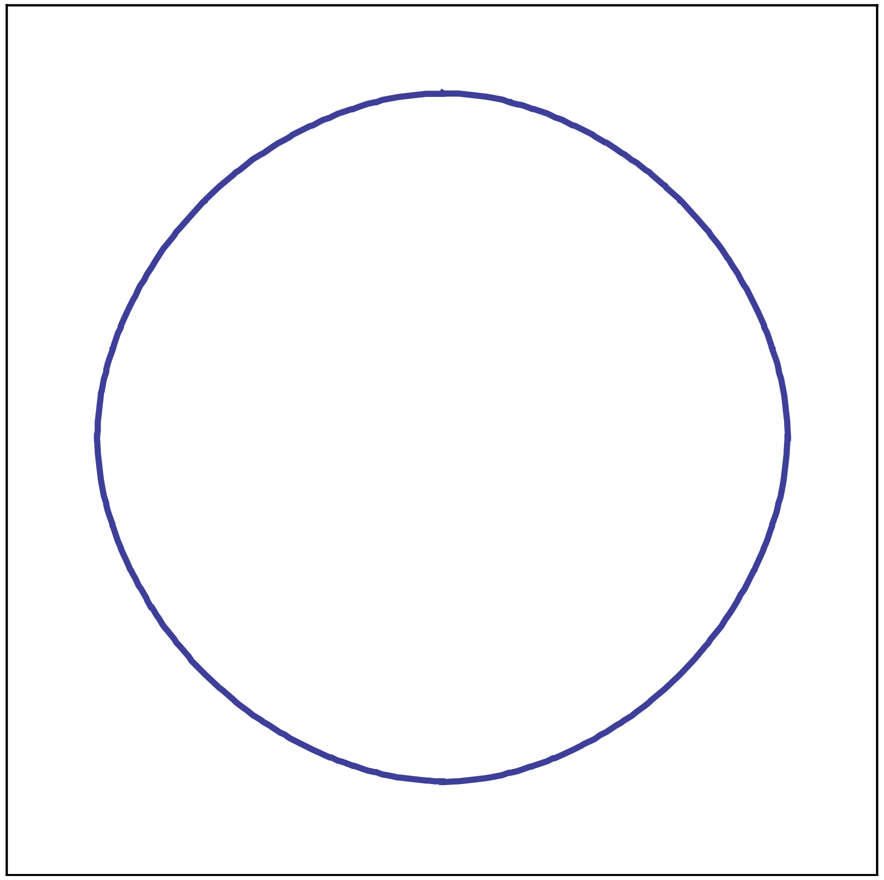


The electron spin polarization obeys

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

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

Fermi surface+antiferromagnetism



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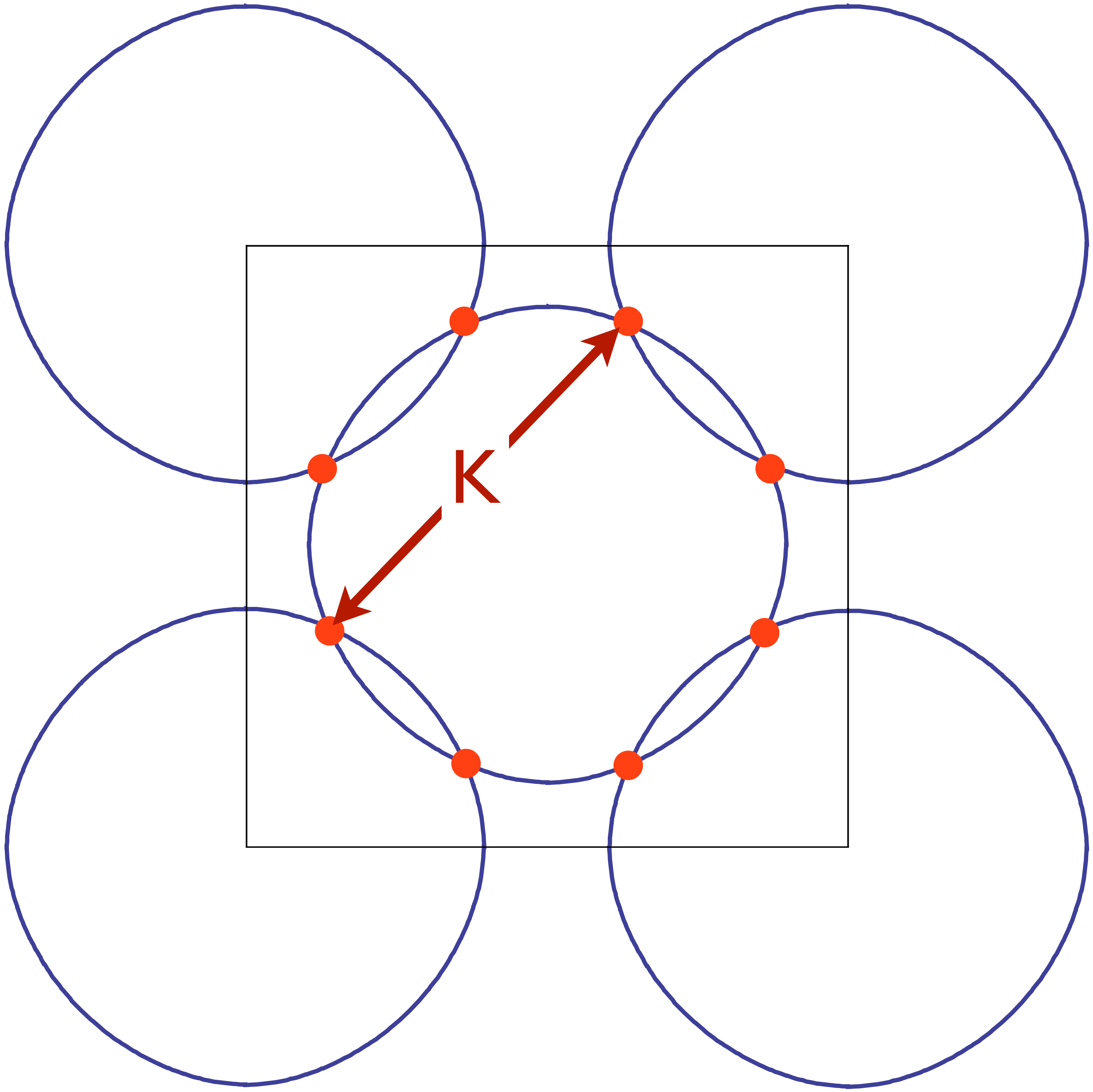
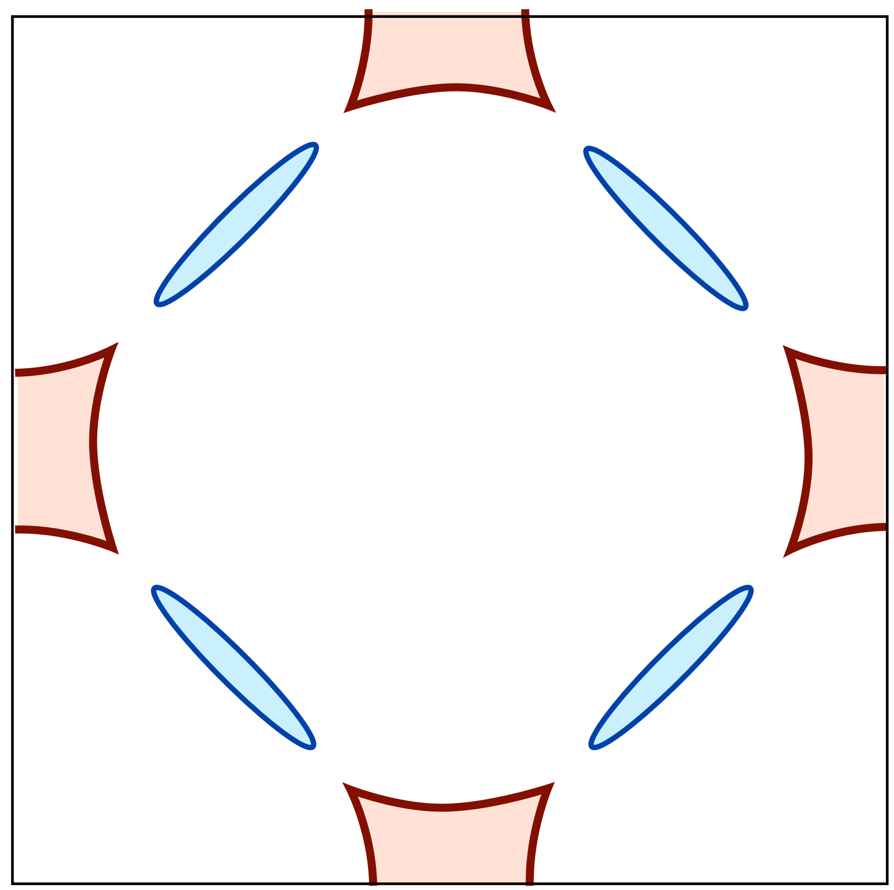


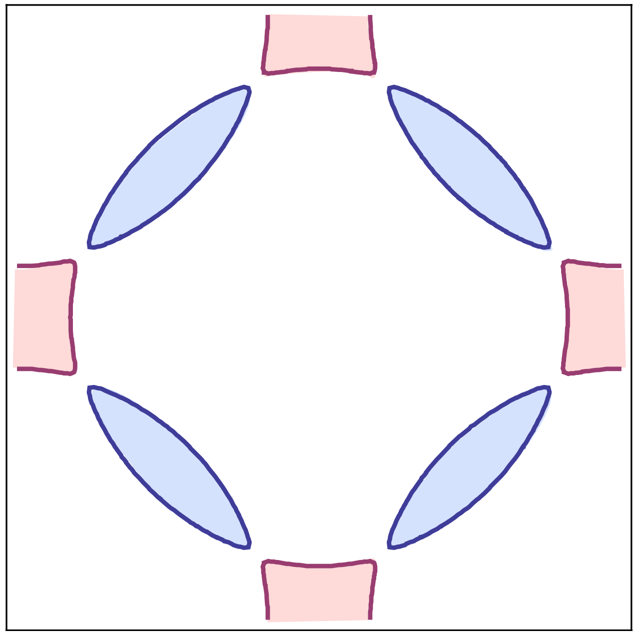
"Hot" spots

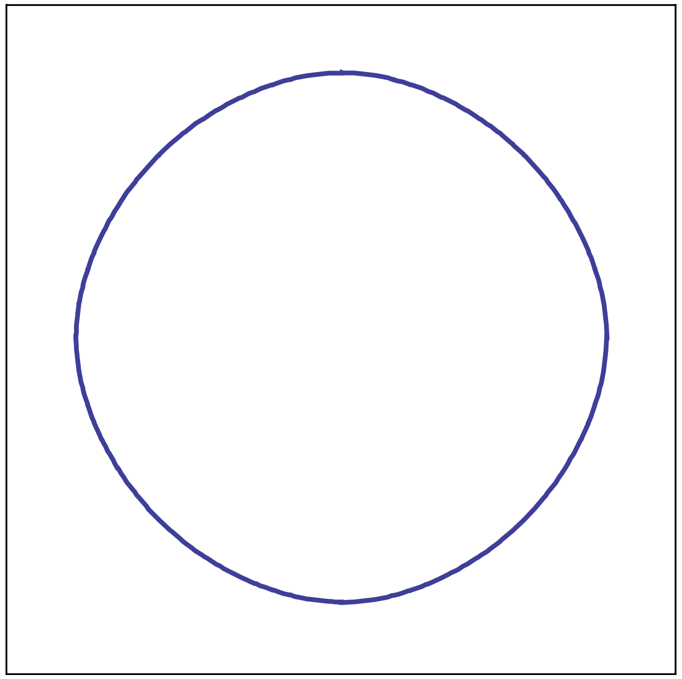
Fermi surface+antiferromagnetism



Electron and hole pockets in
antiferromagnetic phase
with antiferromagnetic order parameter $\langle \vec{\varphi} \rangle \neq 0$

Fermi surface+antiferromagnetism





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

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

Metal with electron and hole pockets

Metal with "large" Fermi surface

r

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

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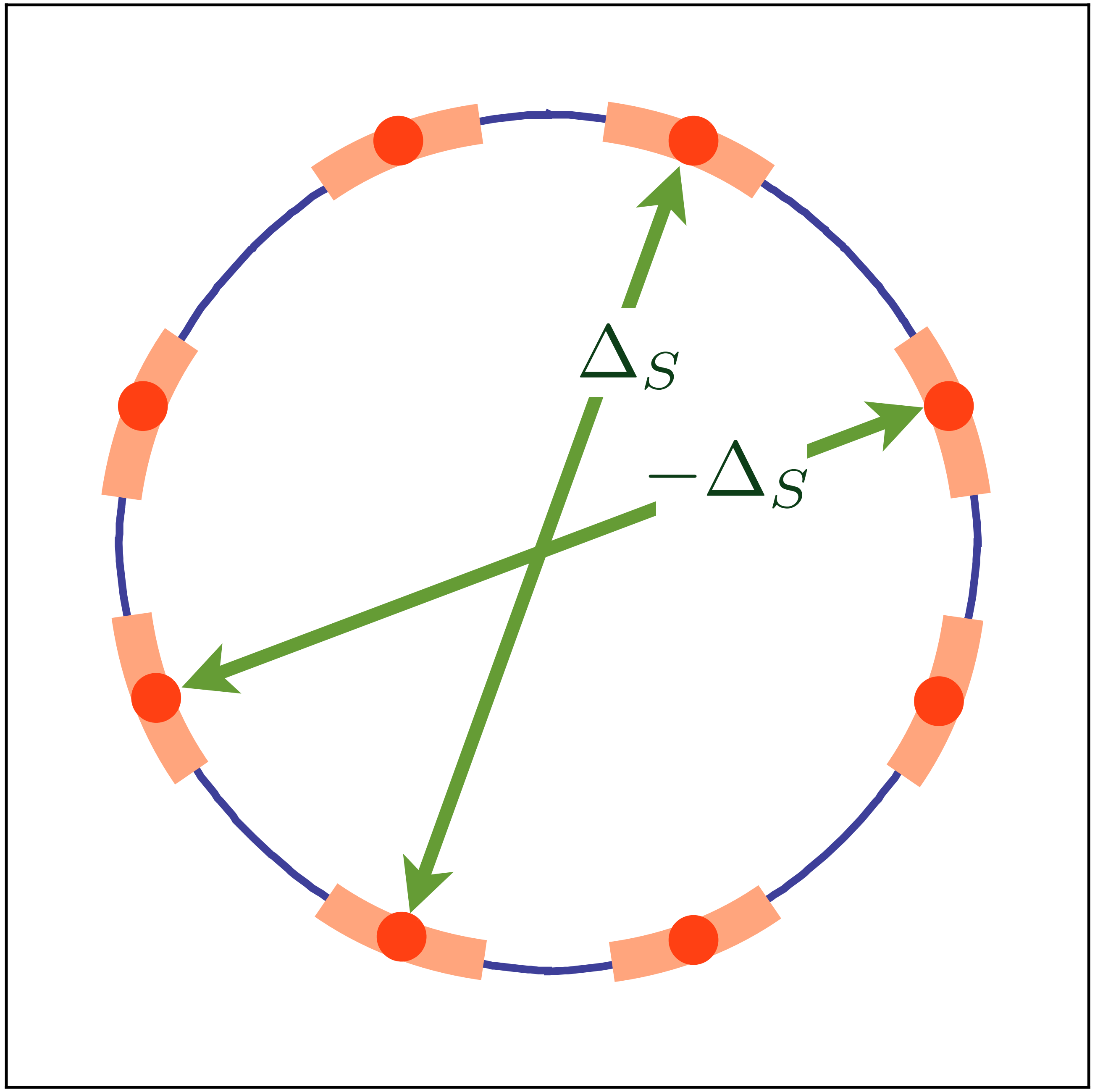
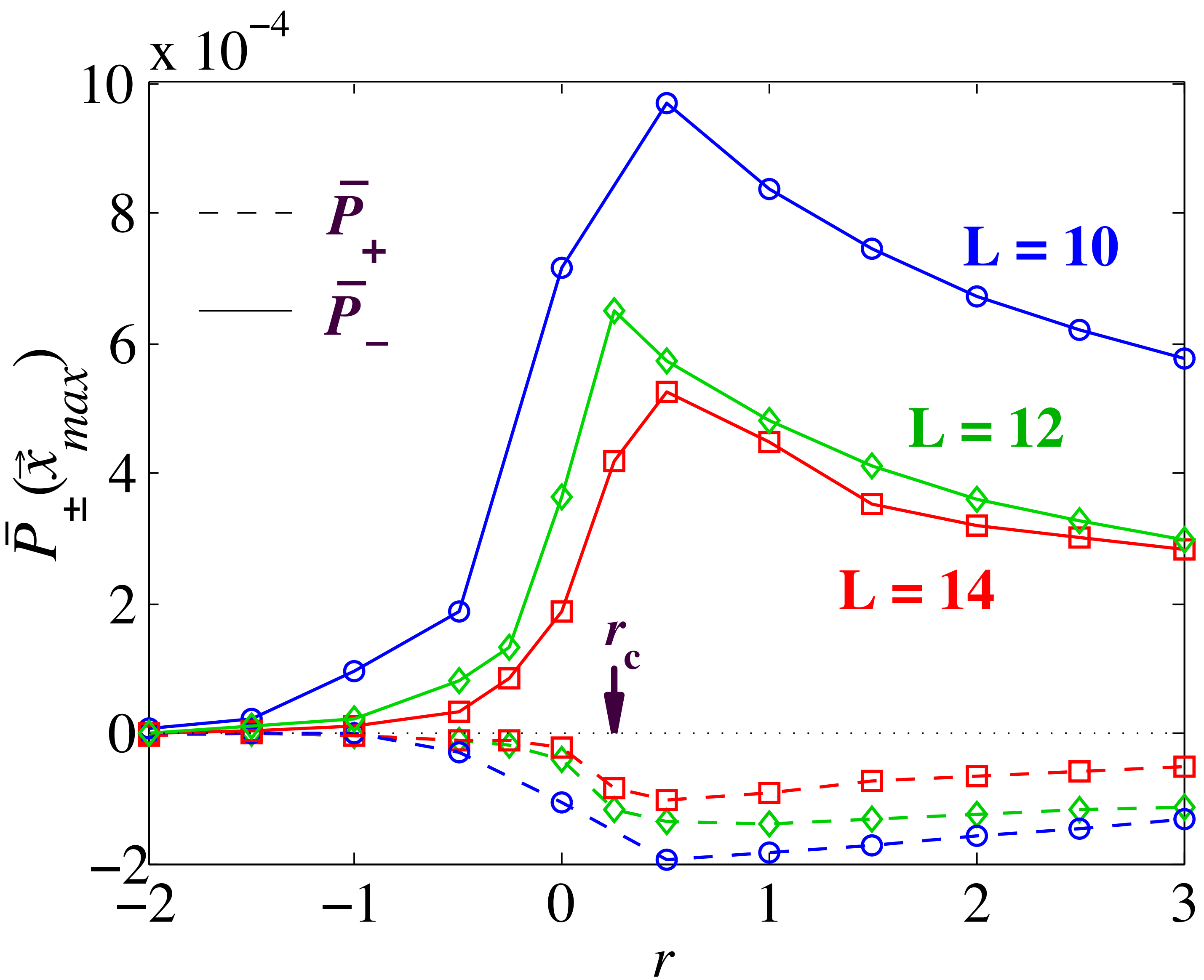


d-wave superconductor: particle-particle pairing at *and near* hot spots, with sign-changing pairing amplitude

