

Metals near the onset of antiferromagnetism: instabilities to d-wave pairing and bond order

Subir Sachdev

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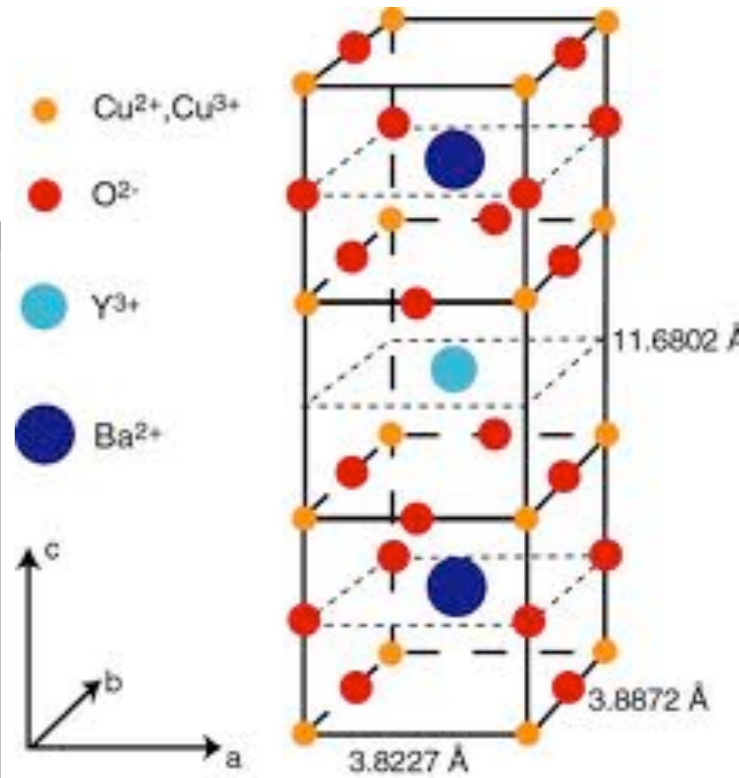
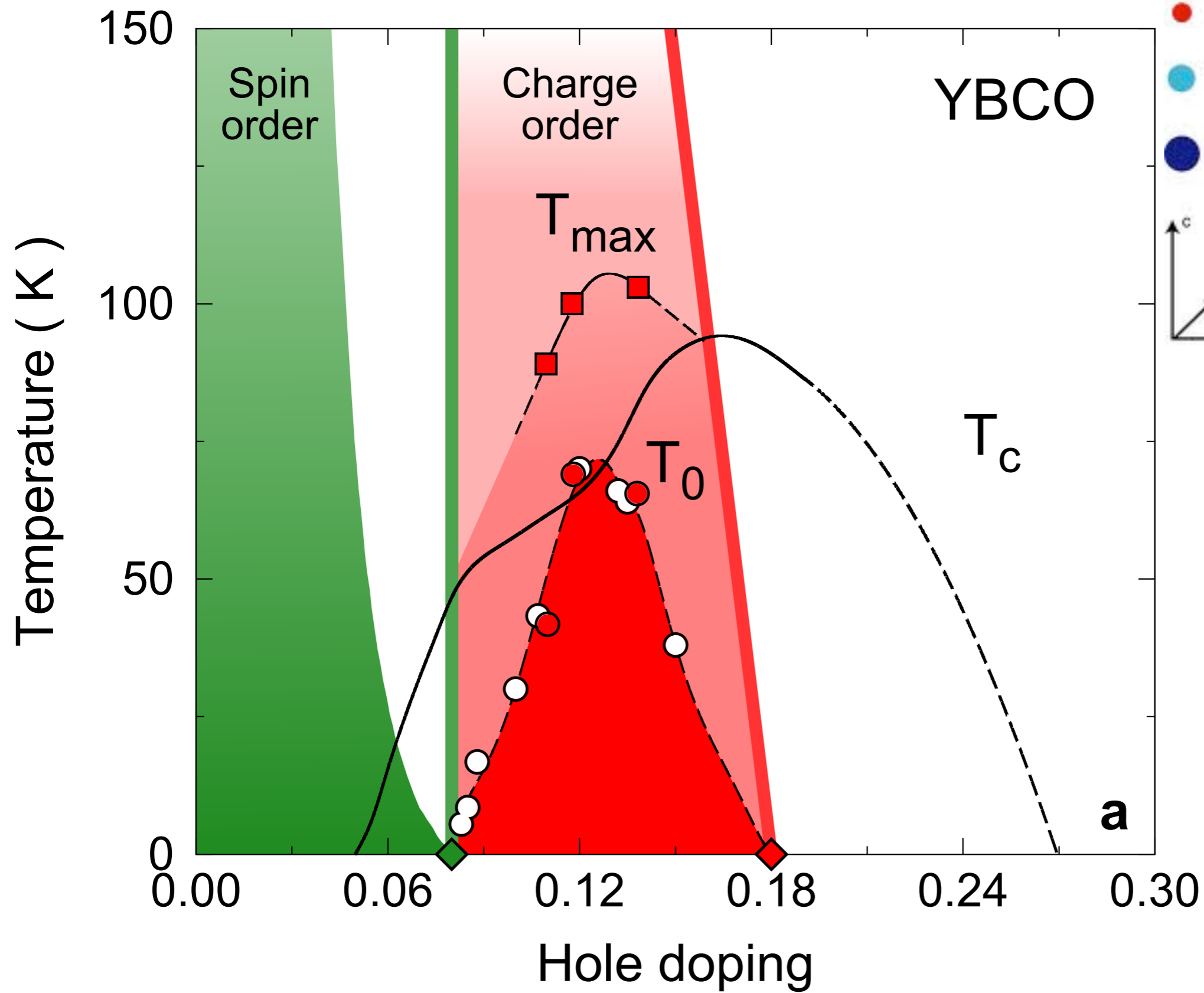