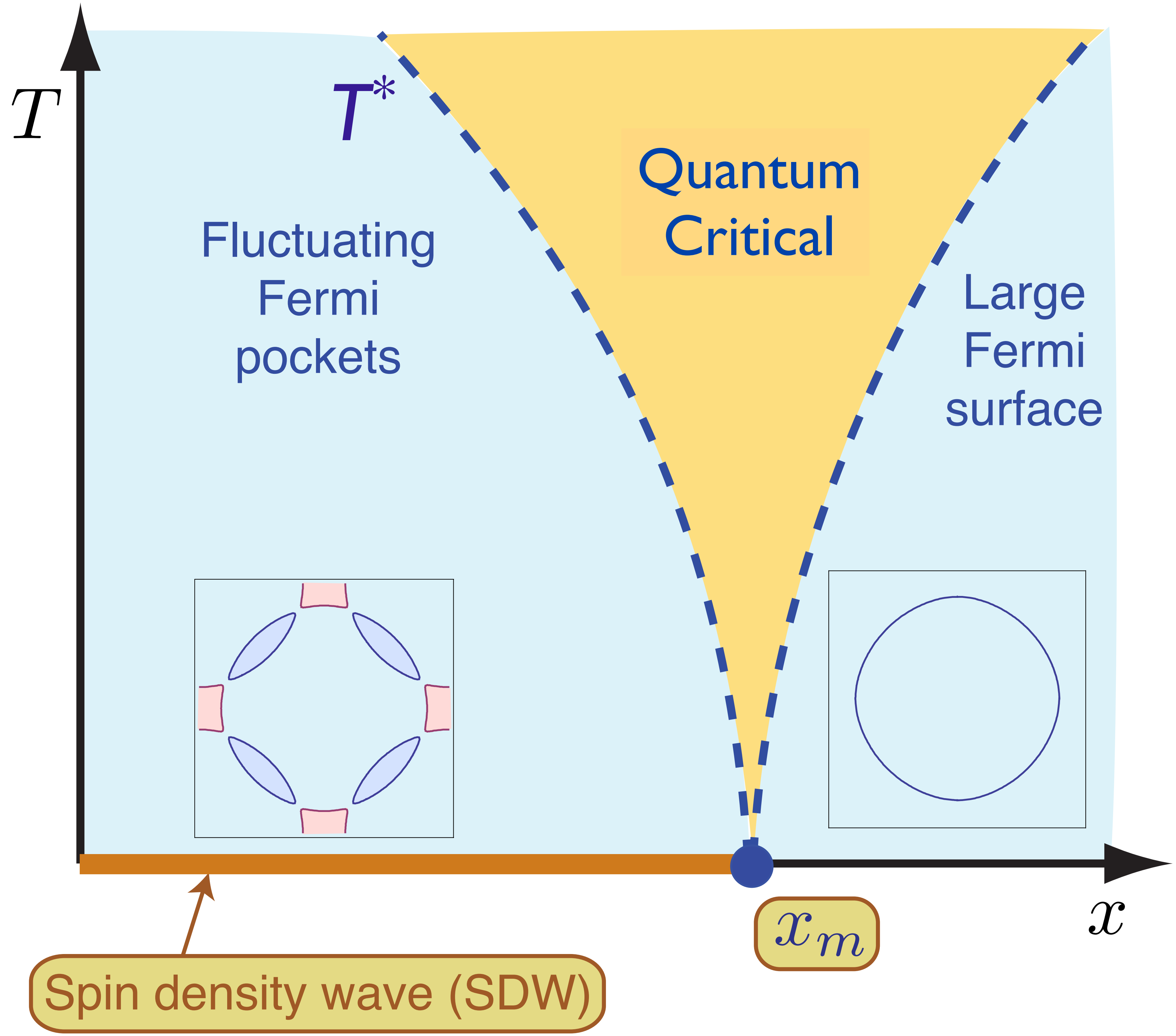
Sign-problem-free Quantum Monte Carlo for antiferromagnetism in metals



s/d pairing amplitudes P_+/P_-
as a function of the tuning parameter r

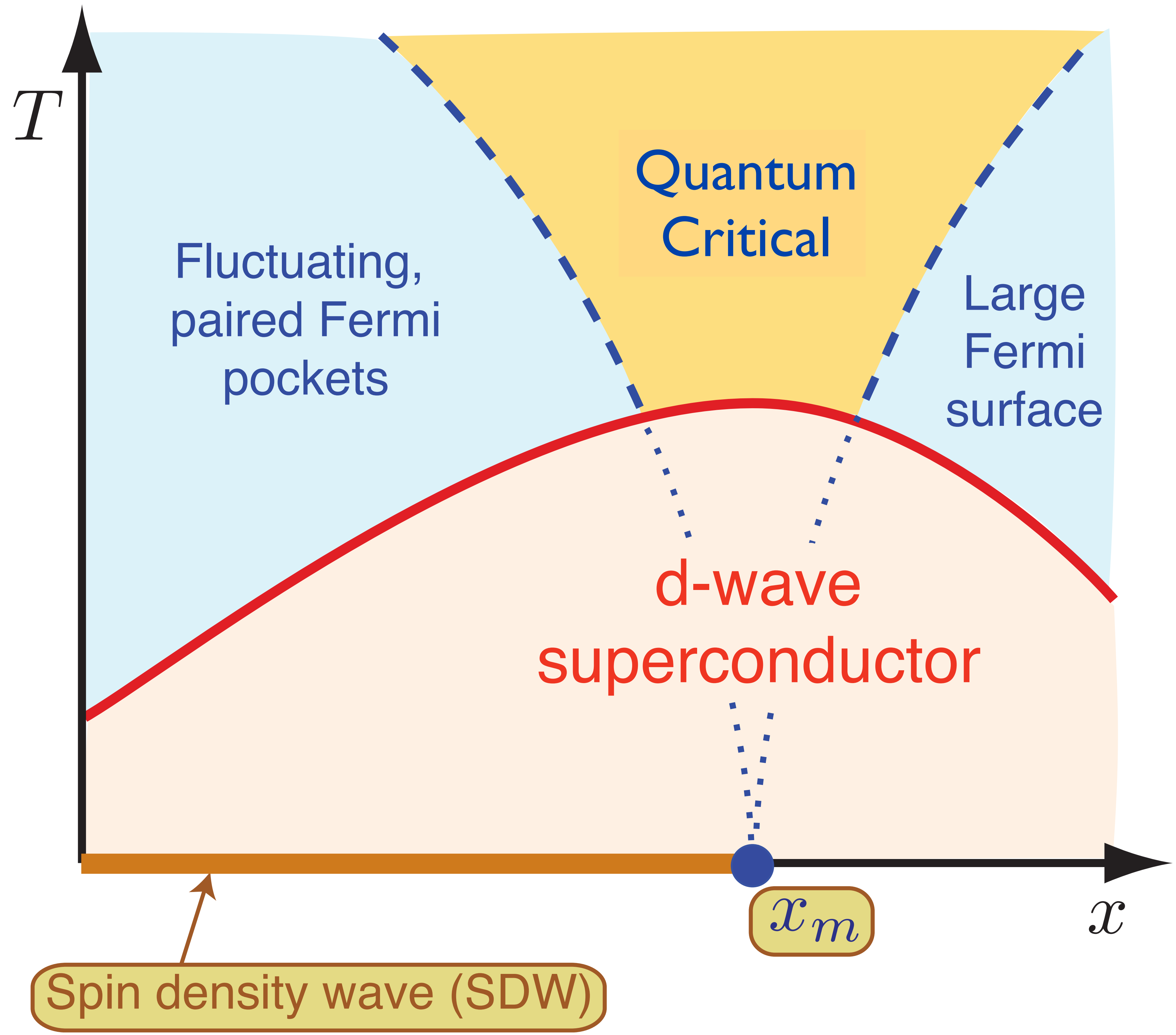
E. Berg, M. Metlitski, and S. Sachdev, *Science* **338**, 1606 (2012).

Fermi surface+antiferromagnetism

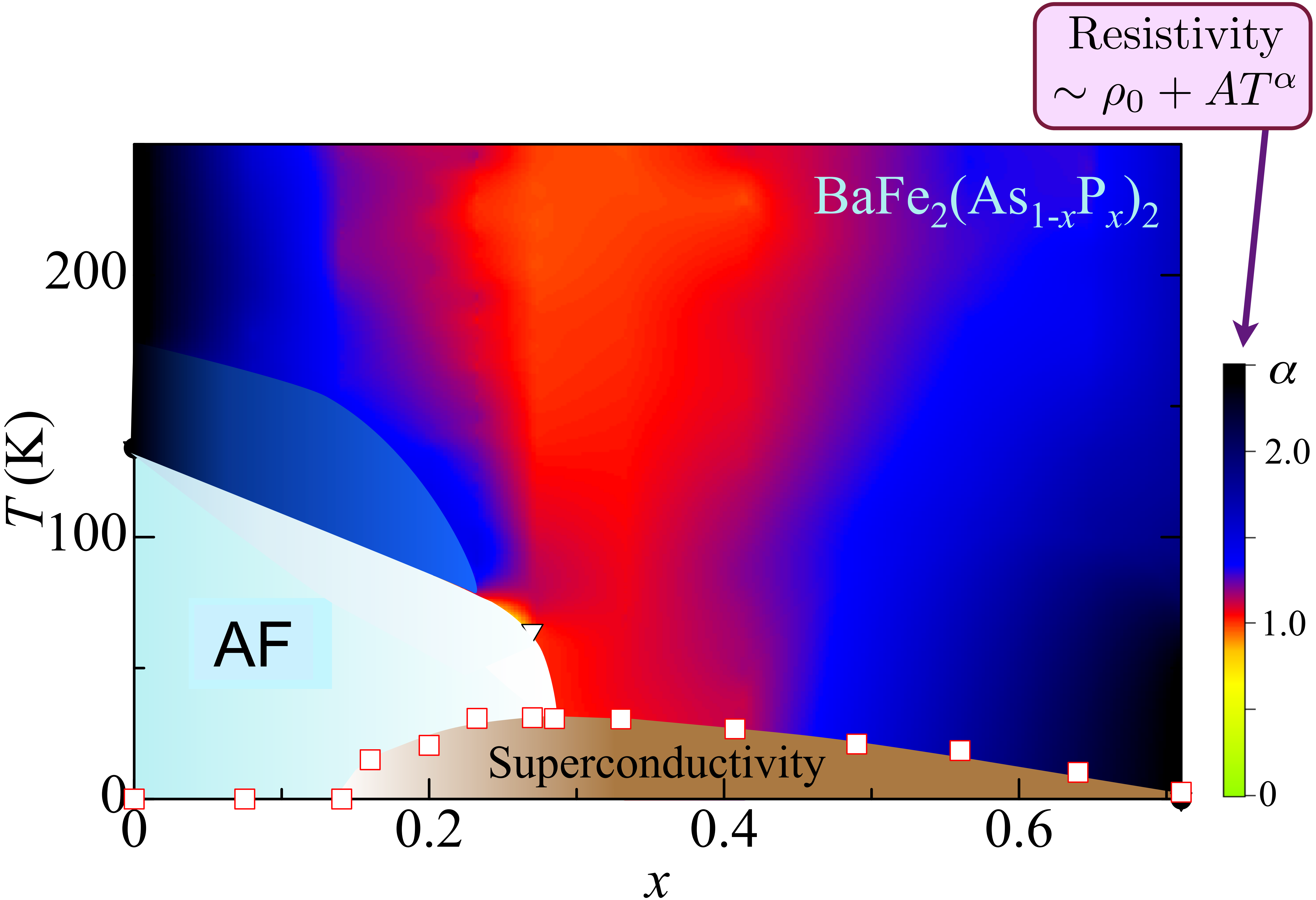


Underlying SDW ordering quantum critical point in **metal** at $x = x_m$

Fermi surface+antiferromagnetism



QCP for the onset of SDW order is actually within a superconductor



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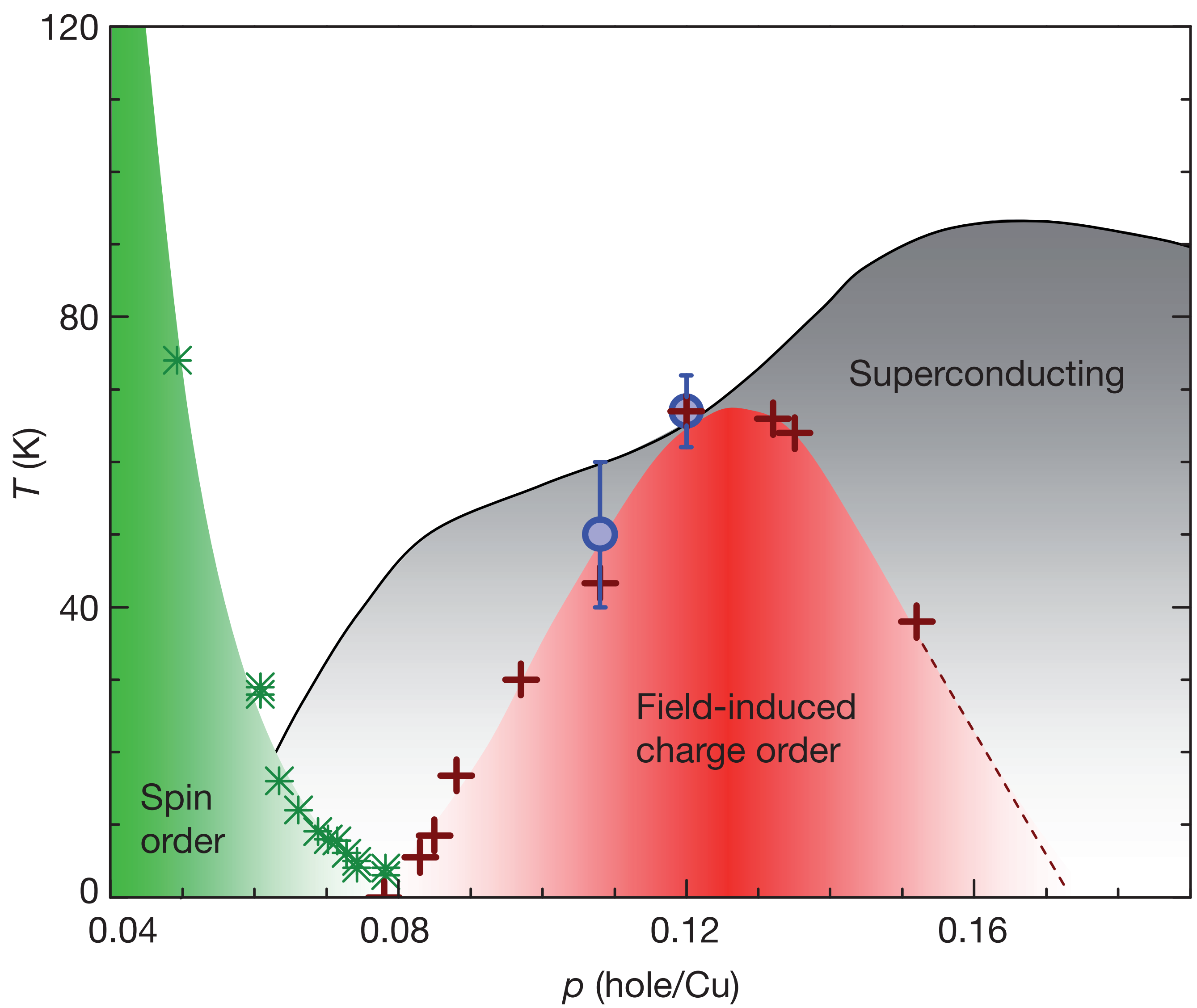
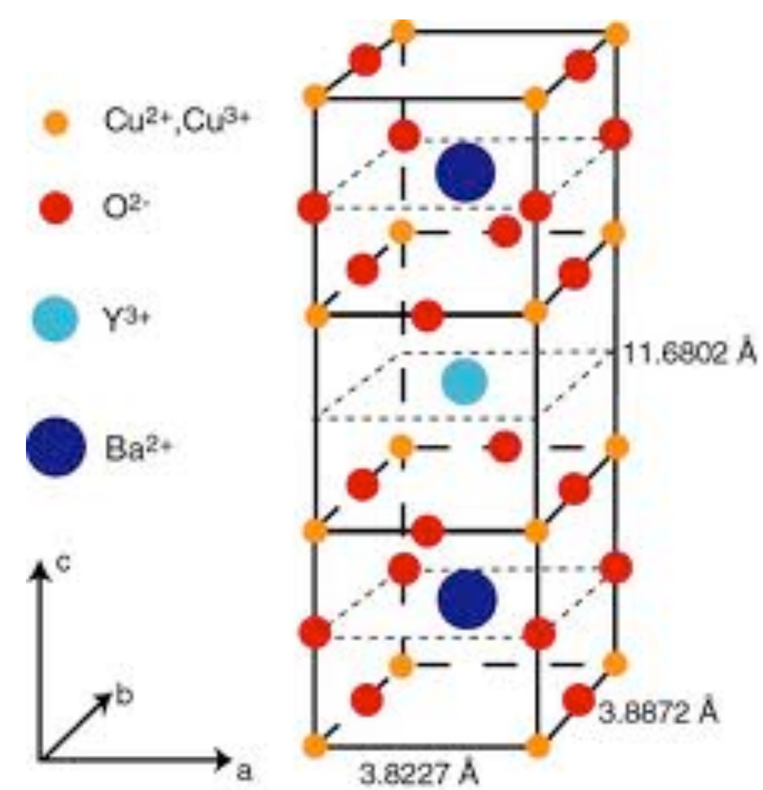
Magnetic-field-induced charge-stripe order in the high-temperature superconductor $YBa_2Cu_3O_y$

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





1. Pseudospin symmetry between d-wave superconductivity and bond order

Continuum field theory with exact pseudospin symmetry

2. Approximate pseudospin symmetry on the lattice t-J model

Pseudogap and bond order in the underdoped cuprates

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Pseudogap and bond order in the underdoped cuprates

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

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

which is invariant under independent SU(2) pseudospin transformations on each site

$$\Psi_{i\alpha} \to U_i \Psi_{i\alpha}$$

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)

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

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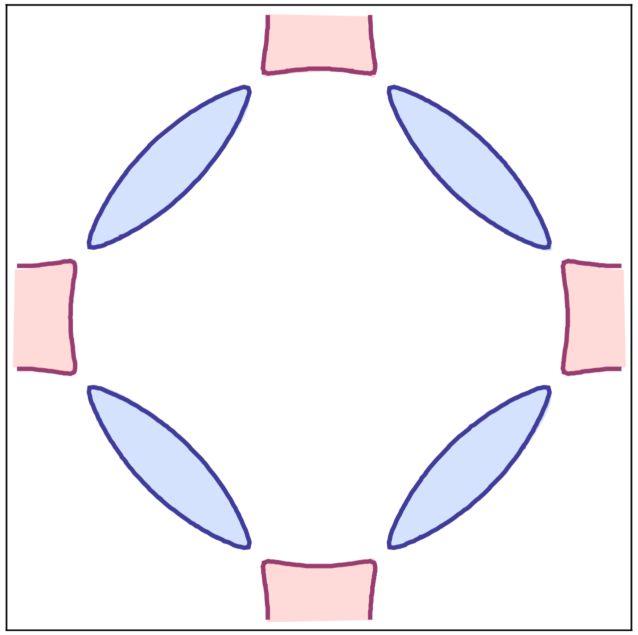
$$\Psi_{i\alpha} \to U_i \Psi_{i\alpha}$$

We will start with the Néel state, and find important consequences of the pseudospin symmetry in metals with antiferromagnetic correlations.

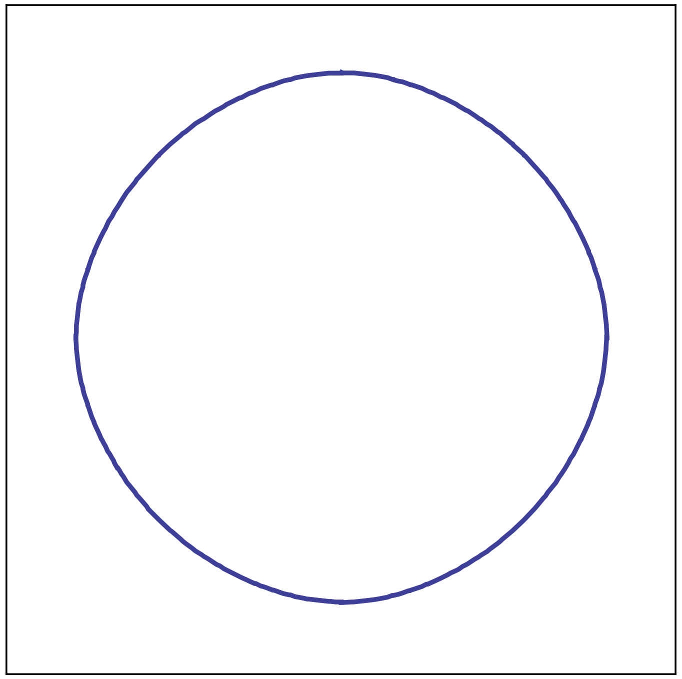
M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)

Fermi surface+antiferromagnetism



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

Metal with electron and hole pockets



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Metal with "large" Fermi surface

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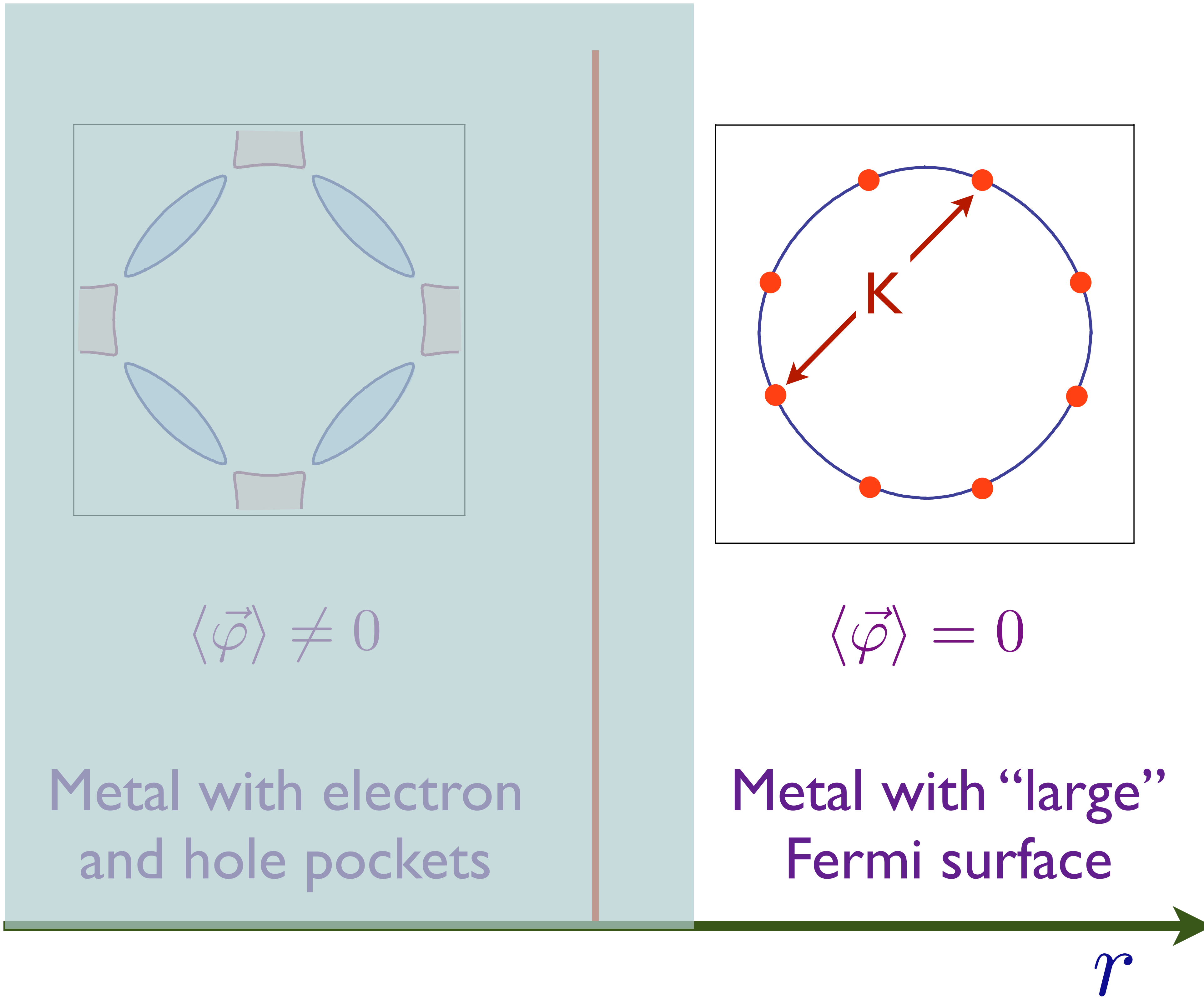
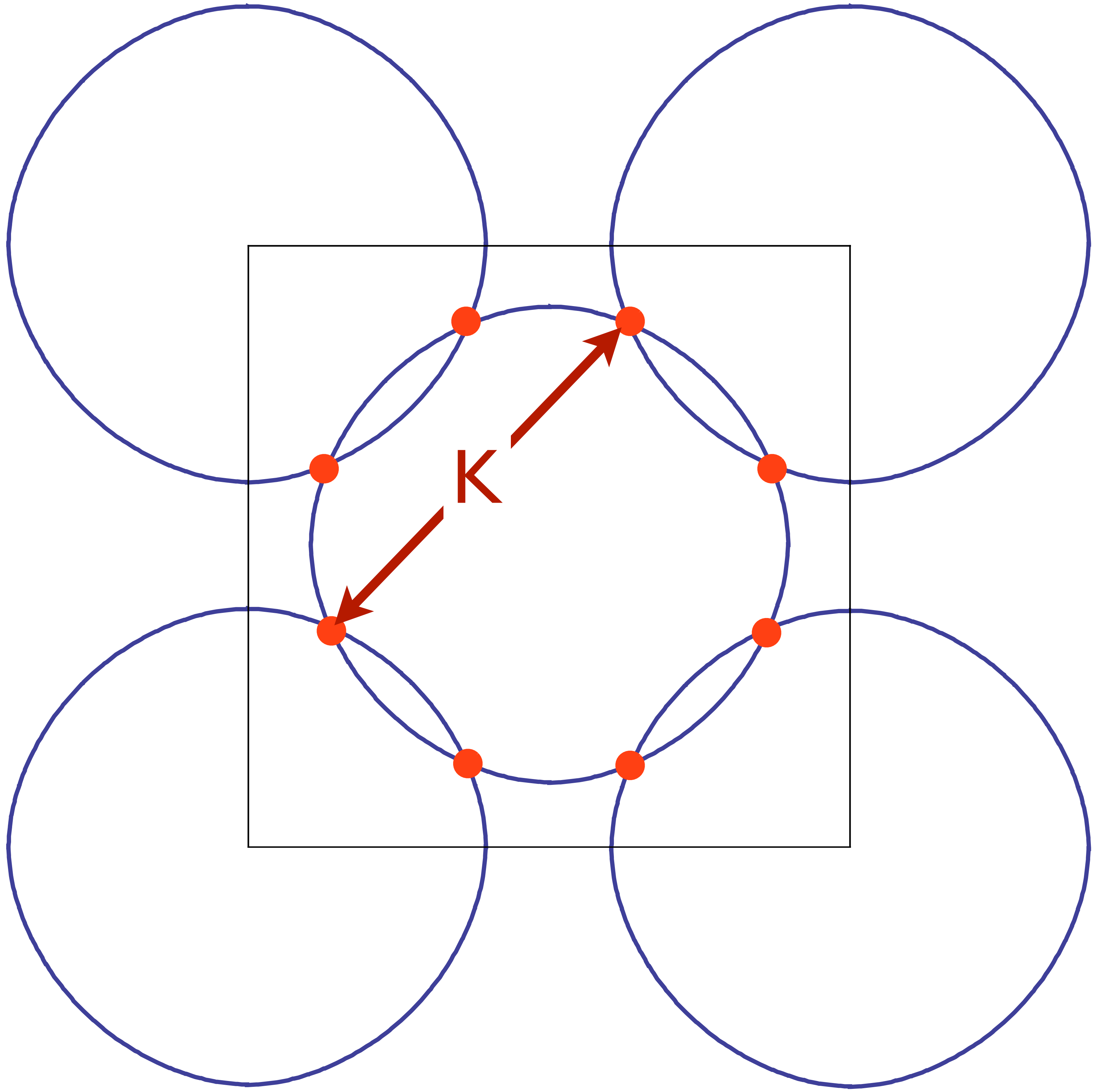


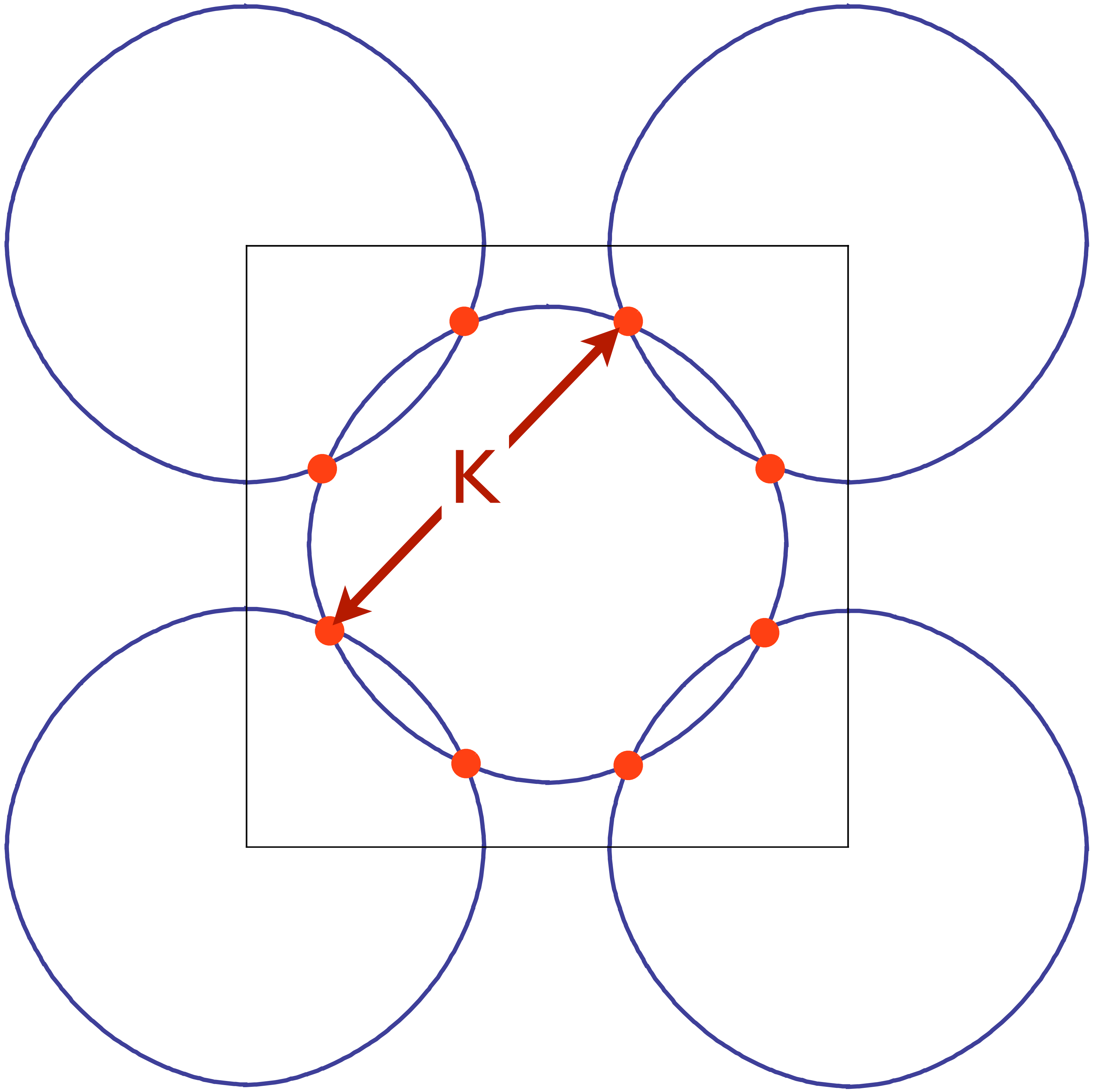
Rest of the talk

Fermi surface+antiferromagnetism



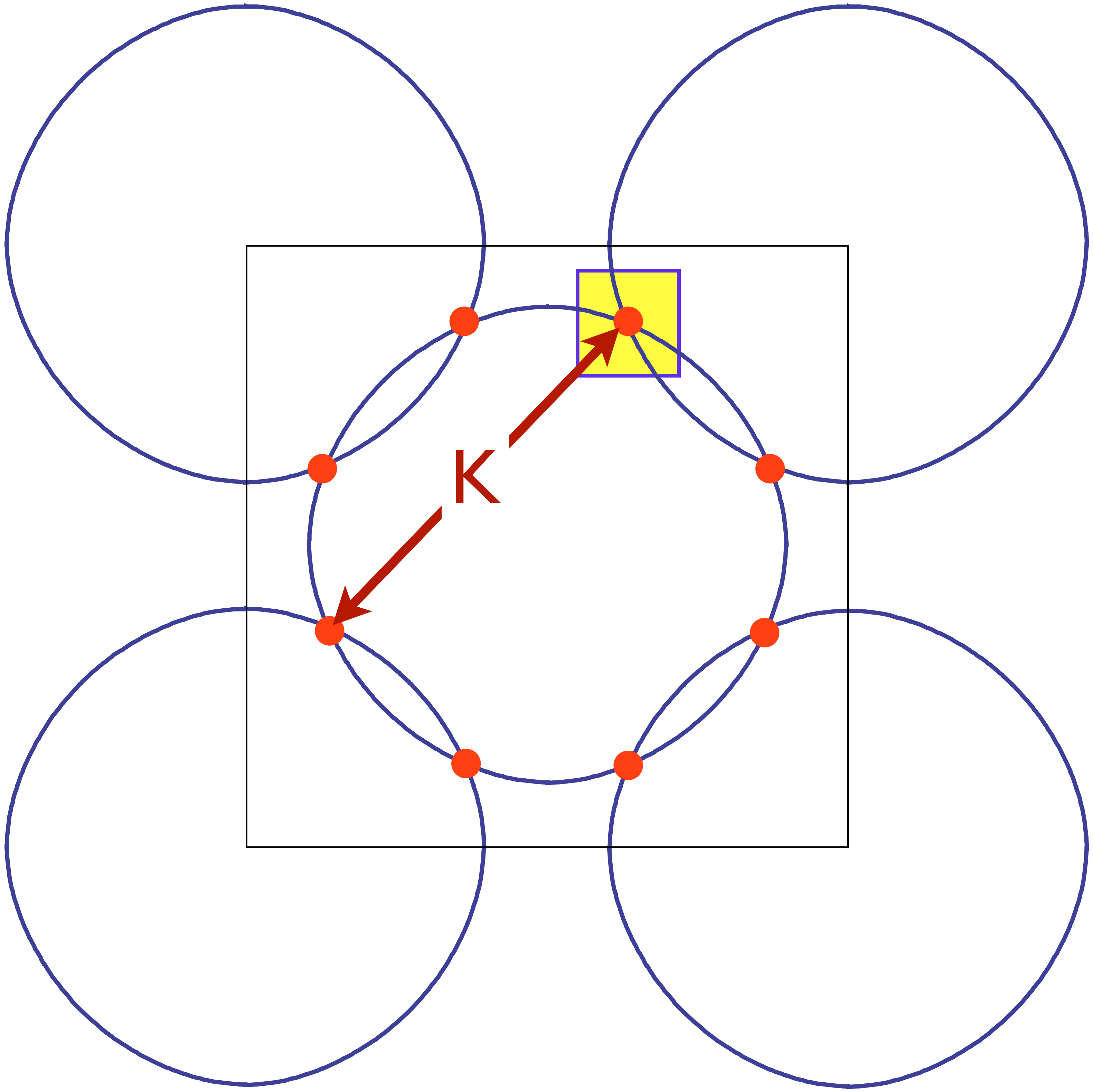
"Hot" spots

Fermi surface+antiferromagnetism



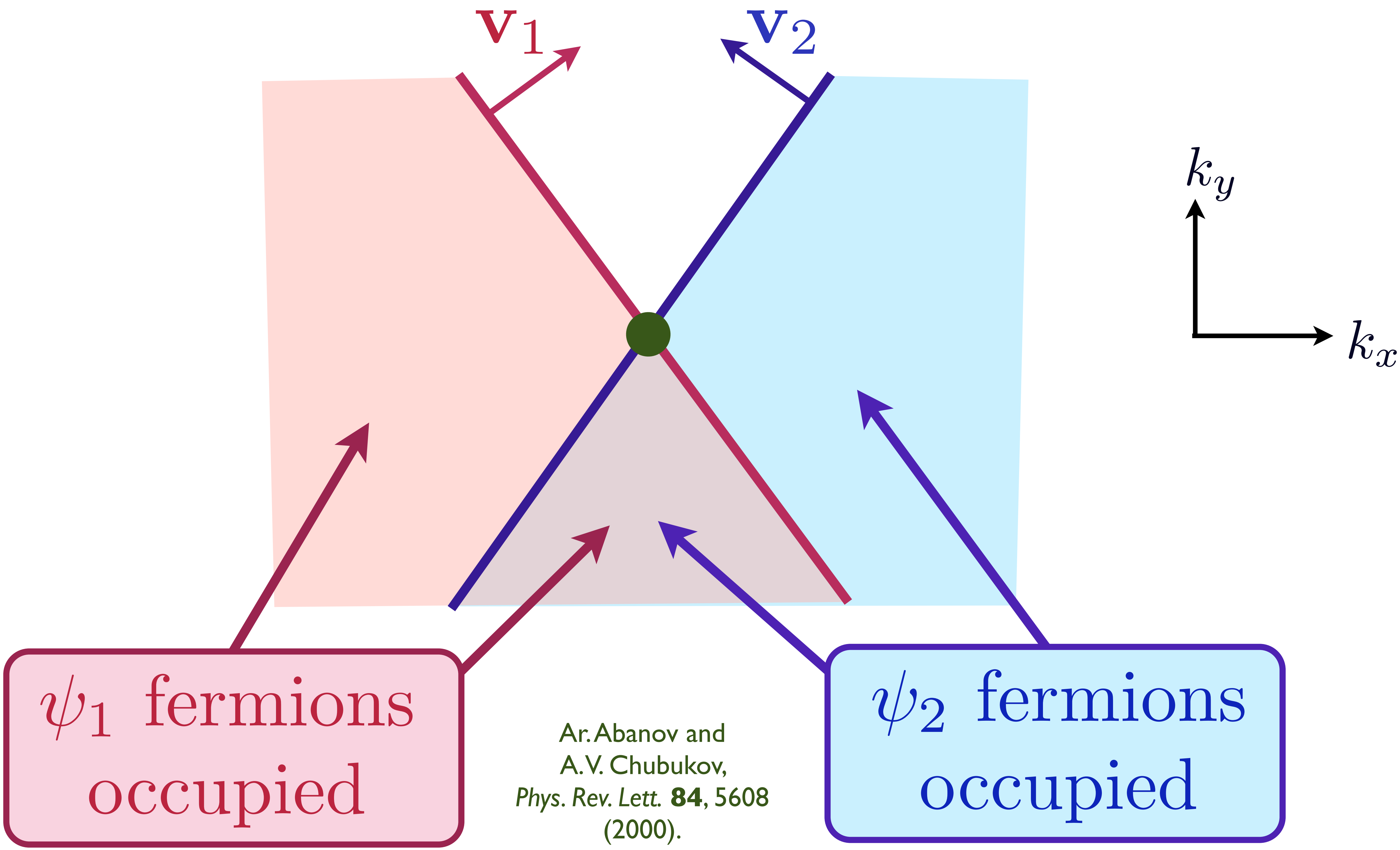
Low energy theory for critical point near hot spots

Fermi surface+antiferromagnetism



Low energy theory for critical point near hot spots

$$\mathcal{S} = \int d^2r d\tau \Big[\psi^\dagger_{1\alpha} \left(\partial_\tau - i\mathbf{v}_1 \cdot \boldsymbol{\nabla}_r\right) \psi_{1\alpha} + \psi^\dagger_{2\alpha} \left(\partial_\tau - i\mathbf{v}_2 \cdot \boldsymbol{\nabla}_r\right) \psi_{2\alpha}$$
$$+ \frac{1}{2} \left(\boldsymbol{\nabla}_r \vec{\varphi}\right)^2 + \frac{s}{2}\vec{\varphi}^2 + \frac{u}{4}\vec{\varphi}^4 - \lambda \vec{\varphi} \cdot \left(\psi^\dagger_{1\alpha} \vec{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi^\dagger_{2\alpha} \vec{\sigma}_{\alpha\beta} \psi_{1\beta} \right) \Big]$$



Ar. Abanov and A.V. Chubukov, *Phys. Rev. Lett.* **84**, 5608 (2000).

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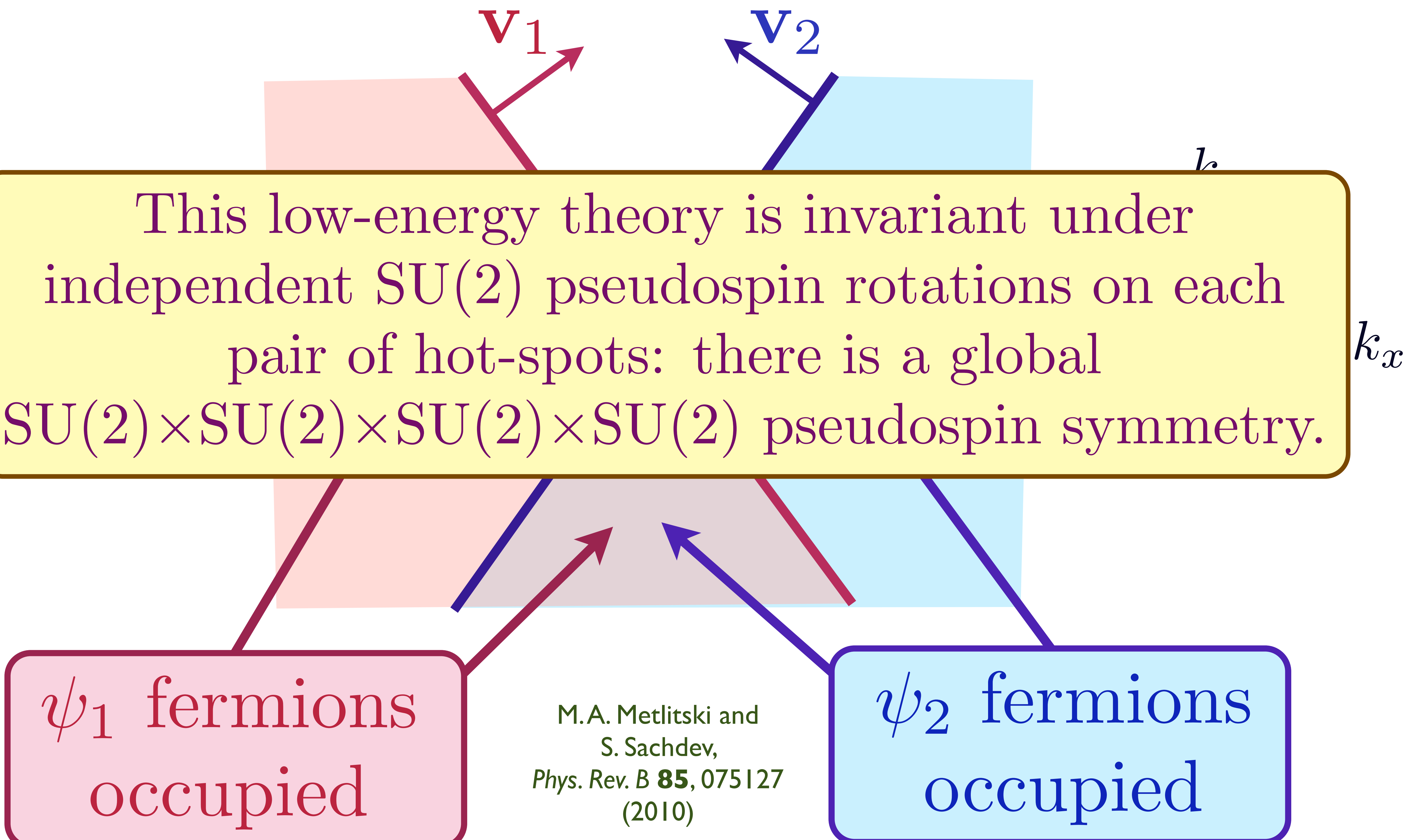

This low-energy theory is invariant under independent SU(2) pseudospin rotations on each pair of hot-spots: there is a global SU(2)×SU(2)×SU(2)×SU(2) pseudospin symmetry.