Max Metlitski



Erez Berg



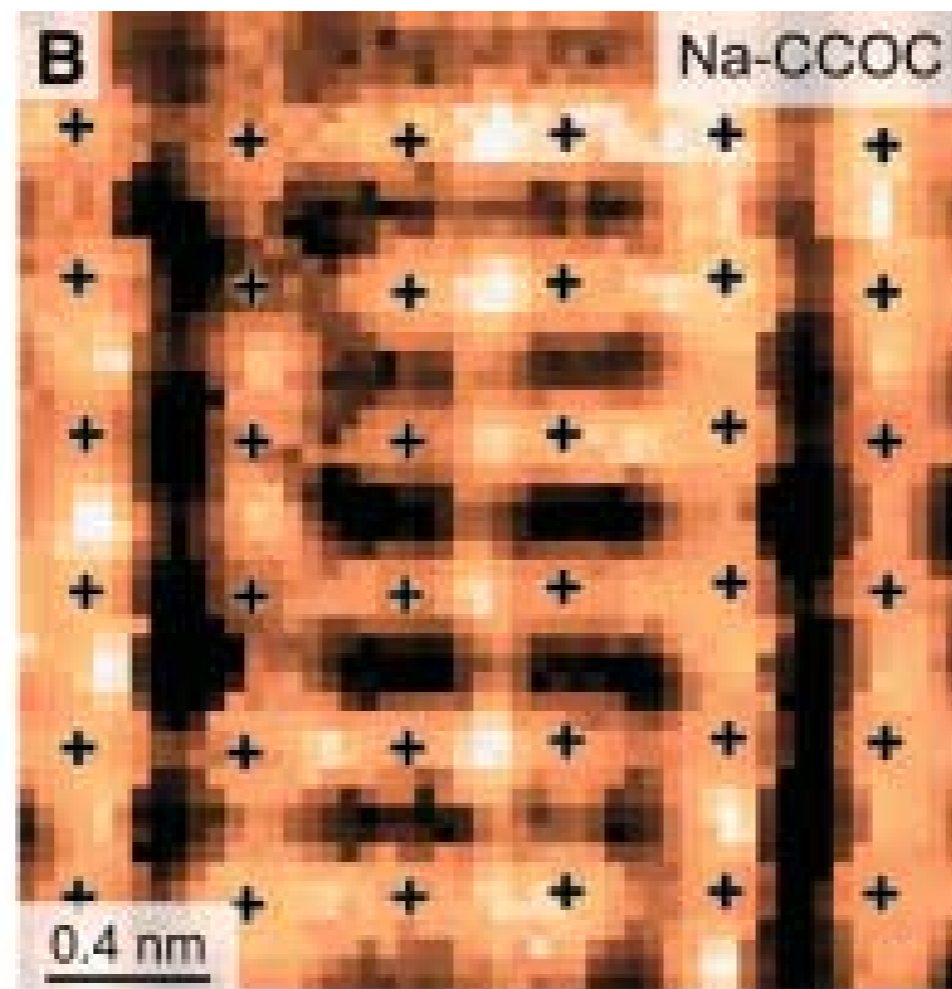


G. Grissonanche et al., preprint

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*}

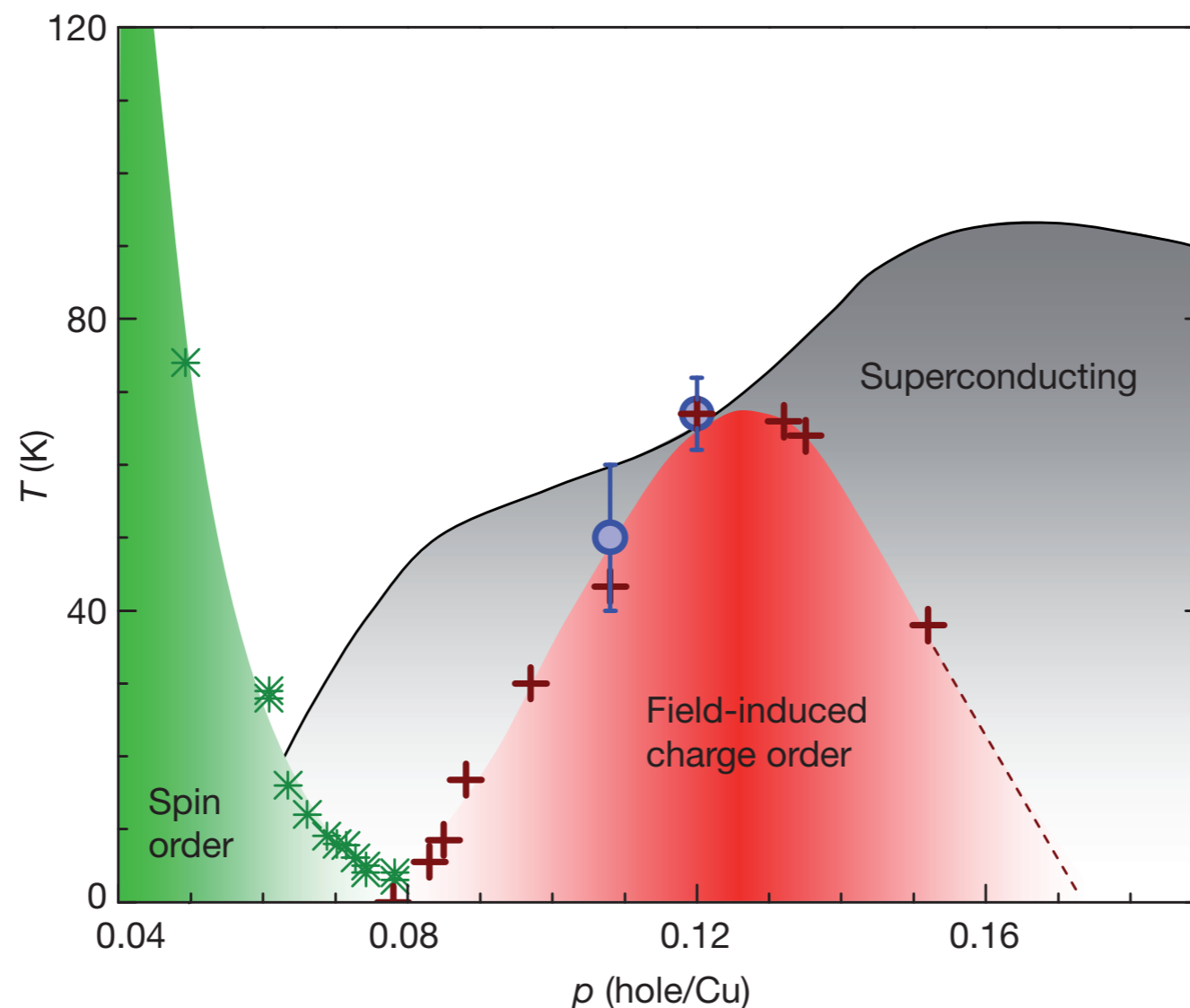
9 MARCH 2007 VOL 315 SCIENCE

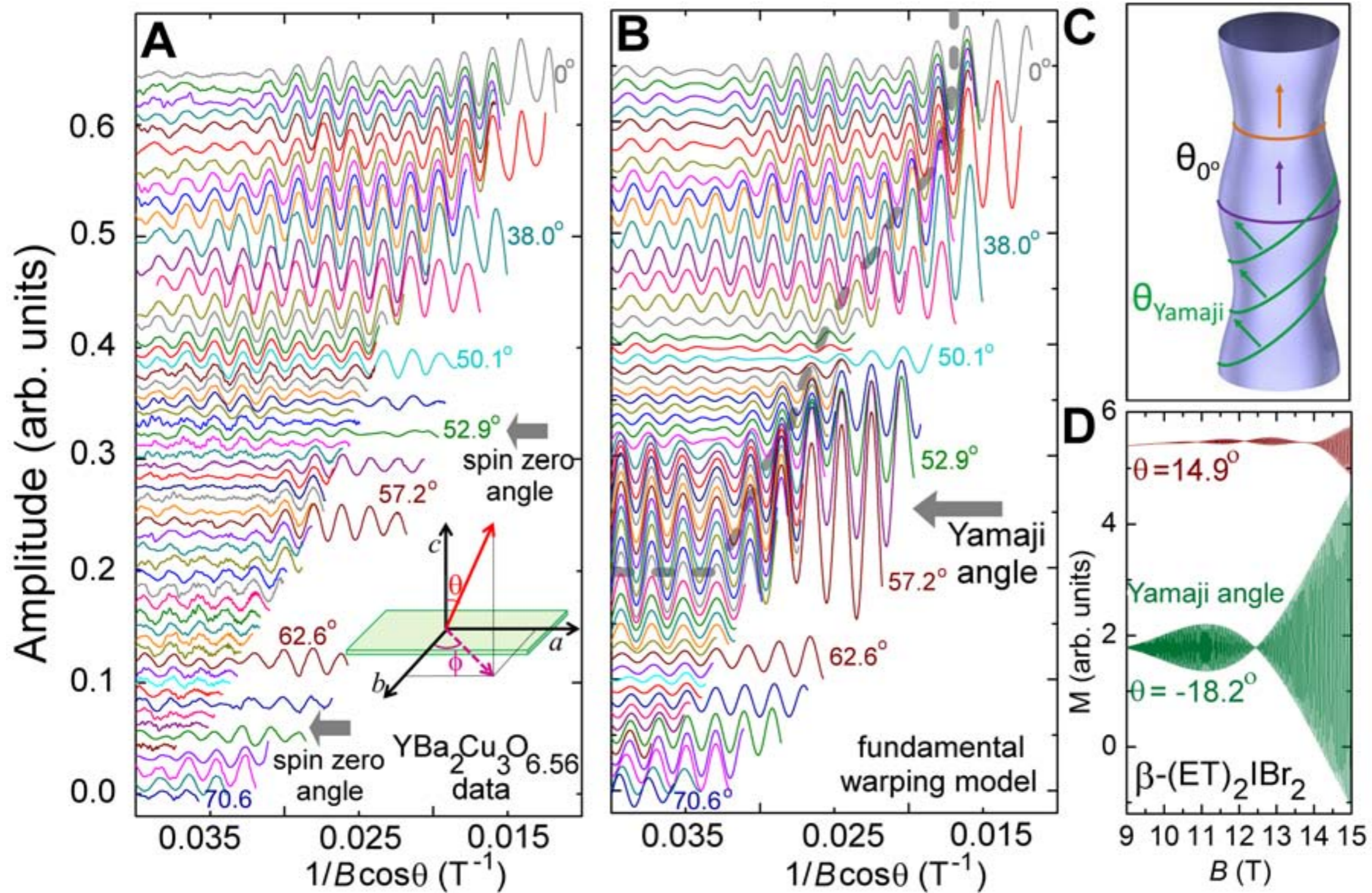


Magnetic-field-induced charge-stripe order in the high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_y$

Tao Wu¹, Hadrien Mayaffre¹, Steffen Krämer¹, Mladen Horvatić¹, Claude Berthier¹, W. N. Hardy^{2,3}, Ruixing Liang^{2,3}, D. A. Bonn^{2,3} & Marc-Henri Julien¹