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

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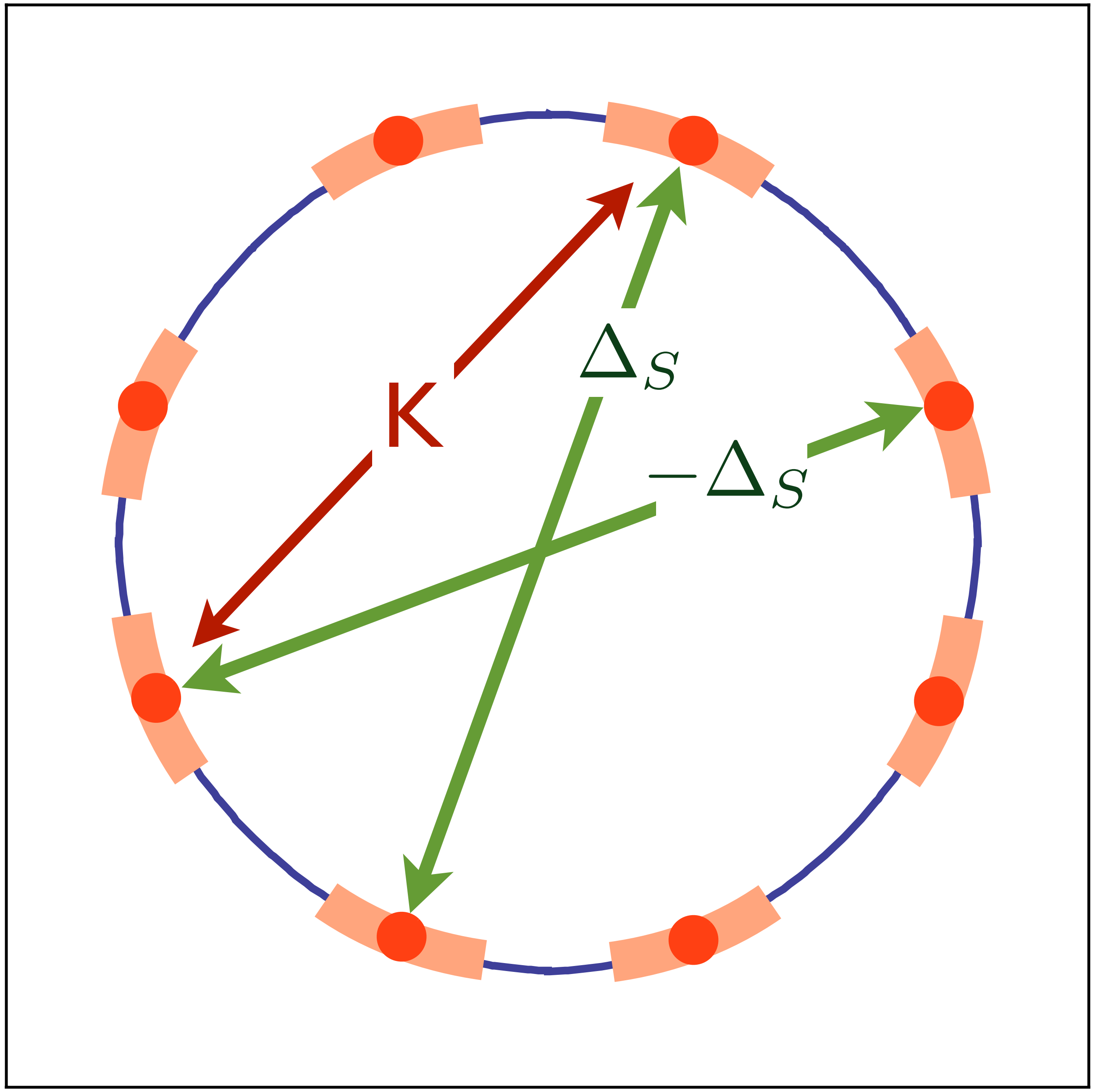
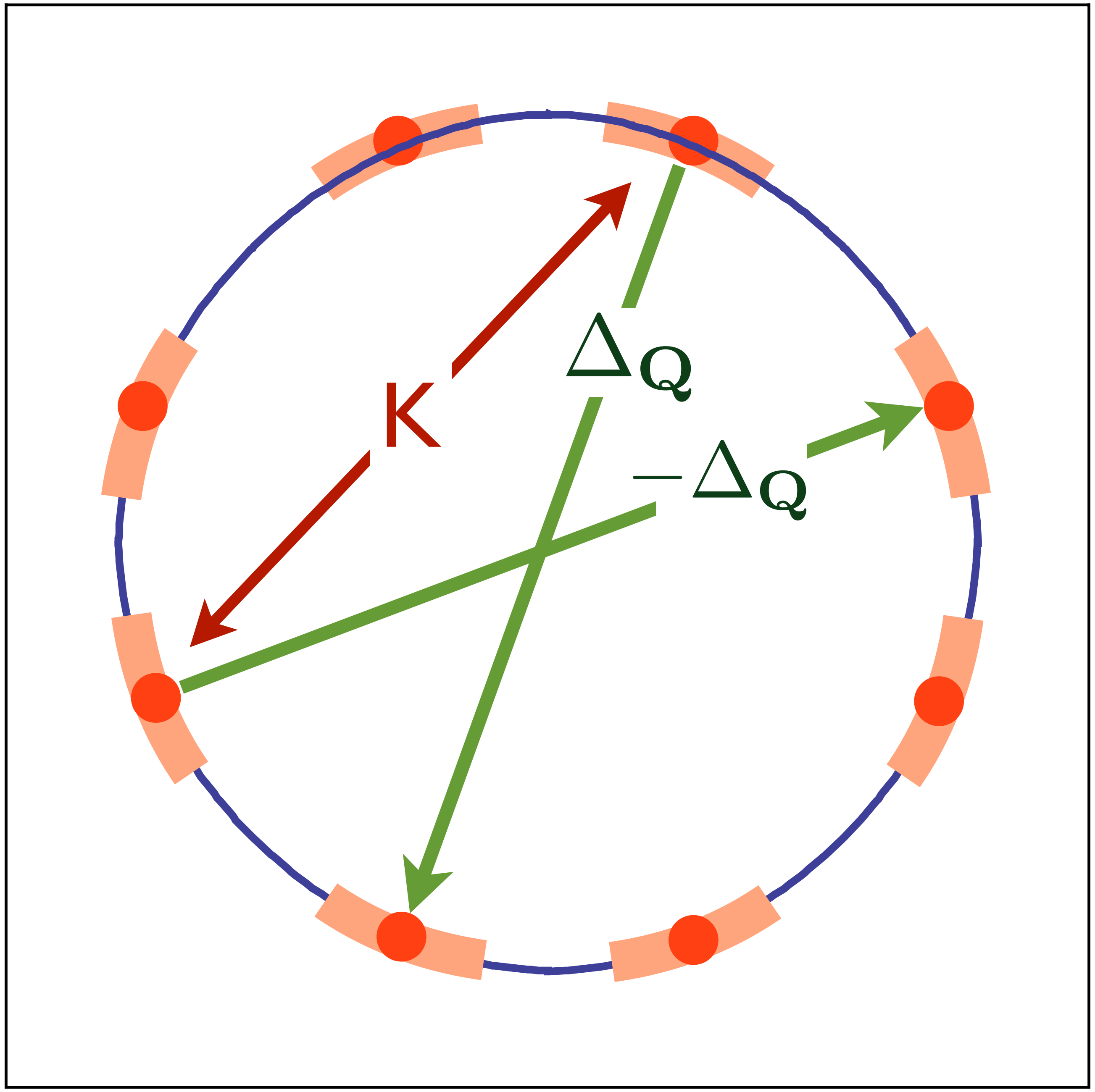


d-wave superconductor: particle-particle pairing at *and near* hot spots, with sign-changing pairing amplitude

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

After pseudospin rotation on *half* the hot-spots

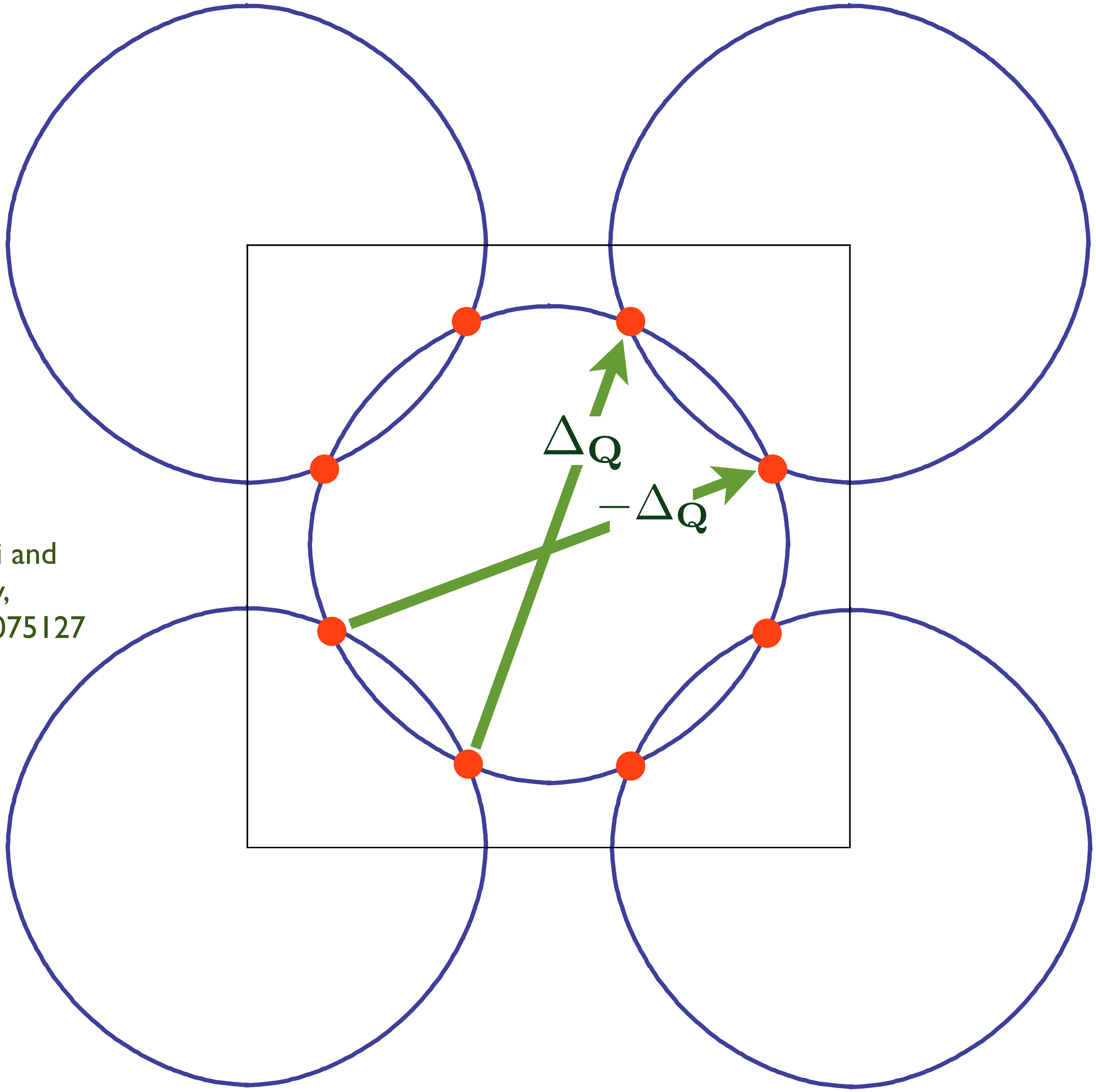
M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)



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

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

Incommensurate *d*-wave bond order



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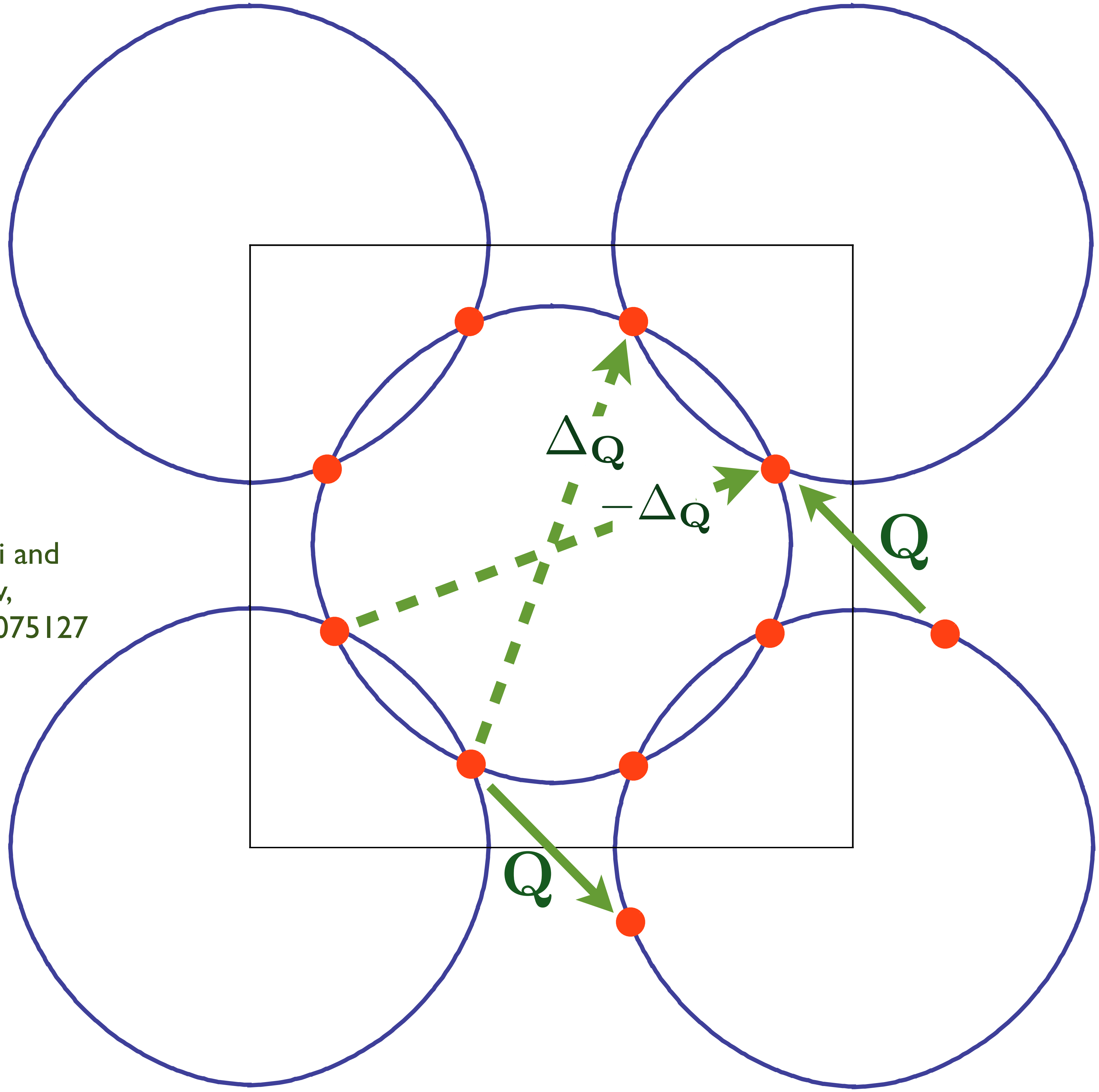

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Incommensurate *d*-wave bond order

Consider modulation in an off-site "density" like variable at sites $\mathbf{r}_i$ and $\mathbf{r}_j$

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

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 neutron/X-ray scattering peak.

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

$$\Delta_{\mathbf{Q}}(\mathbf{k}) = c_s + c_{s'}(\cos k_x + \cos k_y) + c_d(\cos k_x - \cos k_y) + \ldots$$

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

Incommensurate *d*-wave bond order

Consider modulation in an off-site "density" like variable at sites $\mathbf{r}_i$ and $\mathbf{r}_j$

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

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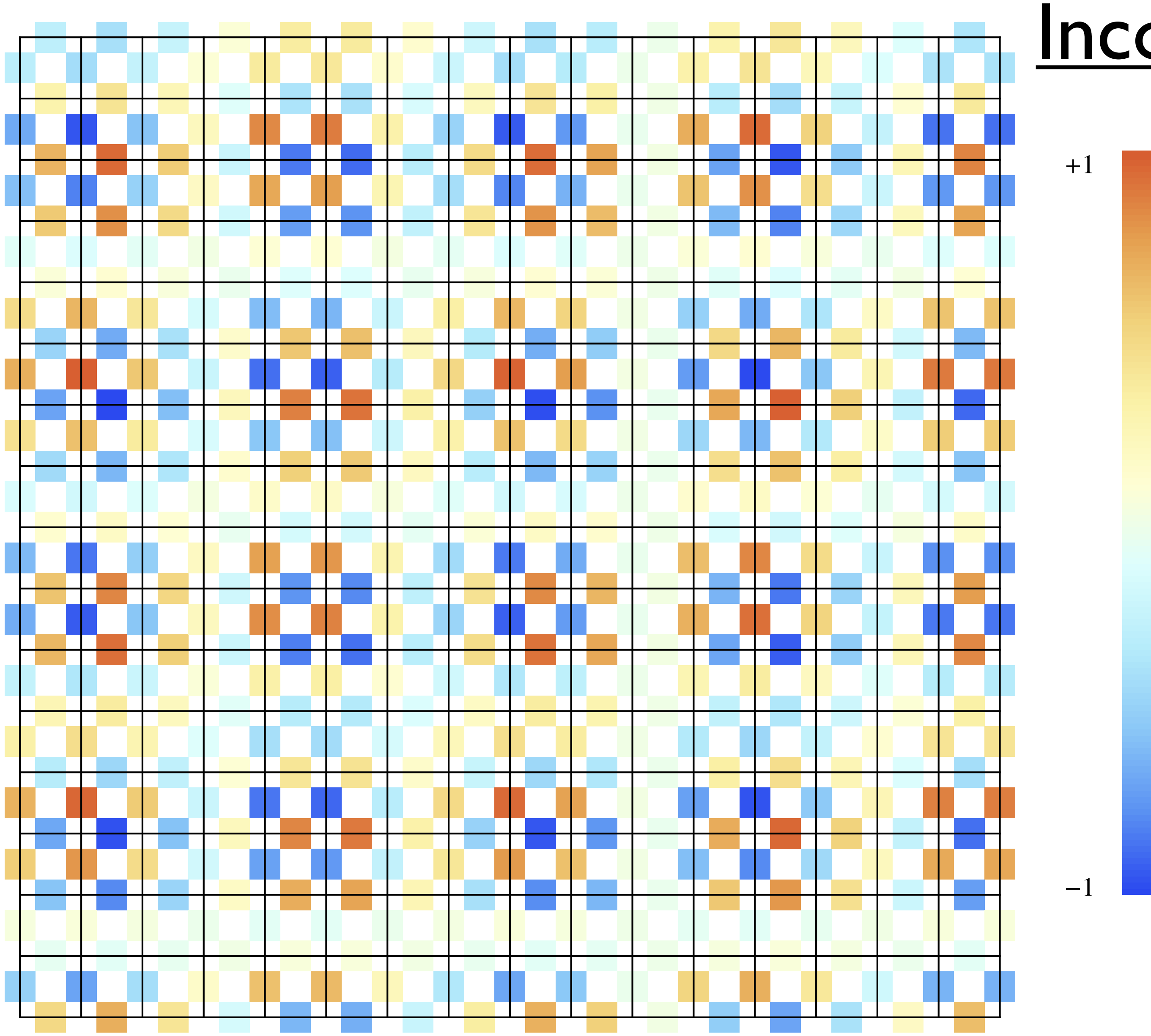
The usual charge-density-wave has only $c_s \neq 0$, and so the density wave is non-zero only if $\mathbf{r}_i = \mathbf{r}_j$.

The bond-ordered state has only c_d non-zero: in this case the density wave is non-zero only if $\mathbf{r}_i$ and $\mathbf{r}_j$ are nearest neighbors.

Incommensurate d-wave bond order



"Bond density" measures amplitude for electrons to be in spin-singlet valence bond.

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

$$\left\langle c_{\mathbf{r}\alpha}^{\dagger} c_{\mathbf{s}\alpha} \right\rangle = \sum_{\mathbf{Q}} \sum_{\mathbf{k}} e^{i\mathbf{Q}\cdot(\mathbf{r}+\mathbf{s})/2} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{s})} \left\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^{\dagger} c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \right\rangle$$

where $\mathbf{Q}$ extends over $\mathbf{Q} = (\pm Q_0, \pm Q_0)$ with $Q_0 = 2\pi/(7.3)$ and

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

Note $\left\langle c_{\mathbf{r}\alpha}^{\dagger} c_{\mathbf{s}\alpha} \right\rangle$ is non-zero *only* when $\mathbf{r}, \mathbf{s}$ are nearest neighbors.

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Continuum field theory with exact pseudospin symmetry

2. Approximate pseudospin symmetry on the lattice t-J model

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$$H_{tJ} = -\sum_{i,j} t_{ij} c^\dagger_{i\alpha} c_{j\alpha} + \sum_{i<j} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

Optimize the free energy w.r.t. a mean field Hamiltonian which allows for spin-singlet charge order ($\Delta_{\mathbf{Q}}(\mathbf{k})$):

$$H_{MF} \quad = \quad -\sum_{i,j} t_{ij} c^\dagger_{i\alpha} c_{j\alpha} + \sum_{\mathbf{k},\mathbf{Q}} \Delta_{\mathbf{Q}}(\mathbf{k}) c^\dagger_{\mathbf{k}+\mathbf{Q}/2,\alpha} c_{\mathbf{k}-\mathbf{Q}/2,\alpha}$$

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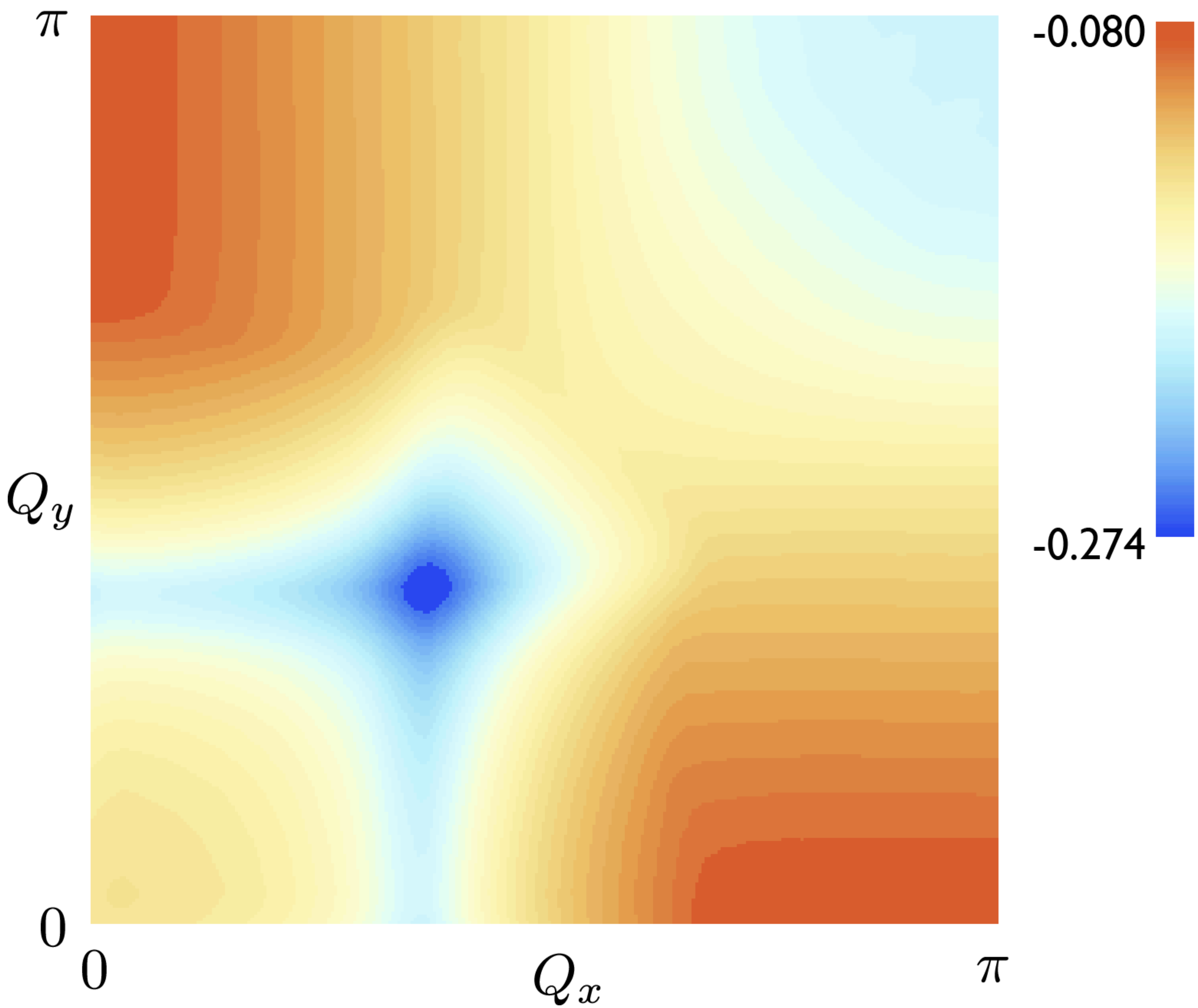
Expanding the free energy in powers of the order parameters we obtain

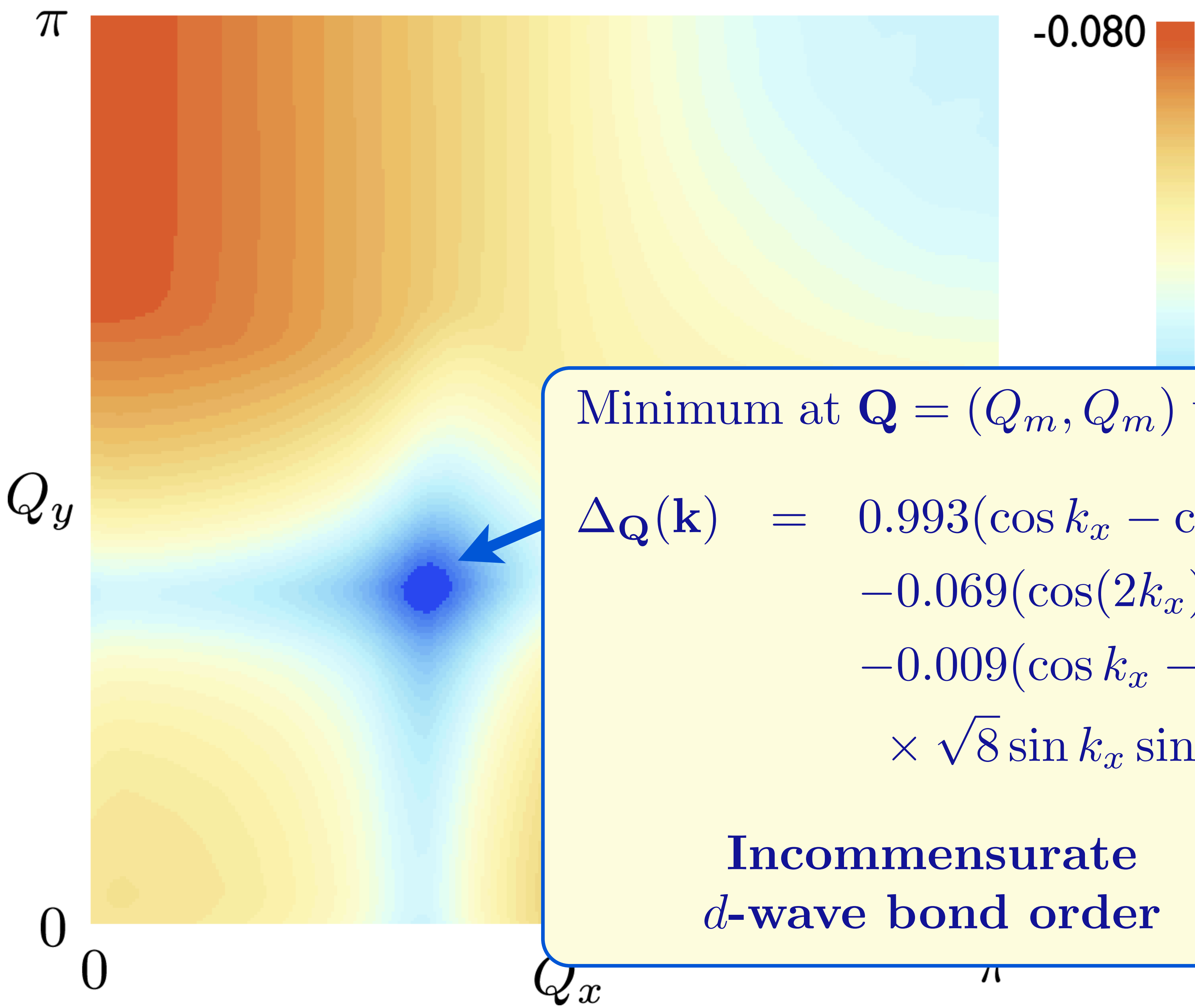
$$F = F_0 + \sum_{\mathbf{k},\mathbf{Q}} \Delta^*_{\mathbf{Q}}(\mathbf{k}) \mathcal{M}_{\mathbf{Q}}(\mathbf{k},\mathbf{k}') \Delta_{\mathbf{Q}}(\mathbf{k}')$$

We compute the eigenvalues, $1+\lambda_{\mathbf{Q}}$, and eigenfunctions, $\Delta_{\mathbf{Q}}(\mathbf{k})$ of the kernel $\mathcal{M}_{\mathbf{Q}}(\mathbf{k},\mathbf{k}')$



Charge-ordering eigenvalue $\lambda_{\mathbf{Q}}/J_0$.

S. Sachdev and R. La Placa, arXiv:1303.2114



Minimum at $\mathbf{Q} = (Q_m, Q_m)$ with

$$\begin{aligned}\Delta_{\mathbf{Q}}(\mathbf{k}) \;=\; & 0.993(\cos k_x - \cos k_y) \\ & -0.069(\cos(2k_x) - \cos(2k_y)) \\ & -0.009(\cos k_x - \cos k_y) \\ & \times \sqrt{8}\sin k_x \sin k_y\end{aligned}$$

Incommensurate
***d*-wave bond order**

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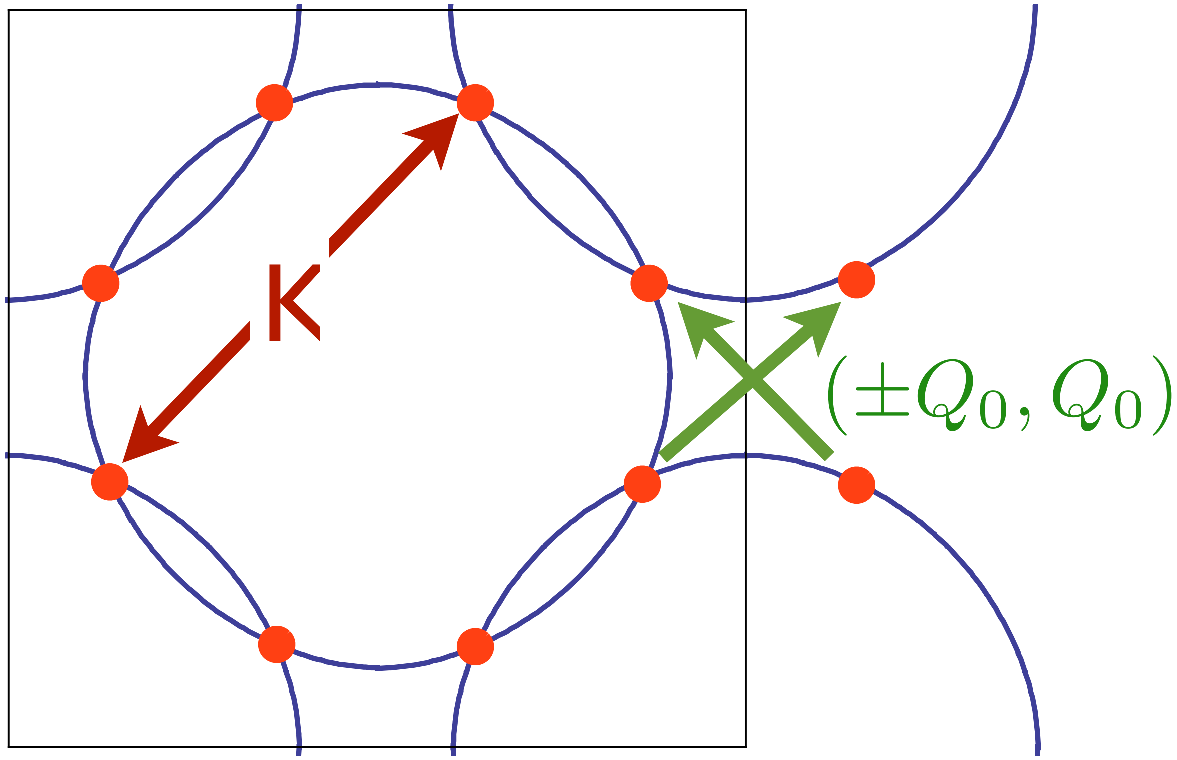
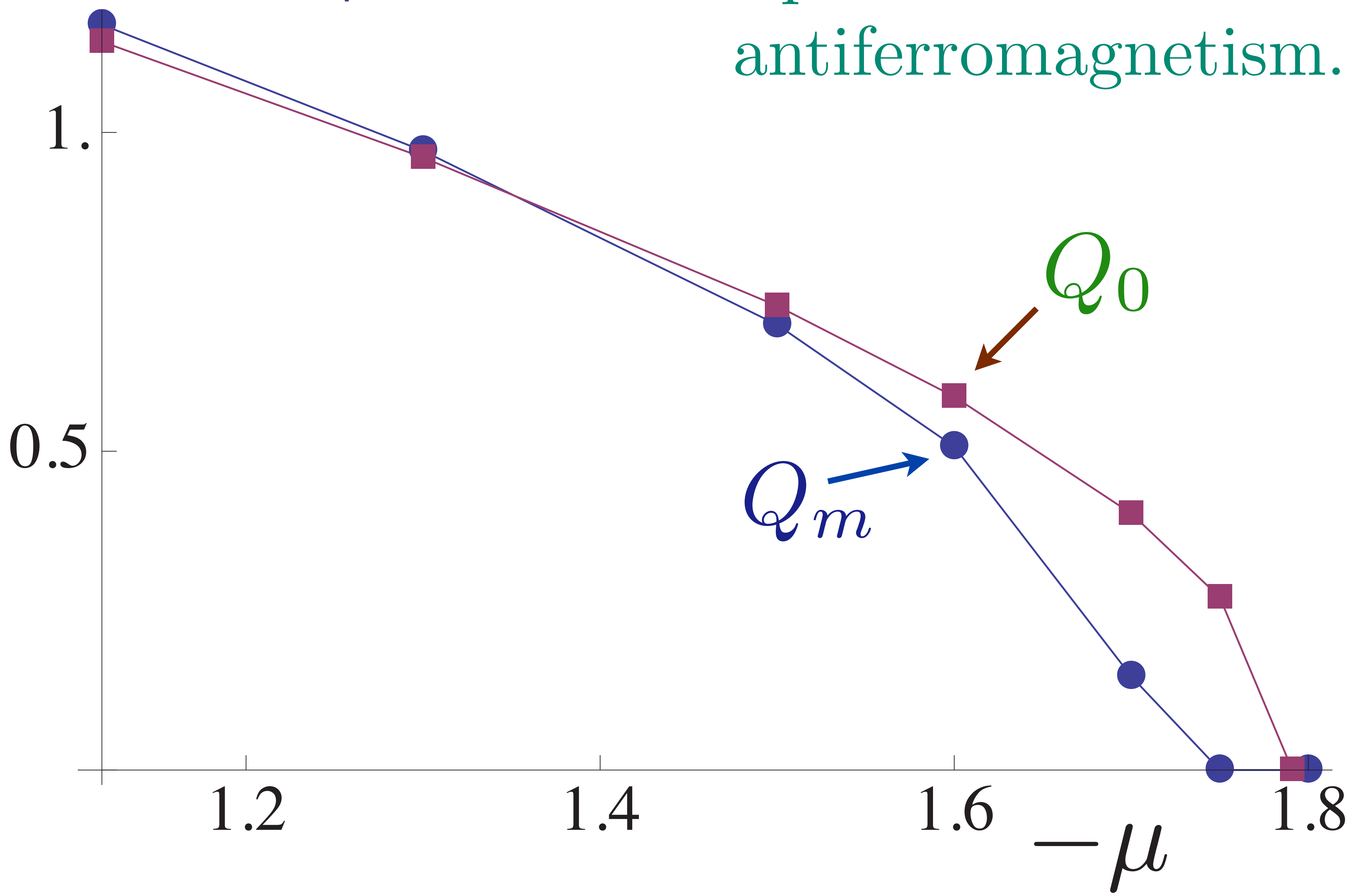
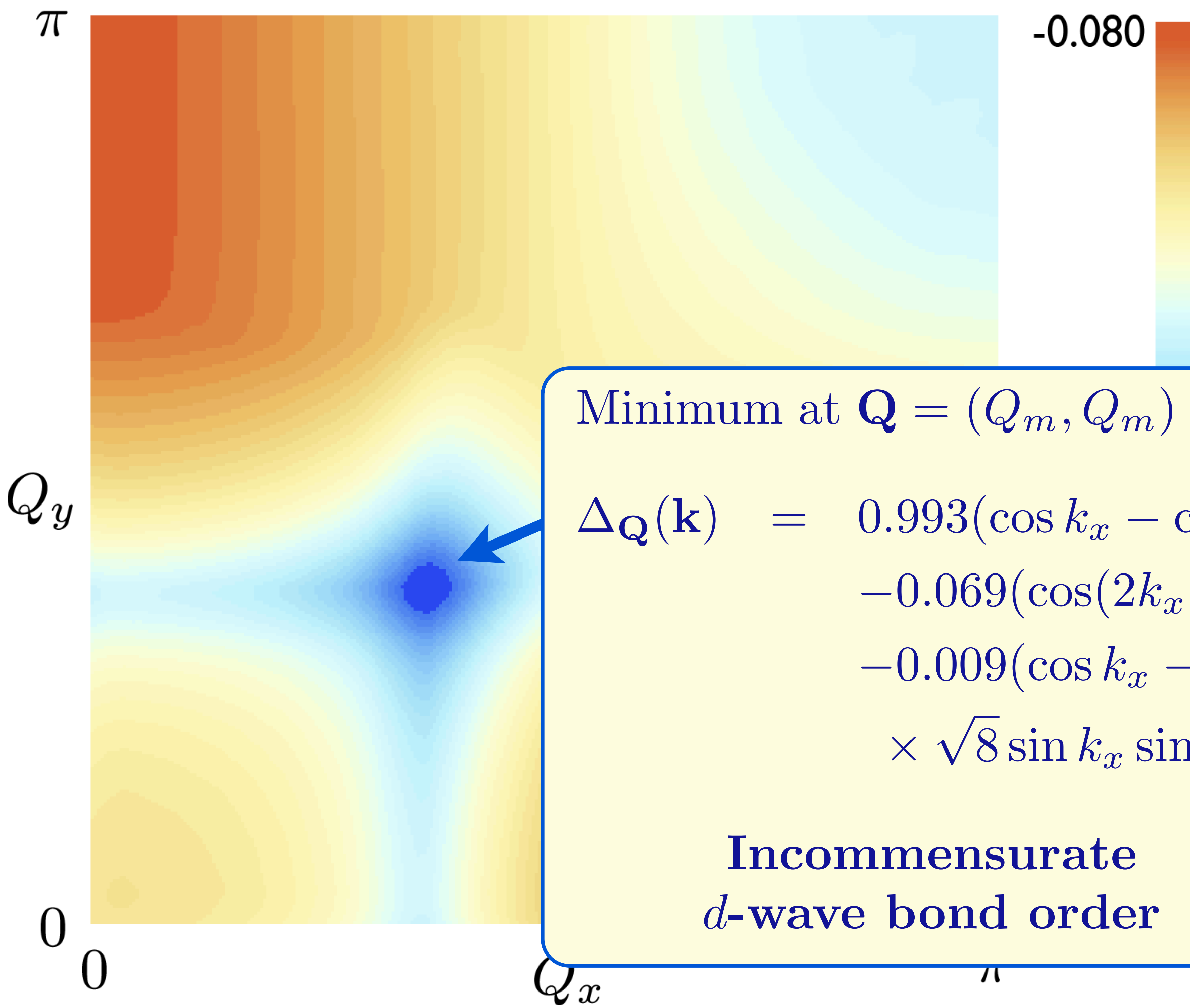


Remarkable agreement between the value of Q_m from Hartree-Fock in a metal with short-range *incommensurate* spin correlations, and the value of Q_0 from hot spots of *commensurate* antiferromagnetism.