8 SEPTEMBER 2011 | VOL 477 | NATURE | 191





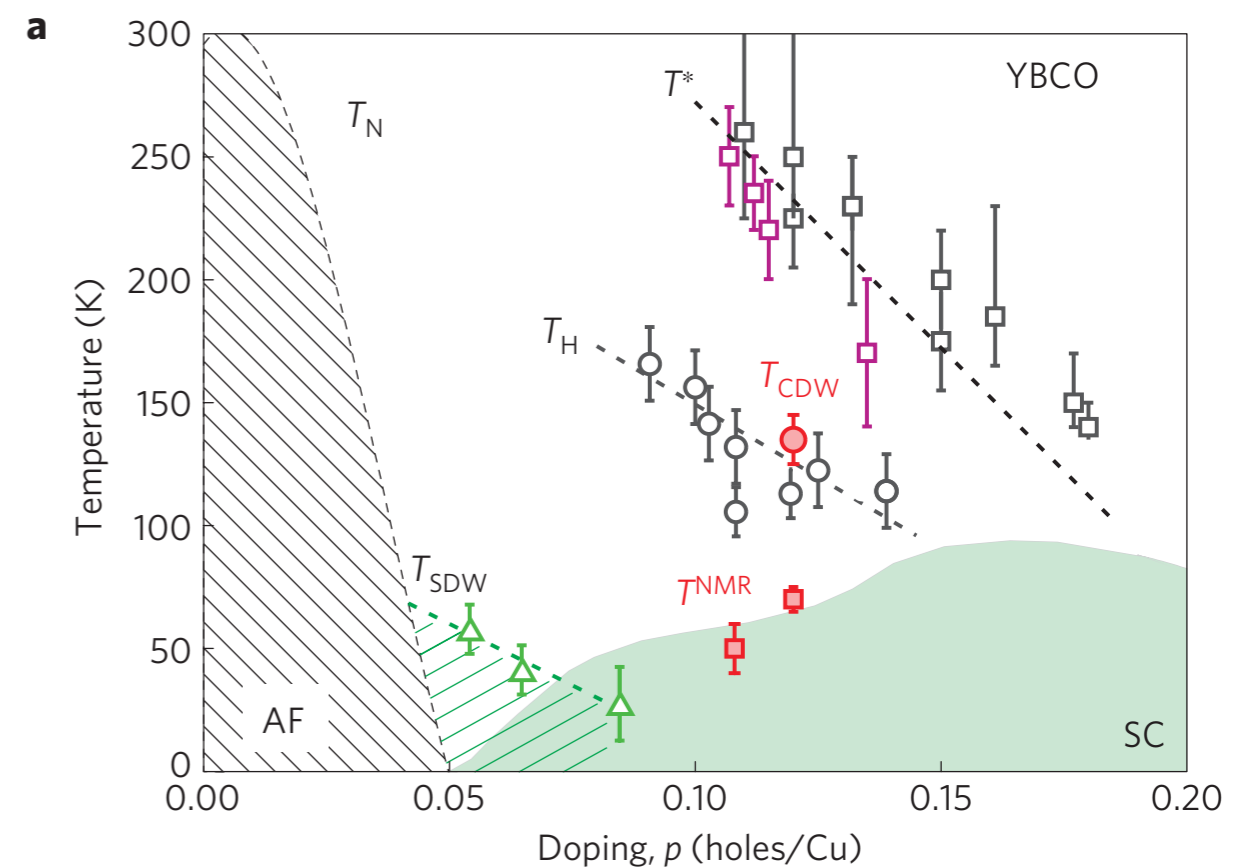
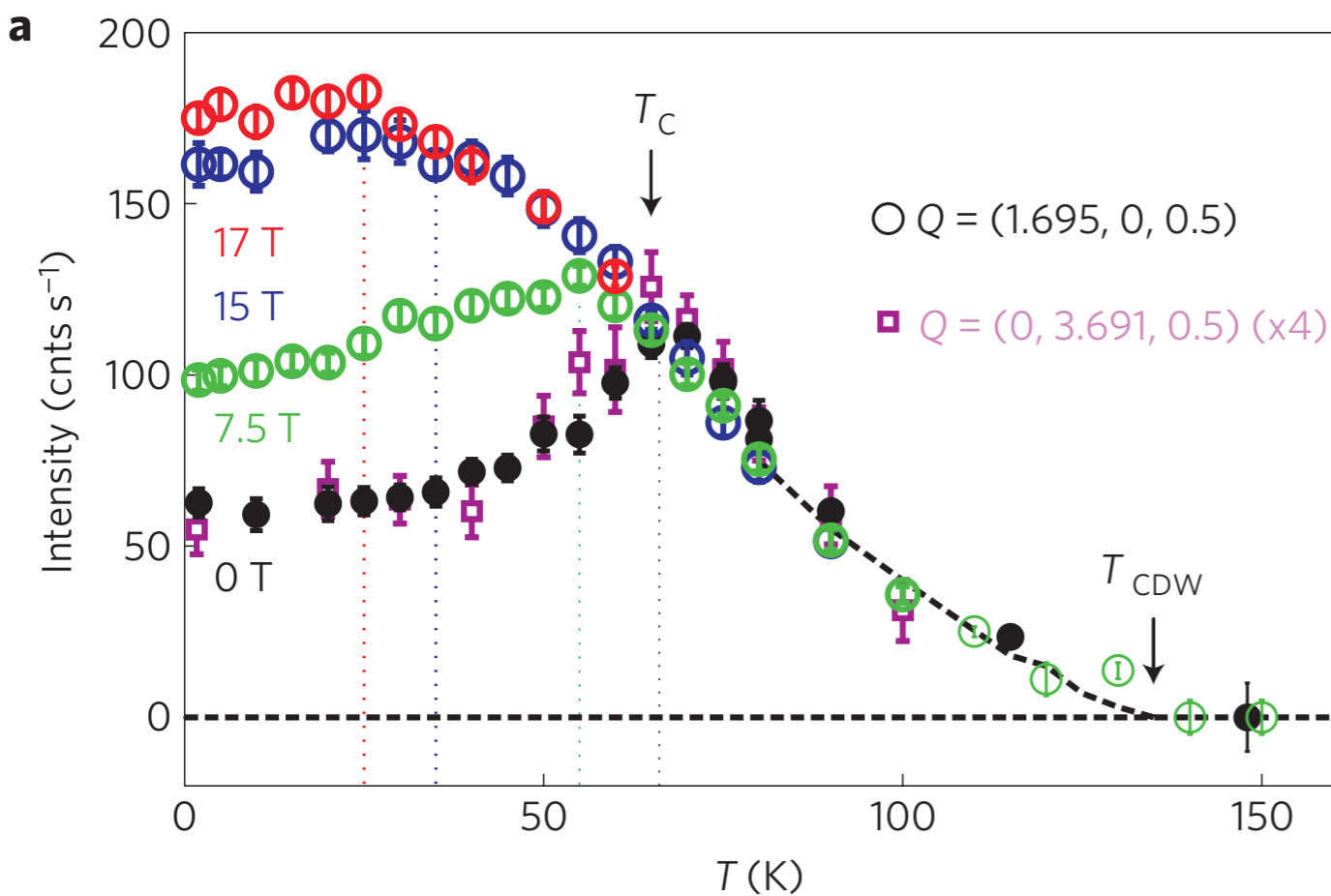
Twofold twisted Fermi surface from staggered order in an underdoped high T_c superconductor

Suchitra E. Sebastian,^{1*} N. Harrison,² F. F. Balakirev,² M. M. Altarawneh,^{2,3}
 Ruixing Liang,^{4,5} D. A. Bonn,^{4,5} W. N. Hardy,^{4,5} G. G. Lonzarich,¹

Direct observation of competition between superconductivity and charge density wave order in $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$

J. Chang^{1,2*}, E. Blackburn³, A. T. Holmes³, N. B. Christensen⁴, J. Larsen^{4,5}, J. Mesot^{1,2}, Ruixing Liang^{6,7}, D. A. Bonn^{6,7}, W. N. Hardy^{6,7}, A. Watenphul⁸, M. v. Zimmermann⁸, E. M. Forgan³ and S. M. Hayden⁹

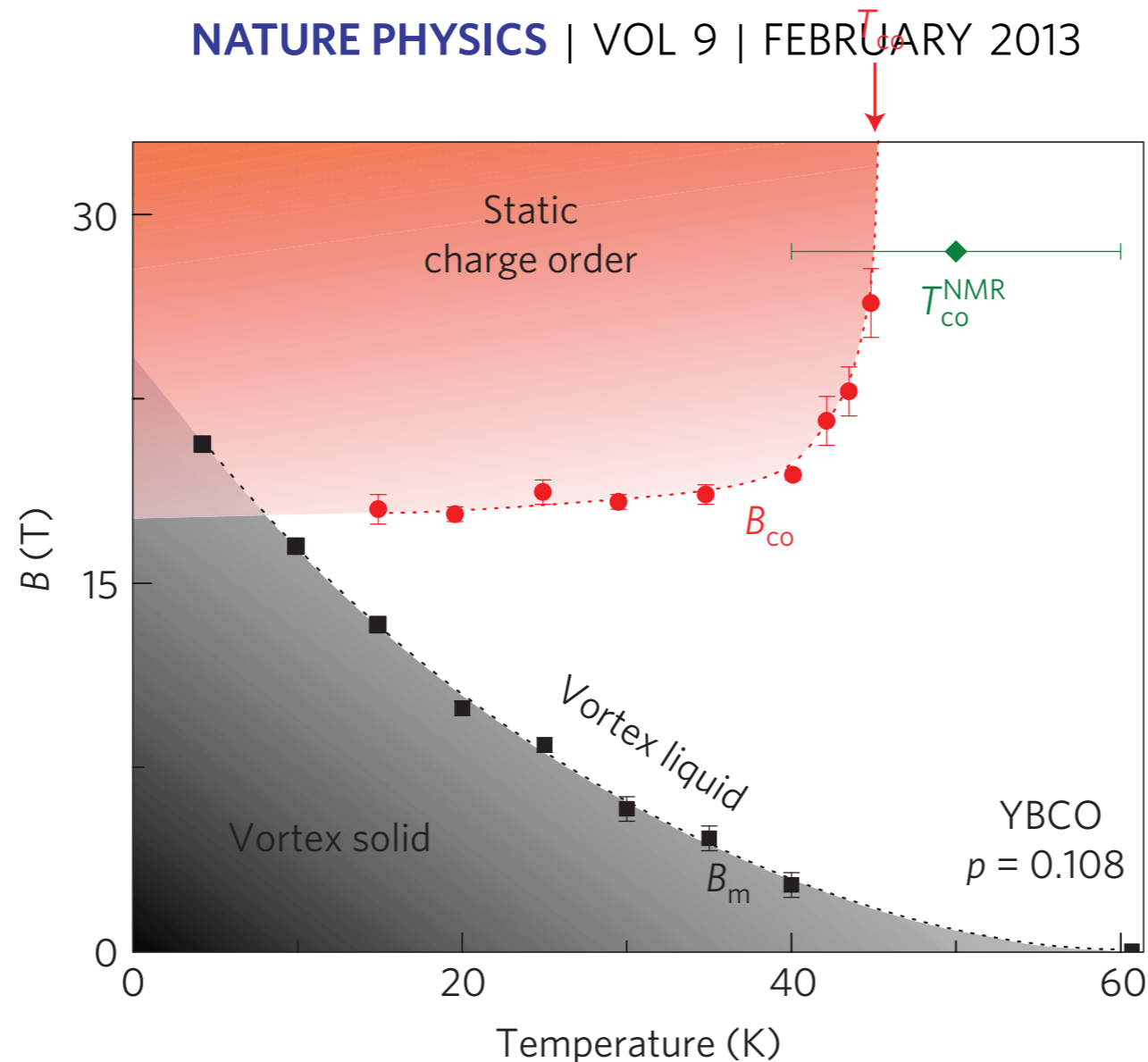
NATURE PHYSICS | VOL 8 | DECEMBER 2012 |



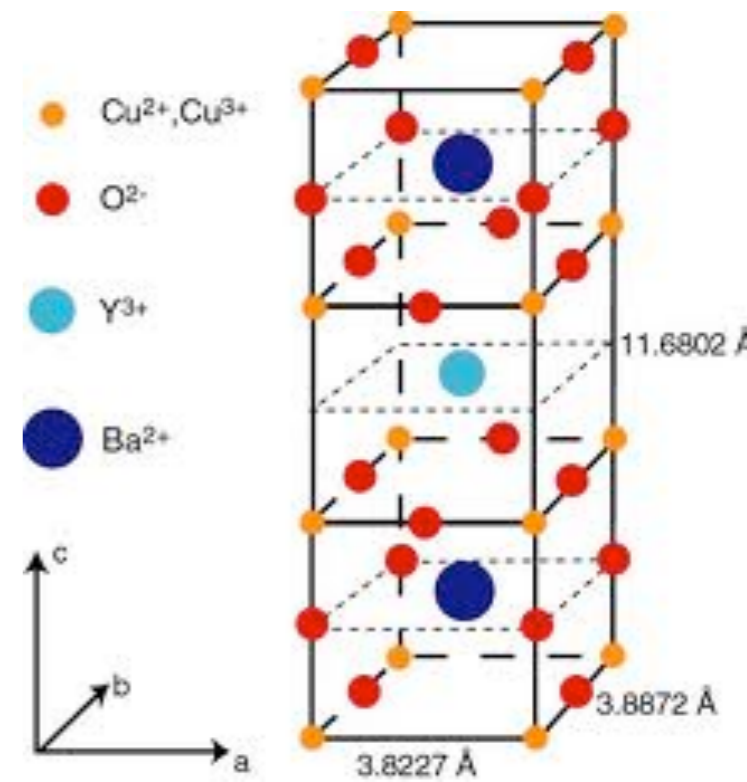
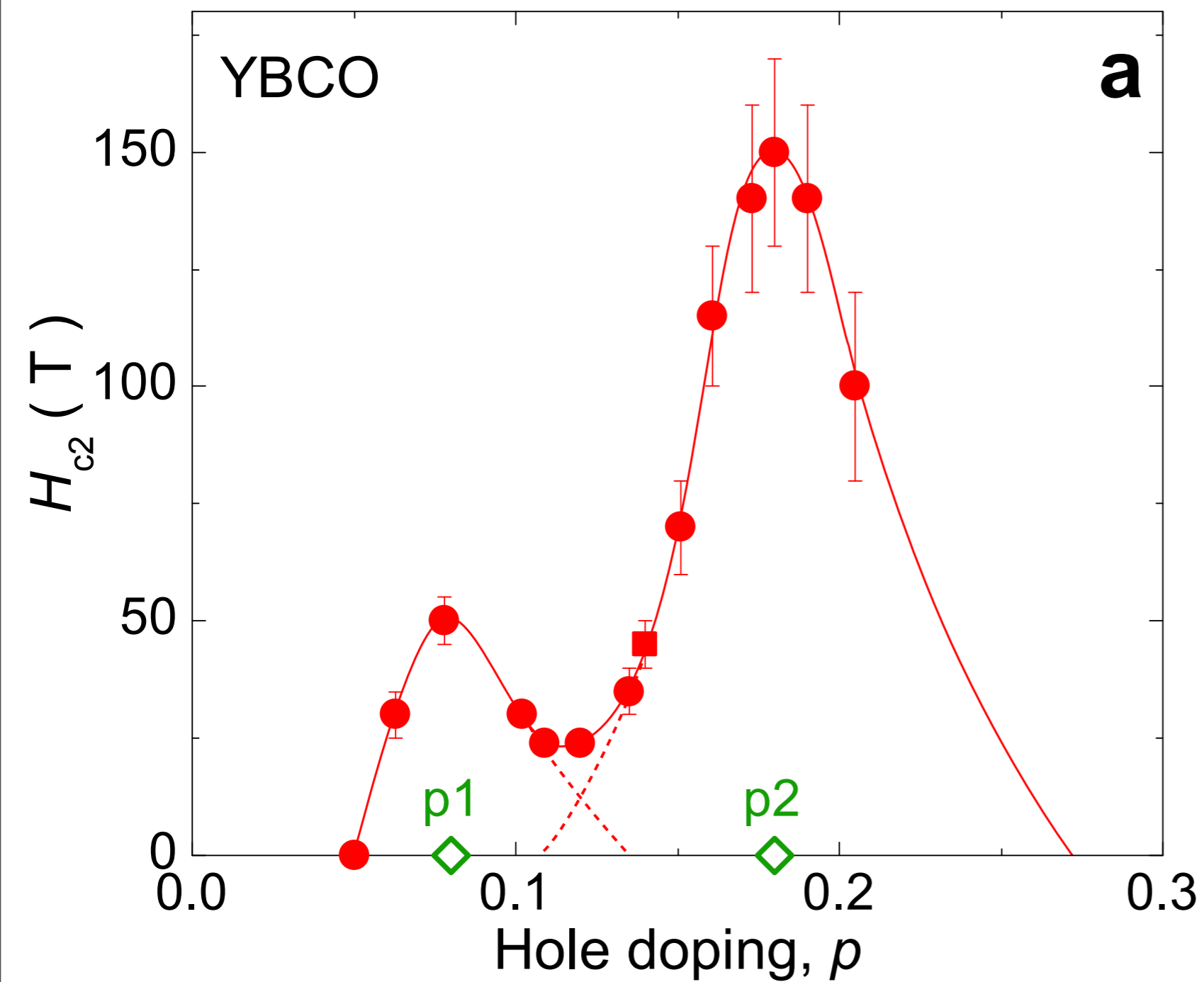
Thermodynamic phase diagram of static charge order in underdoped $\text{YBa}_2\text{Cu}_3\text{O}_y$