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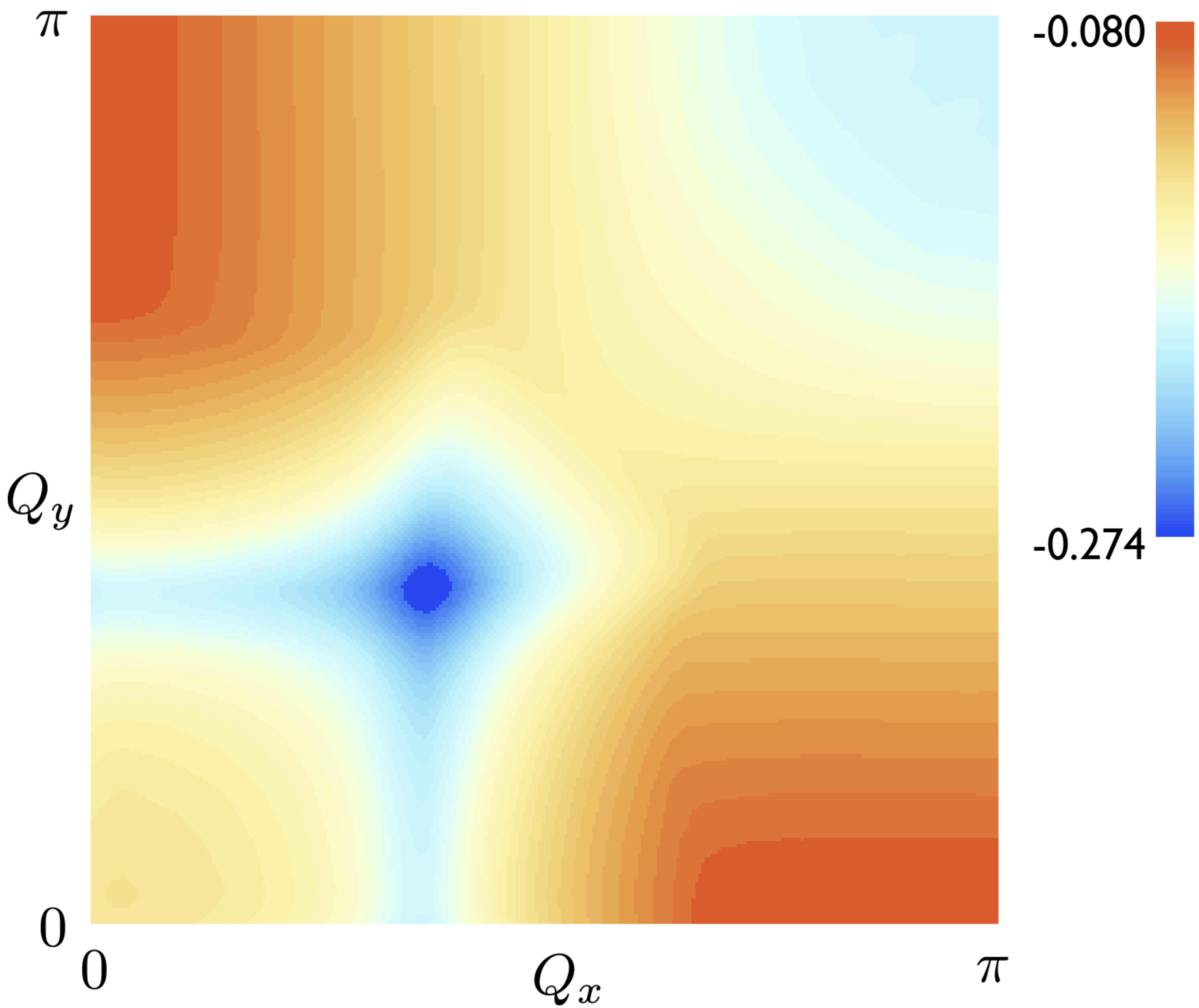

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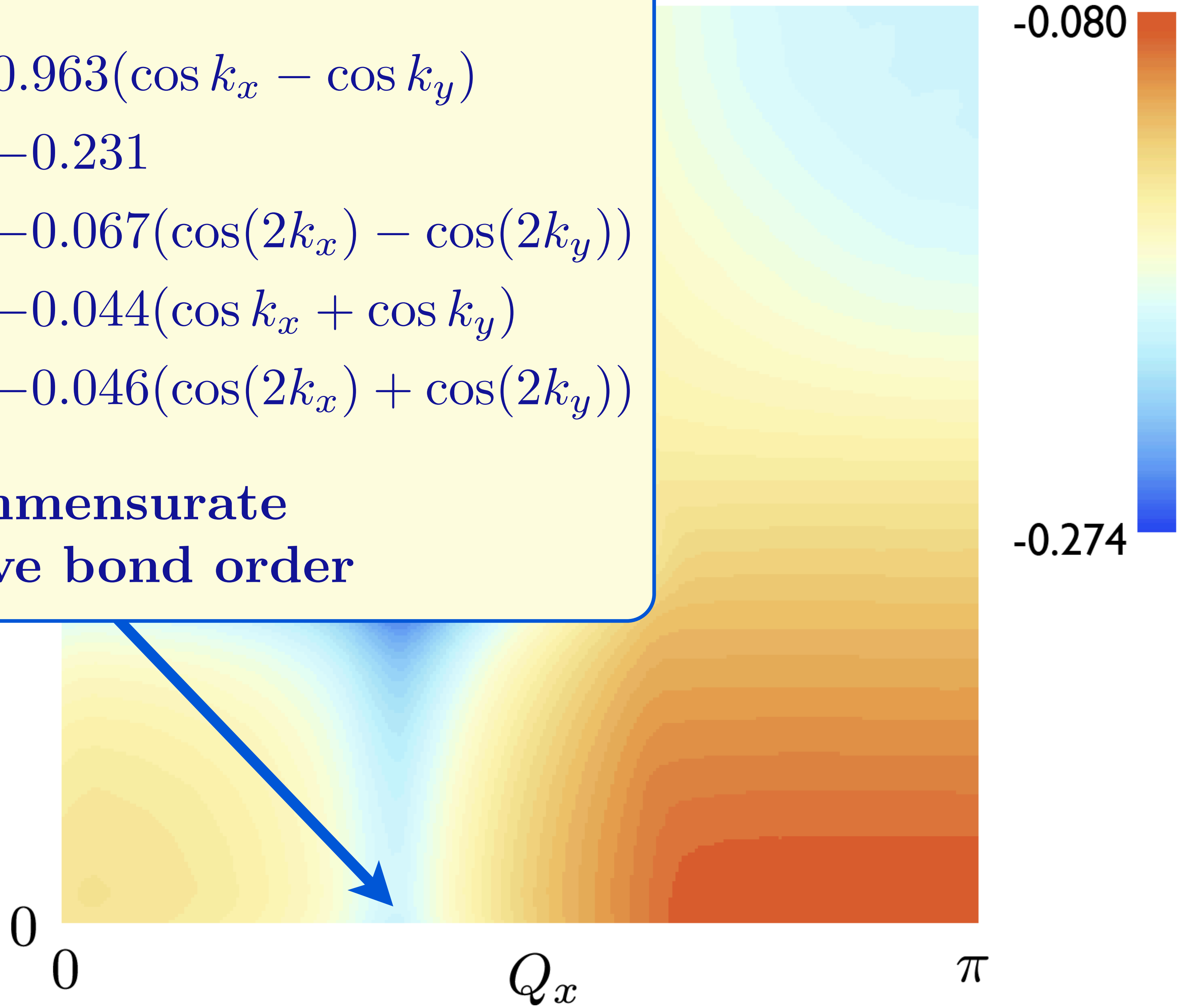
$\mathbf{Q} = (Q_m, 0)$ with

$$\Delta_{\mathbf{Q}}(\mathbf{k}) = 0.963(\cos k_x - \cos k_y) - 0.231 - 0.067(\cos(2k_x) - \cos(2k_y)) - 0.044(\cos k_x + \cos k_y) - 0.046(\cos(2k_x) + \cos(2k_y))$$

Incommensurate
d_{+s}-wave bond order



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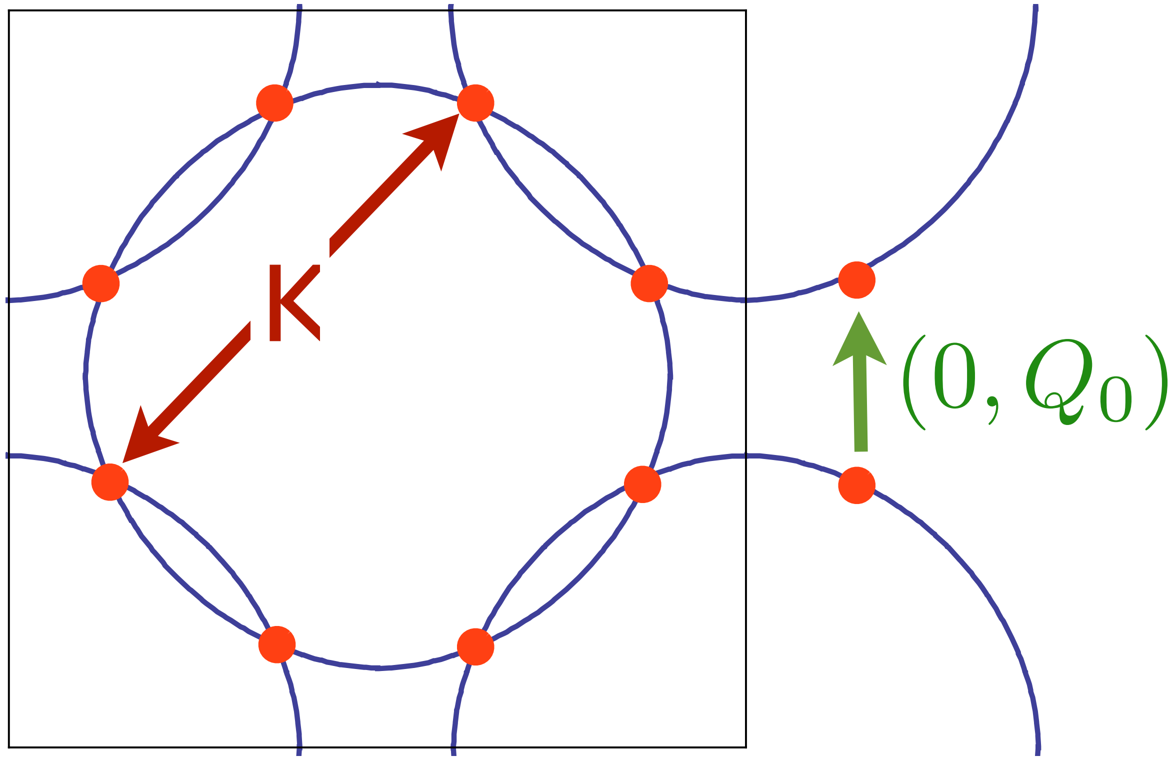

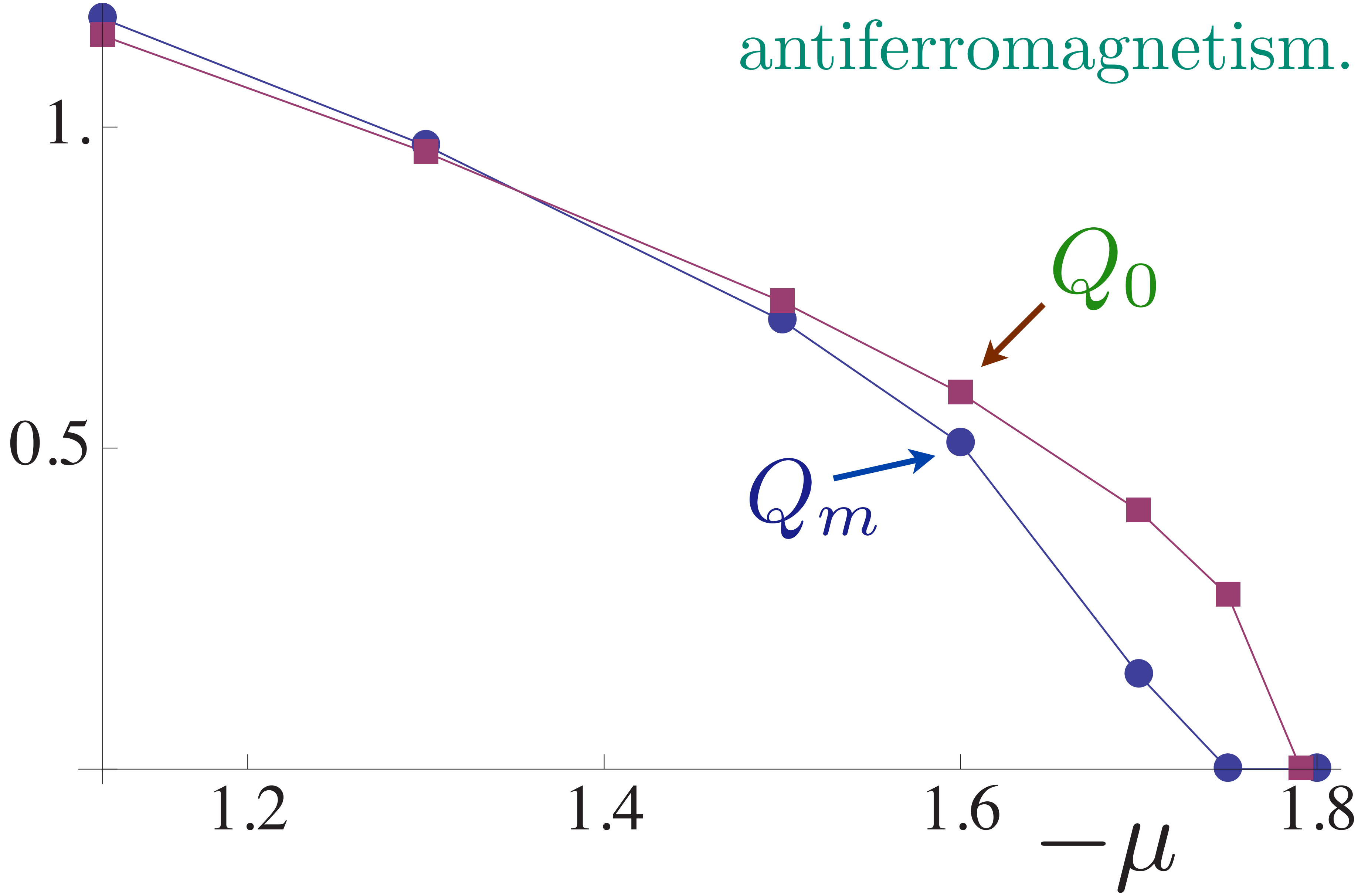

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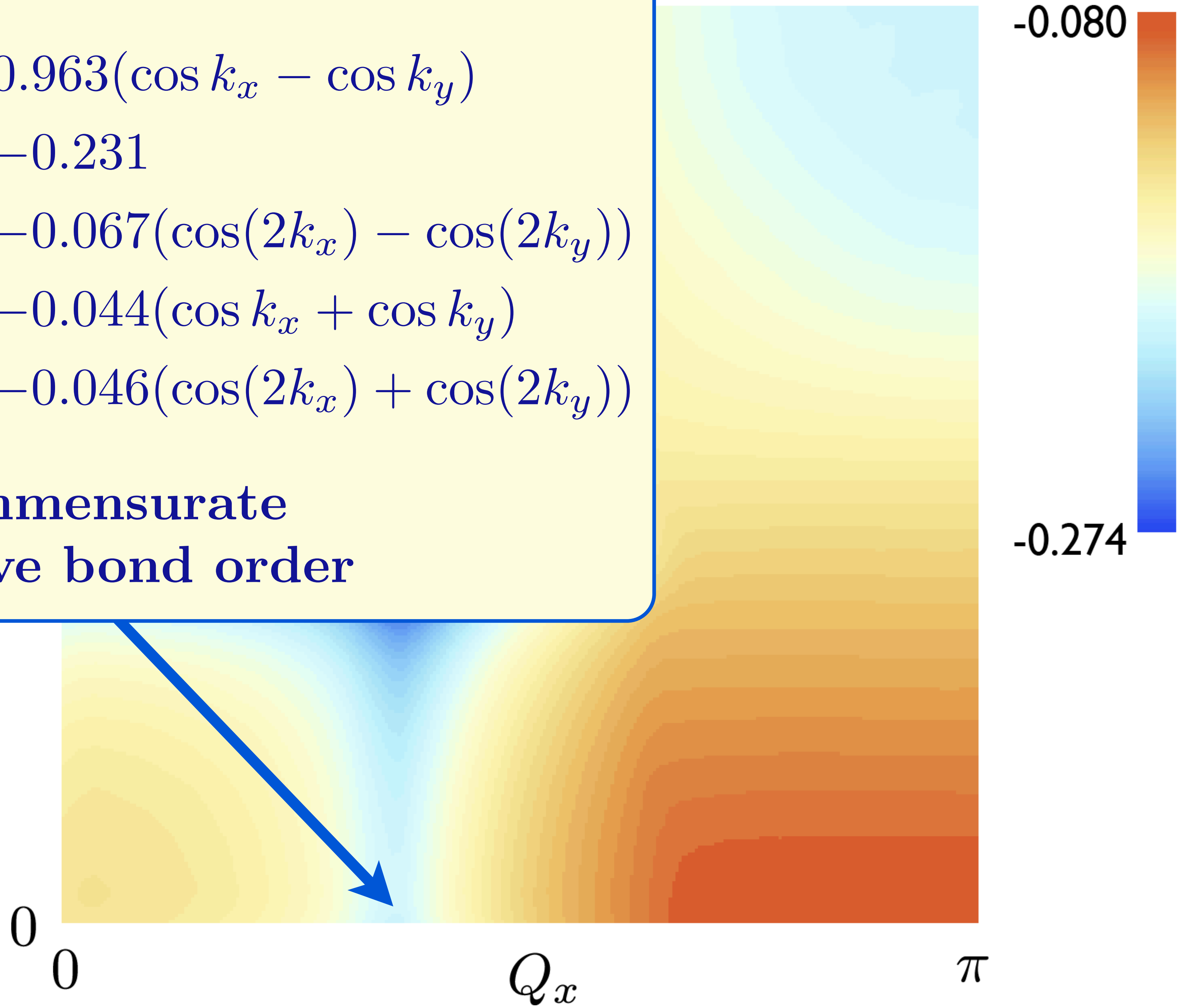

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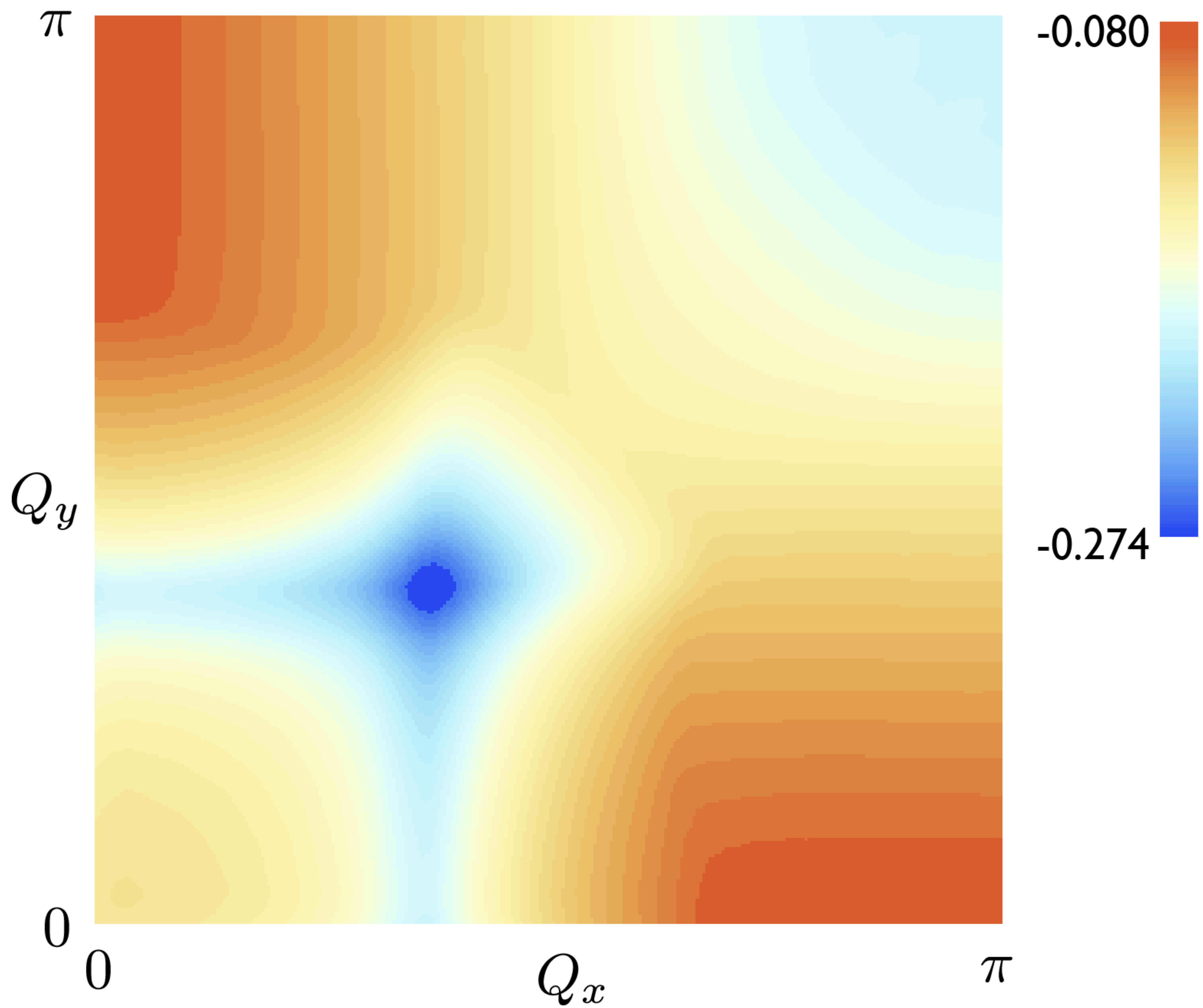