David LeBoeuf^{1*}, S. Krämer², W. N. Hardy^{3,4}, Ruixing Liang^{3,4}, D. A. Bonn^{3,4} and Cyril Proust^{1,4*}

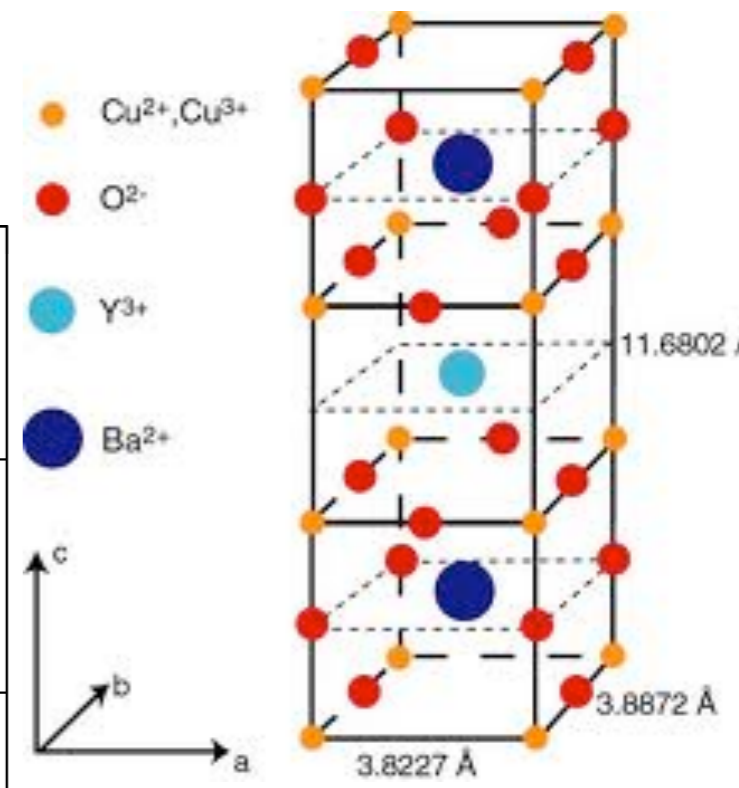
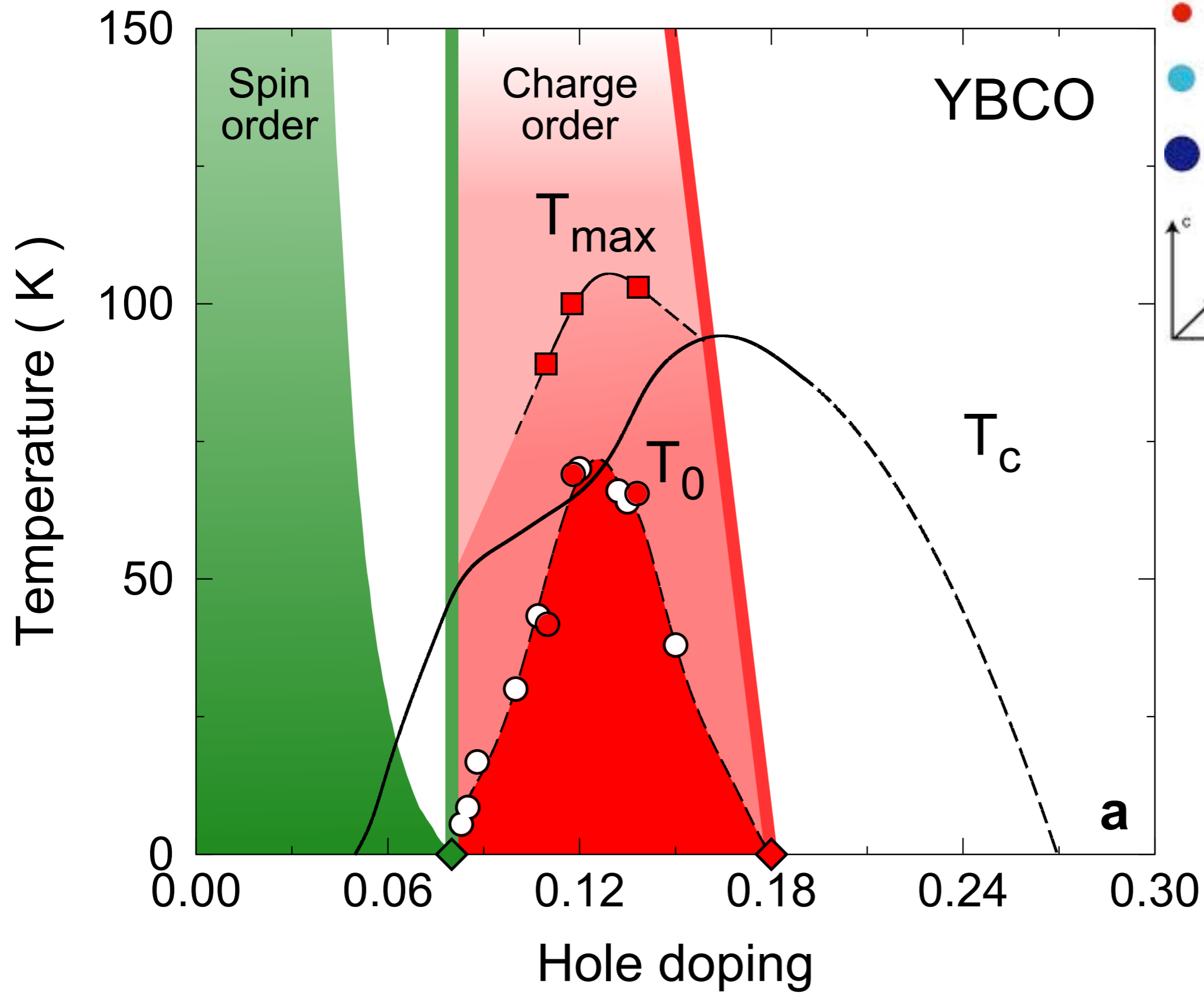
NATURE PHYSICS | VOL 9 | FEBRUARY 2013



The comparison of different acoustic modes indicates that the charge modulation is biaxial, which differs from a uniaxial stripe charge order.



G. Grissonanche et al., preprint



G. Grissonnanche et al., preprint

Outline

1. Antiferromagnetism in metals:
low energy theory
2. d-wave superconductivity
3. Emergent pseudospin symmetry,
and bond order
4. Quantum Monte Carlo
without the sign problem

Outline

1. Antiferromagnetism in metals:
low energy theory

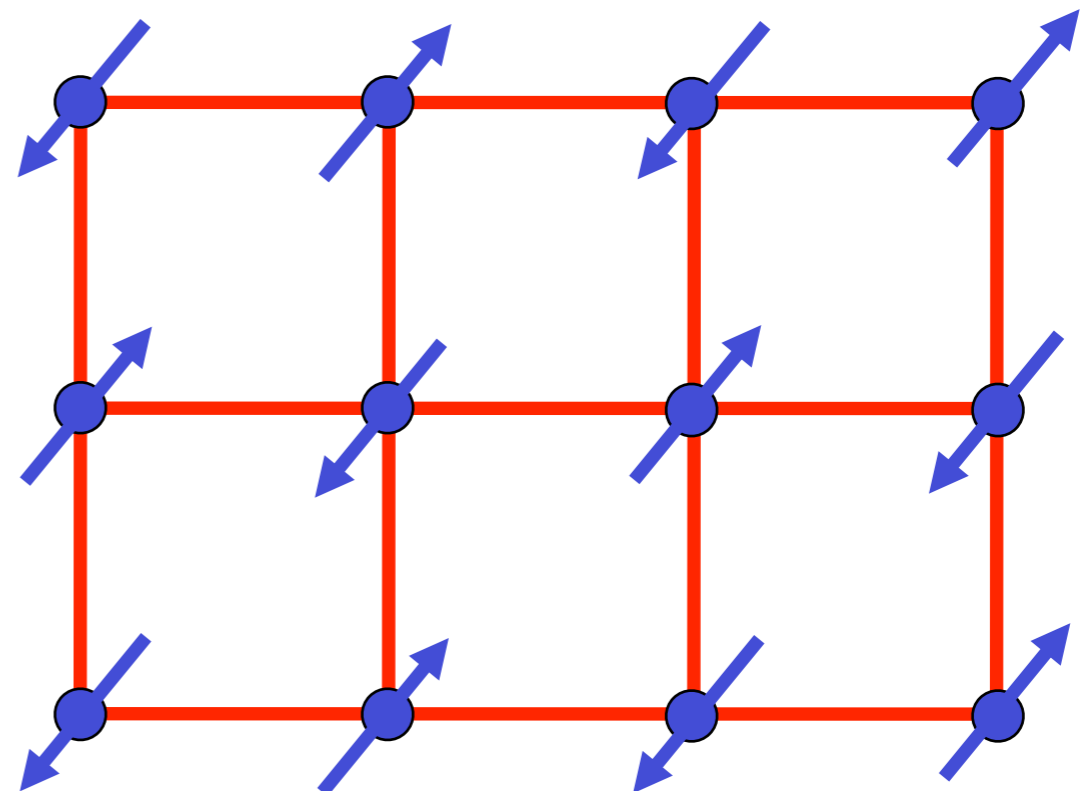
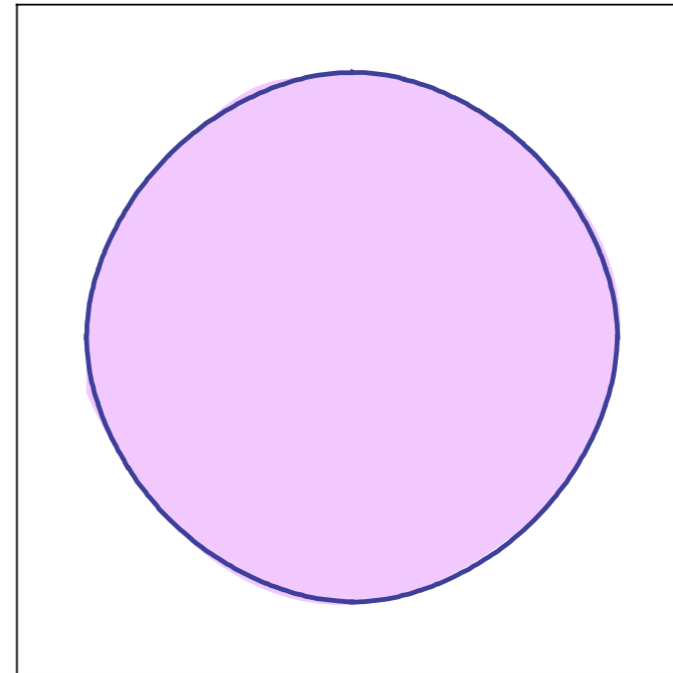
2. d-wave superconductivity

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without the sign problem

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} is the ordering wavevector.

The Hubbard Model

$$H = - \sum_{i < j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + U \sum_i \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_i c_{i\alpha}^\dagger c_{i\alpha}$$

$t_{ij} \rightarrow$ “hopping”. $U \rightarrow$ local repulsion, $\mu \rightarrow$ chemical potential

Spin index $\alpha = \uparrow, \downarrow$

$$n_{i\alpha} = c_{i\alpha}^\dagger c_{i\alpha}$$

$$c_{i\alpha}^\dagger c_{j\beta} + c_{j\beta} c_{i\alpha}^\dagger = \delta_{ij} \delta_{\alpha\beta}$$

$$c_{i\alpha} c_{j\beta} + c_{j\beta} c_{i\alpha} = 0$$

The Hubbard Model

Decouple U term by a Hubbard-Stratanovich transformation

$$\mathcal{S} = \int d^2r d\tau [\mathcal{L}_c + \mathcal{L}_\varphi + \mathcal{L}_{c\varphi}]$$