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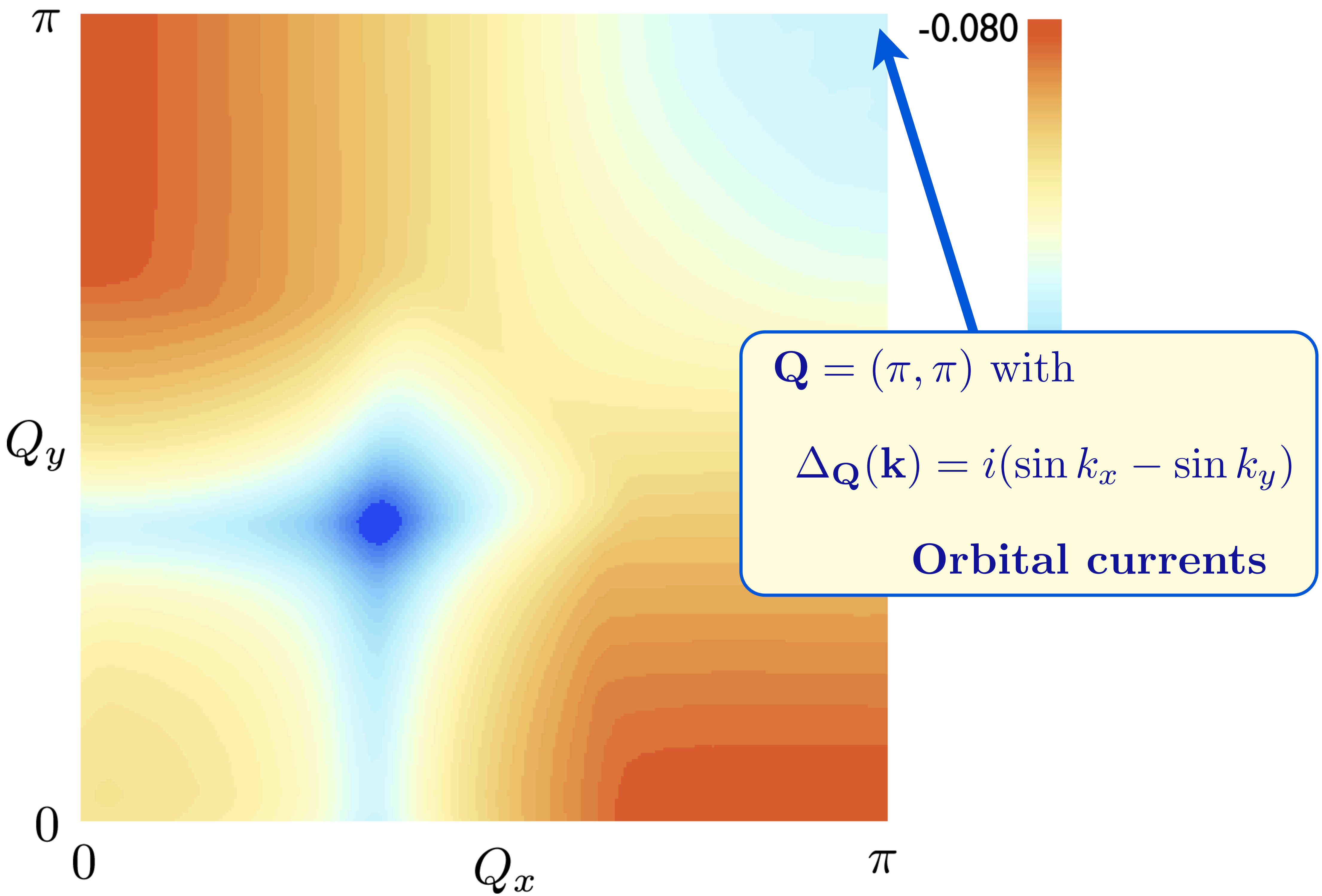

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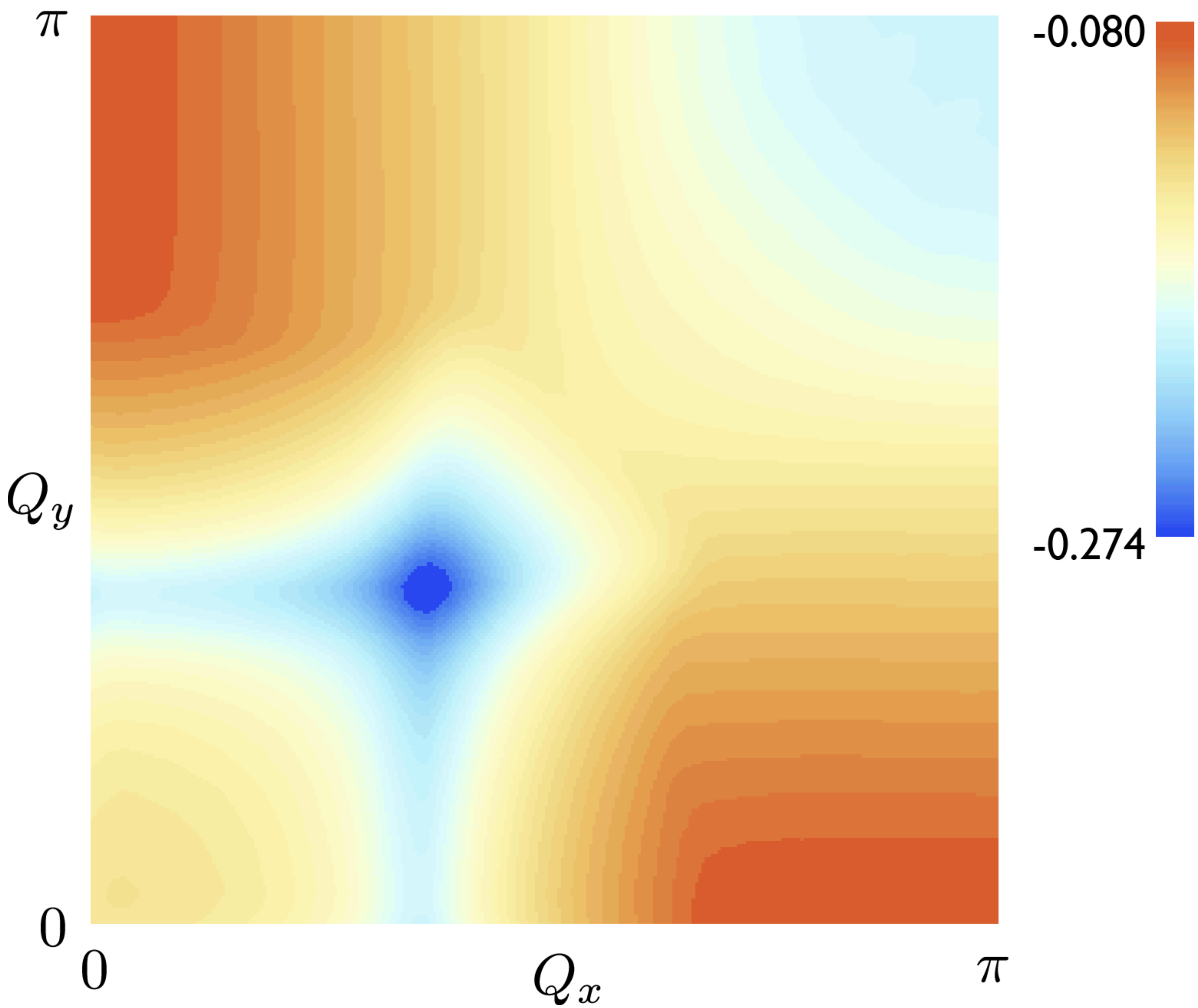

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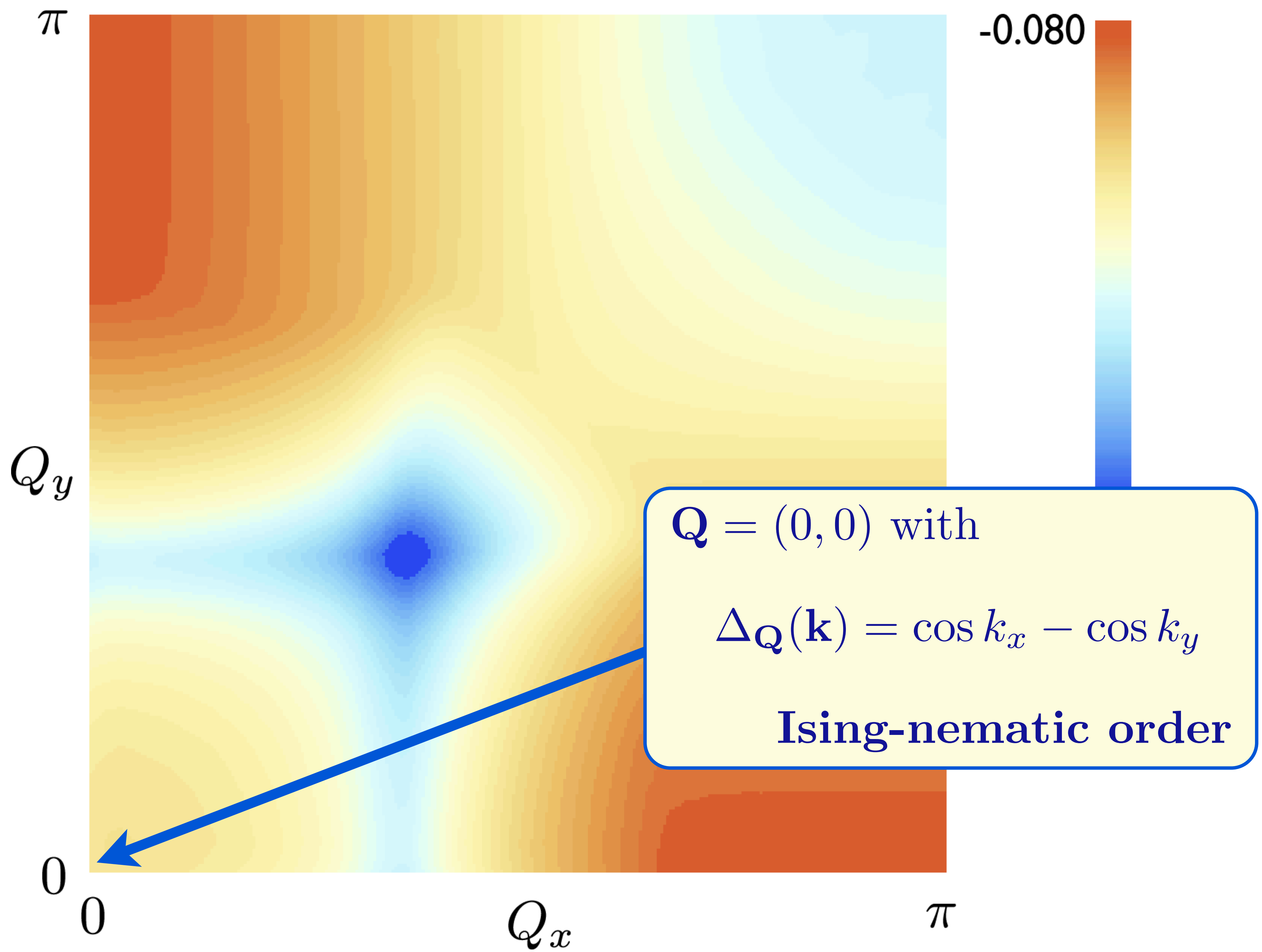

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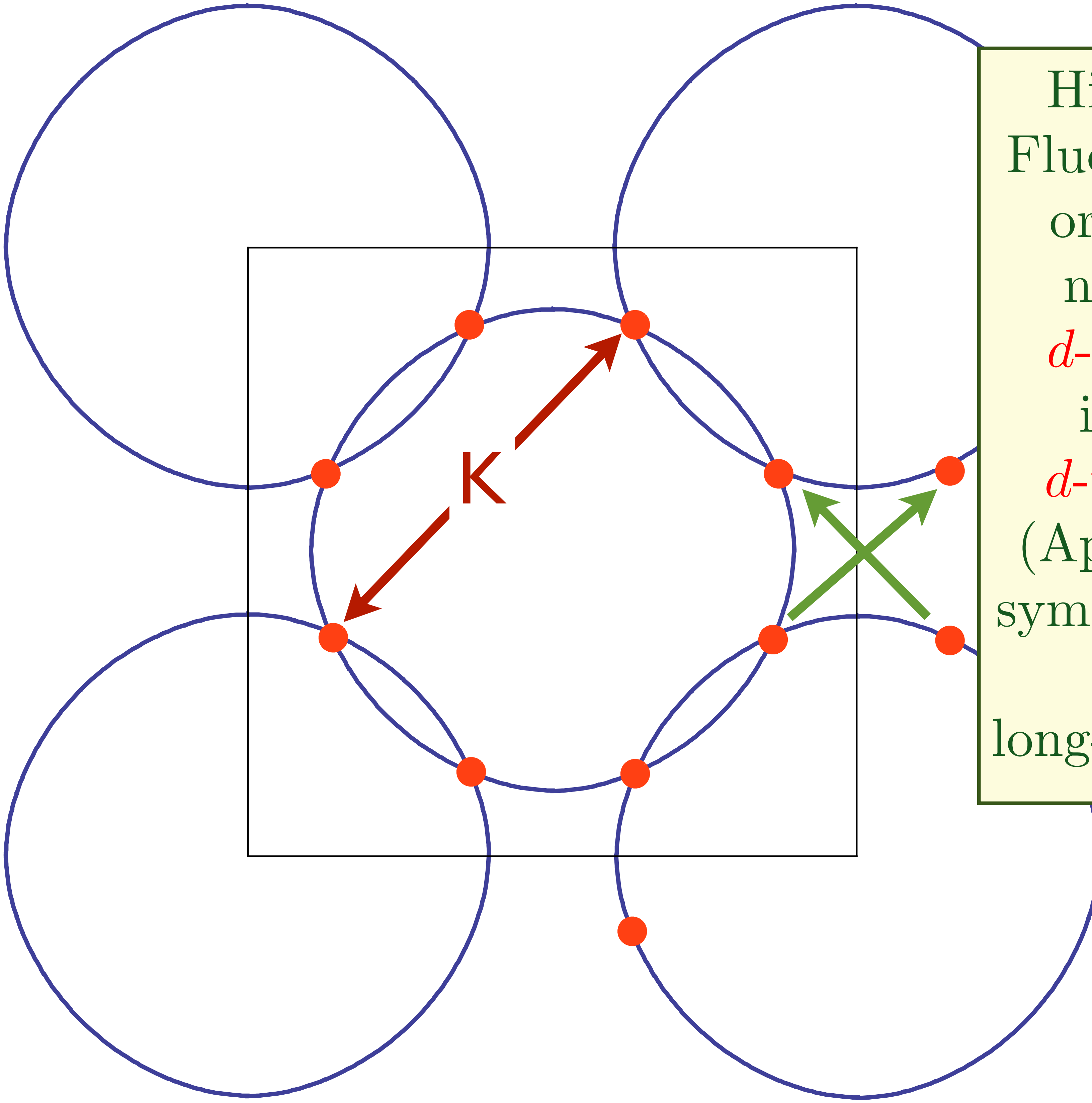
Incommensurate *d*-wave bond order



High T pseudogap: Fluctuating composite order parameter of nearly degenerate *d*-wave pairing and incommensurate *d*-wave bond order. (Approximate) SU(2) symmetry of composite order prevents long-range order $T > 0$.

K. B. Efetov, H. Meier, and C. Pepin, Nature Physics, to appear, arXiv:1210.3276

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

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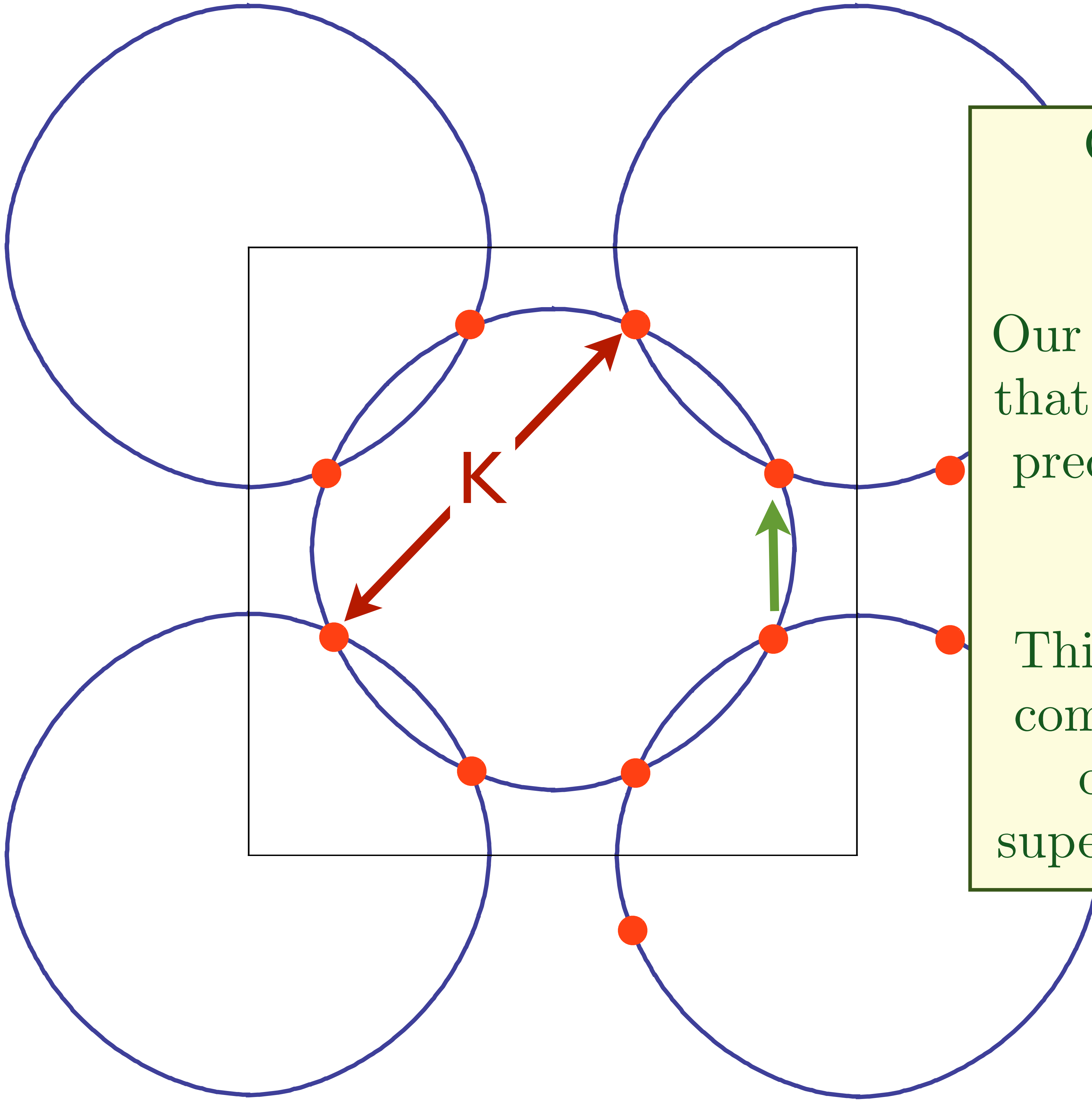


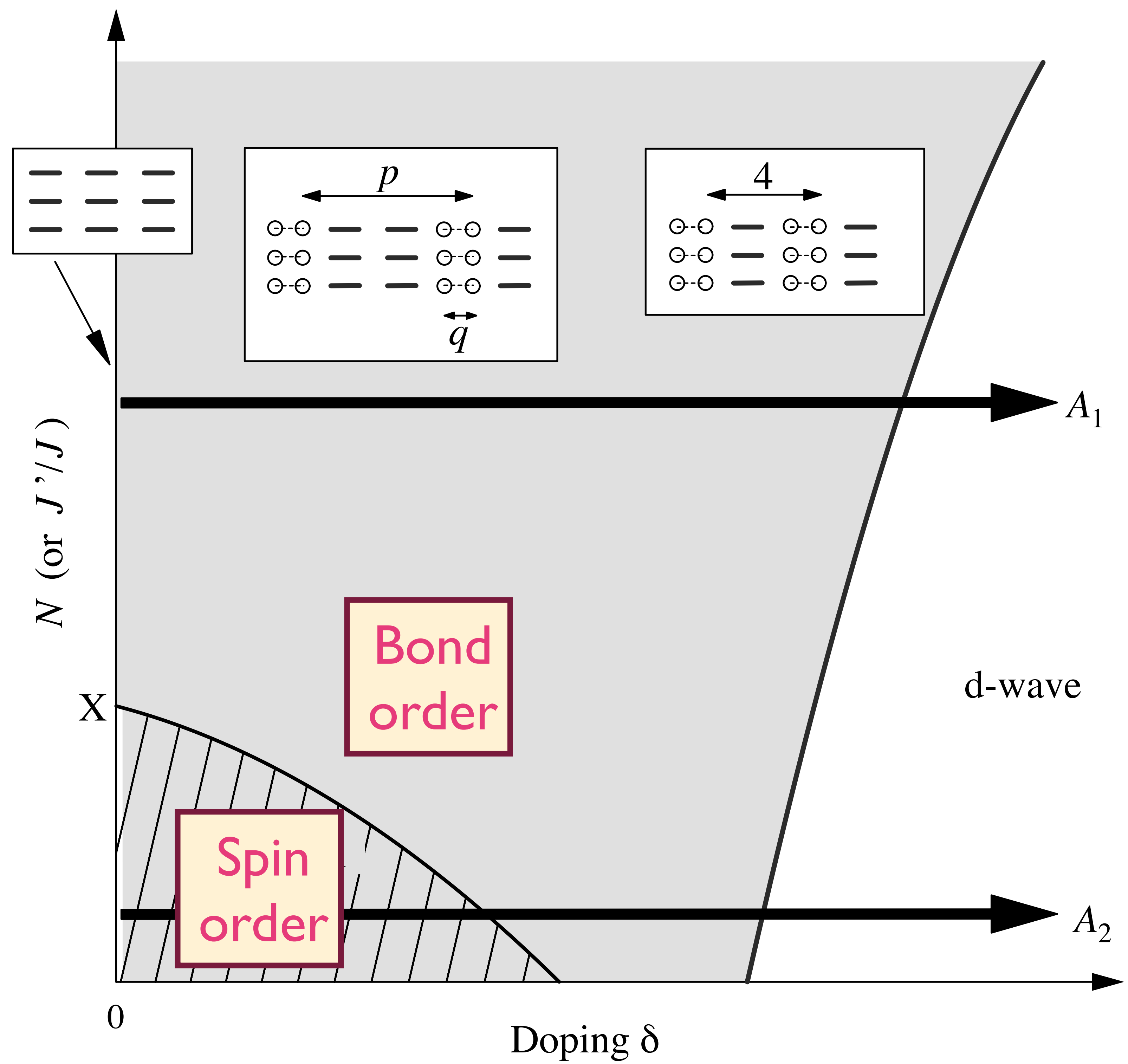
Observed low T ordering.

Our computations show that the charge order is predominantly d-wave also at this $\mathbf{Q}$.

This $\mathbf{Q}$ is preferred in computations of bond order within the superconducting phase.

S. Sachdev and R. La Placa, arXiv:1303.2114
M. Vojta and S. Sachdev, Physical Review Letters **83**, 3916 (1999)
M. Vojta and O. Rosch, Physical Review B 77, 094504 (2008)

Evidence bond order is along (1,0), (0,1) directions in low *T* superconducting phase



M. Vojta and S. Sachdev, Physical Review Letters **83**, 3916 (1999)
S. Sachdev and N. Read, Int. J. Mod. Phys. B **5**, 219 (1991)

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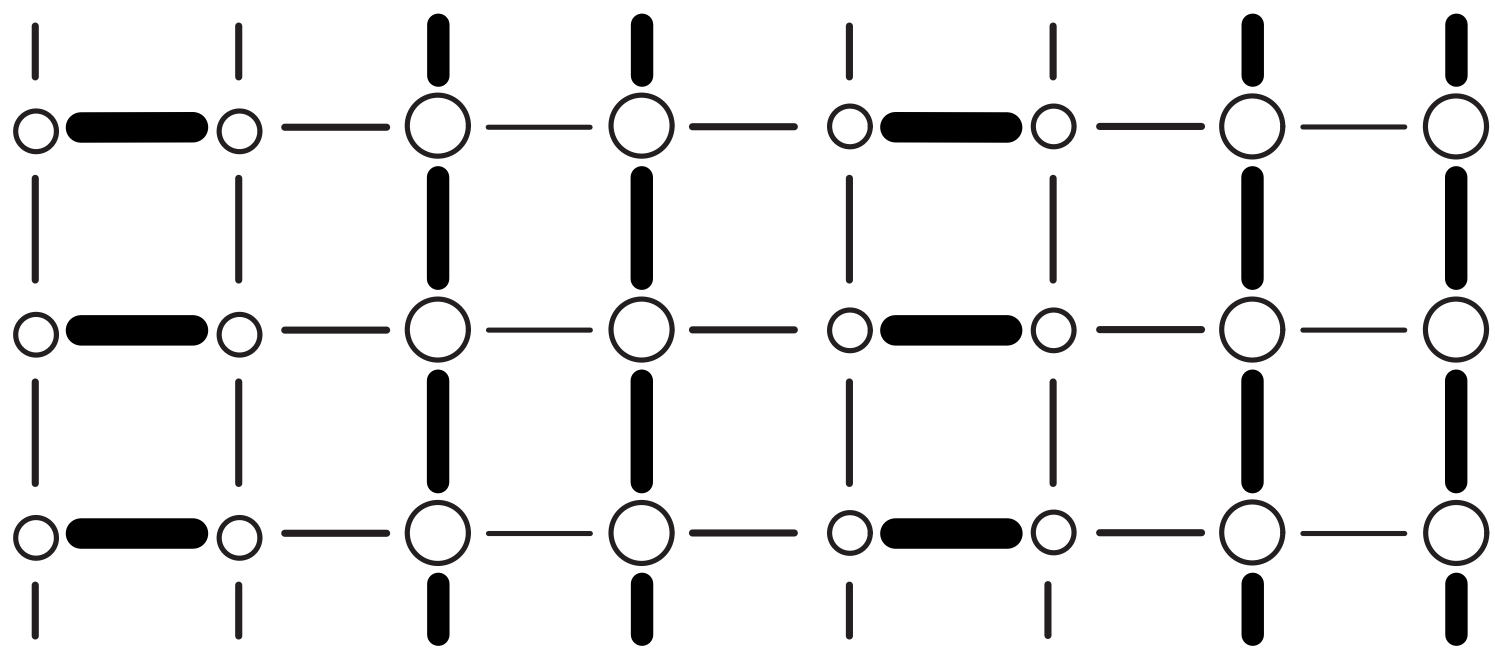
PHYSICAL REVIEW B **77**, 094504 (2008)

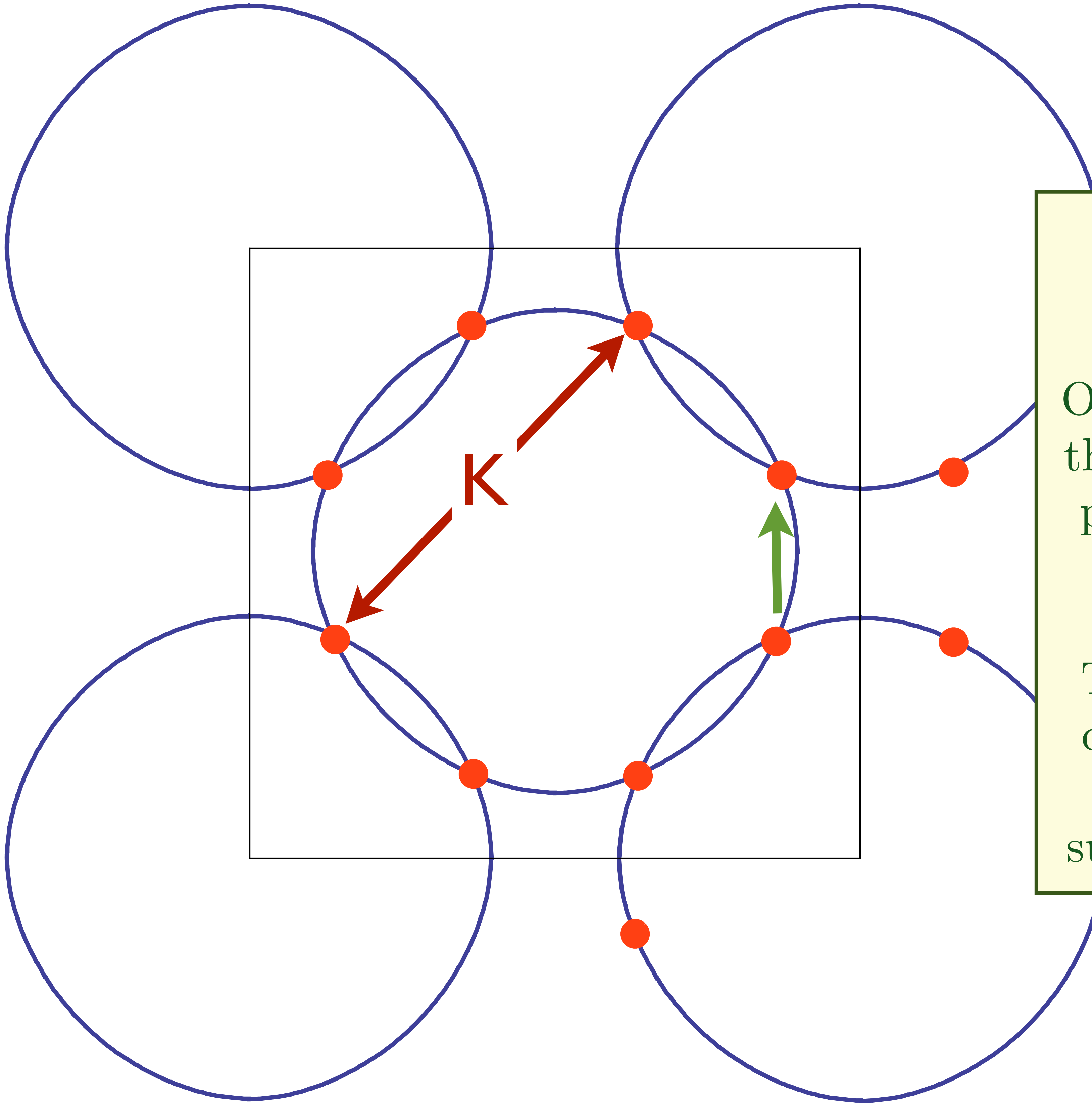
Superconducting *d*-wave stripes in cuprates: Valence bond order coexisting with nodal quasiparticles

Matthias Vojta and Oliver Rösch

We point out that unidirectional bond-centered charge-density-wave states in cuprates involve electronic order in both *s*- and *d*-wave channels, with nonlocal Coulomb repulsion suppressing the *s*-wave component.



Incommensurate *d*-wave bond order



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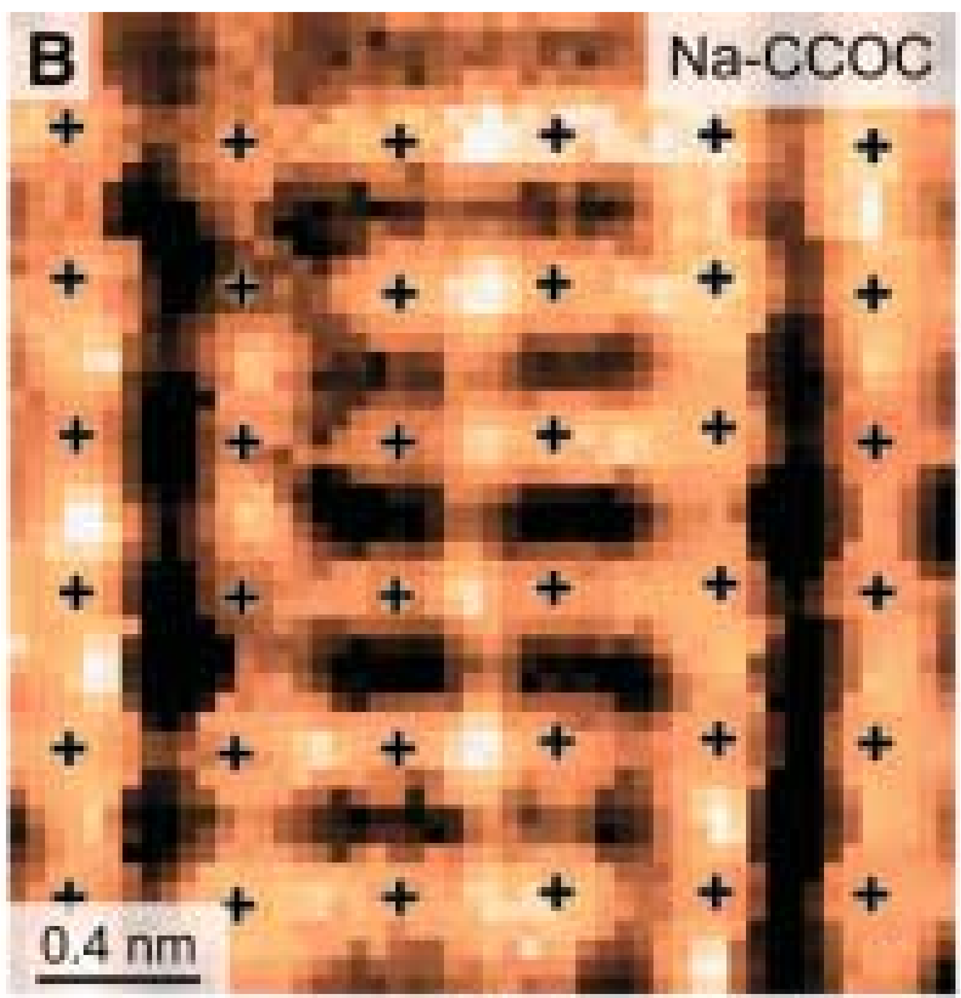
An Intrinsic Bond-Centered Electronic Glass with Unidirectional Domains in Underdoped Cuprates

Y. Kohsaka,[1] C. Taylor,[1] K. Fujita,[1,2] A. Schmidt,[1] C. Lupien,[3] T. Hanaguri,[4] M. Azuma,[5] M. Takano,[5] H. Eisaki,[6] H. Takagi,[2,4] S. Uchida,[2,7] J. C. Davis[1,8]*

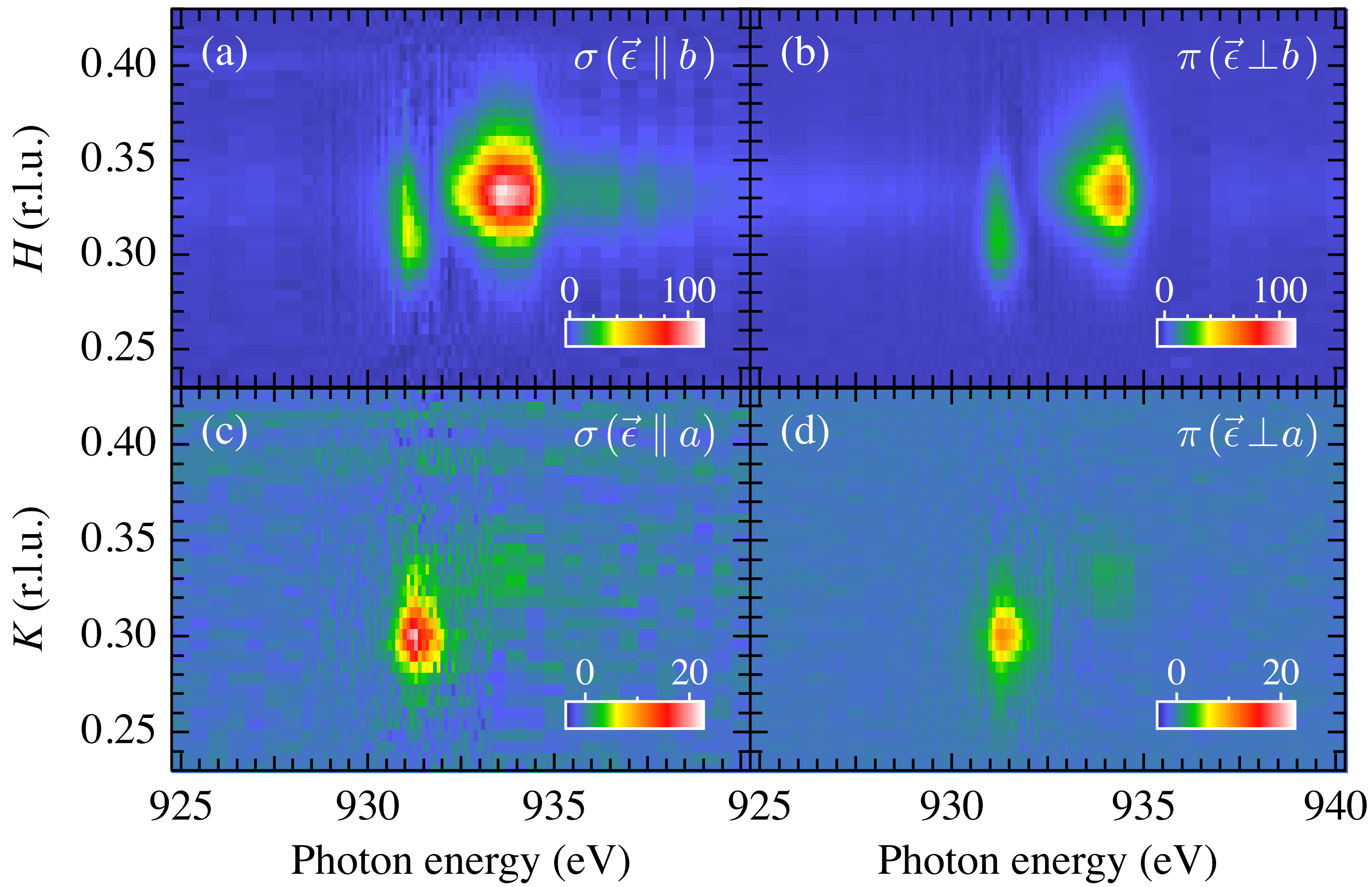
9 MARCH 2007 VOL 315 SCIENCE



Distinct Charge Orders in the Planes and Chains of Ortho-III-Ordered $YBa_2Cu_3O_{6+\delta}$ Superconductors Identified by Resonant Elastic X-ray Scattering

A. J. Achkar,[1] R. Sutarto,[2,3] X. Mao,[1] F. He,[3] A. Frano,[4,5] S. Blanco-Canosa,[4] M. Le Tacon,[4] G. Ghiringhelli,[6] L. Braicovich,[6] M. Minola,[6] M. Moretti Sala,[7] C. Mazzoli,[6] Ruixing Liang,[2] D. A. Bonn,[2] W. N. Hardy,[2] B. Keimer,[4] G. A. Sawatzky,[2] and D. G. Hawthorn[1,*]

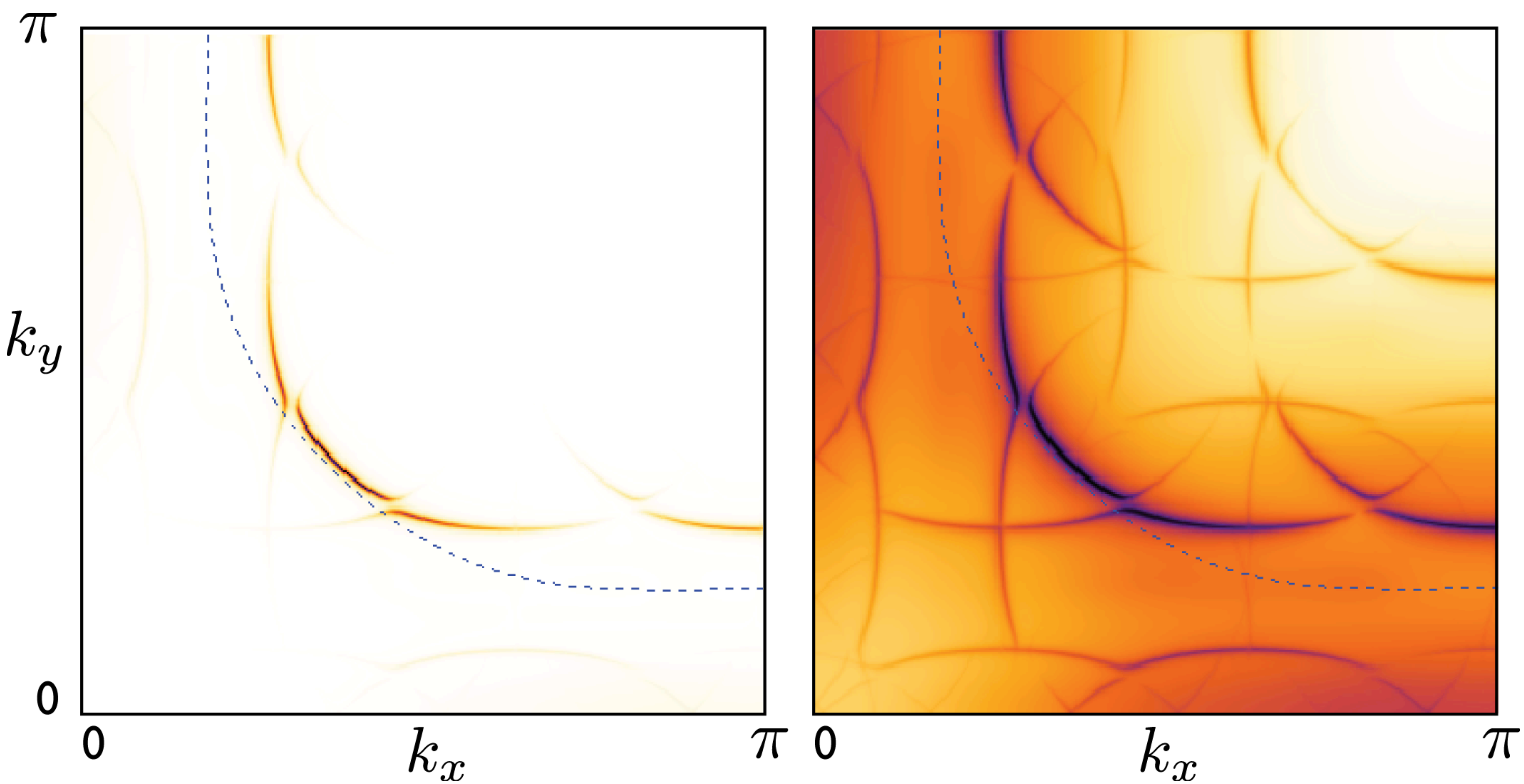
PRL **109,** 167001 (2012)



Moreover, the energy dependence of the CDW order in the planes is shown to result from a spatial modulation of energies of the Cu $2p$ to $3d_{x^2-y^2}$ transition, similar to stripe-ordered 214 cuprates.

These energy shifts are interpreted as a spatial modulation of the electronic structure and may point to a valence-bond-solid interpretation of the stripe phase.

Electron spectral function



$\mathrm{Im}G(\mathbf{k}, \omega + i\eta)$ $\qquad$ $\log \mathrm{Im}G(\mathbf{k}, \omega + i\eta)$

$$\left\langle c^{\dagger}_{\boldsymbol{k}-\boldsymbol{Q}/2,\alpha} c_{\boldsymbol{k}+\boldsymbol{Q}/2,\alpha} \right\rangle \propto \Delta_{\boldsymbol{Q}}(\boldsymbol{k}) = \begin{cases} \Delta_s + \Delta_d(\cos k_x - \cos k_y) & , \quad \boldsymbol{Q} = (\pm Q_0, 0) \\ \Delta_s - \Delta_d(\cos k_x - \cos k_y) & , \quad \boldsymbol{Q} = (0, \pm Q_0) \end{cases}$$

with $\Delta_s/\Delta_d = -0.234$.

S. Sachdev and R. La Placa, arXiv:1303.2114

Summary

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- Antiferromagnetic quantum criticality leads to d-wave superconductivity (supported by sign-problem-free Monte Carlo simulations)

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- Metals with antiferromagnetic spin correlations have nearly degenerate instabilities: to *d*-wave superconductivity, and to a charge density wave with a *d*-wave form factor. This is a promising explanation of the pseudogap regime.