$$\mathcal{L}_c = c_a^\dagger \varepsilon(-i\nabla) c_a$$

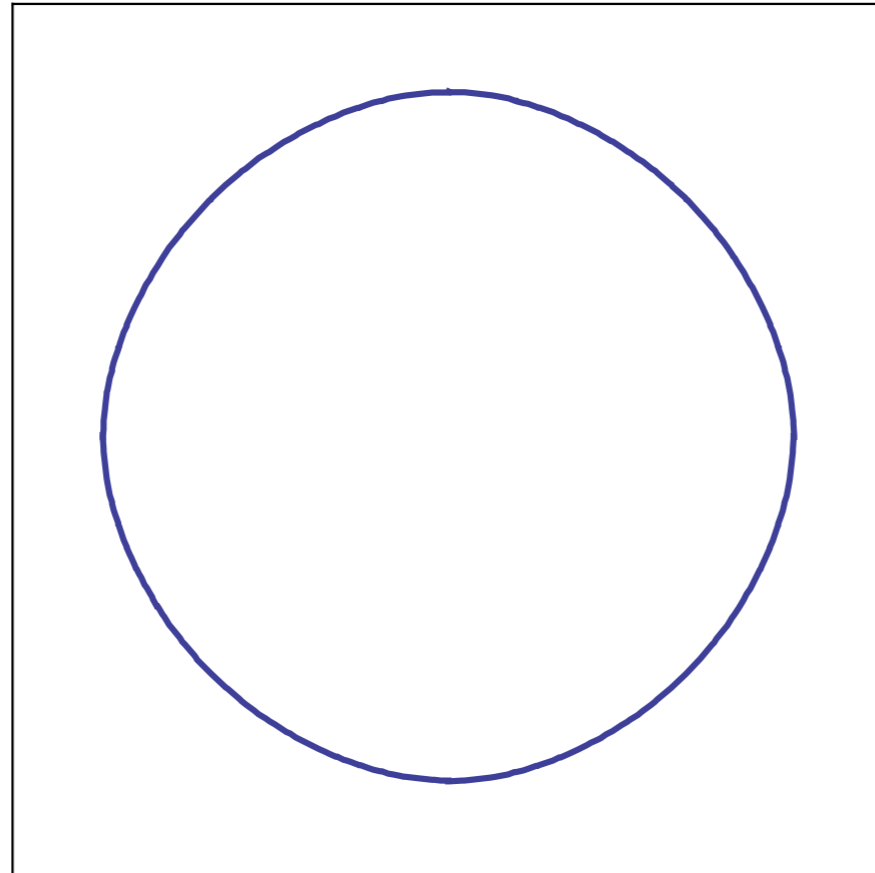
$$\mathcal{L}_\varphi = \frac{1}{2} (\nabla \varphi_\alpha)^2 + \frac{r}{2} \varphi_\alpha^2 + \frac{u}{4} (\varphi_\alpha^2)^2$$

$$\mathcal{L}_{c\varphi} = \lambda \varphi_\alpha e^{i\mathbf{K}\cdot\mathbf{r}} c_a^\dagger \sigma_{ab}^\alpha c_b.$$

“Yukawa” coupling between fermions and antiferromagnetic order:

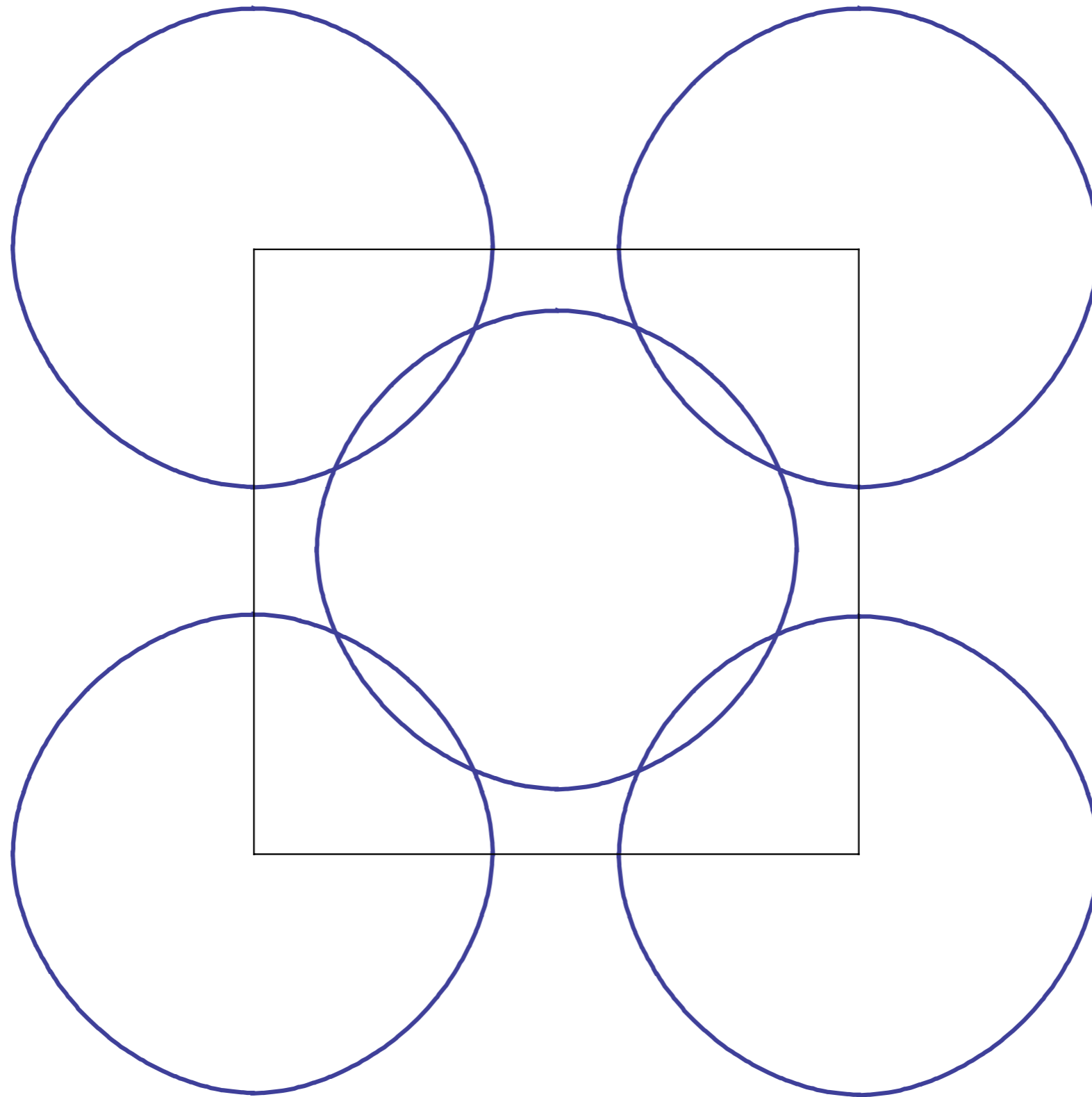
$$\lambda^2 \sim U, \text{ the Hubbard repulsion}$$

Fermi surface+antiferromagnetism



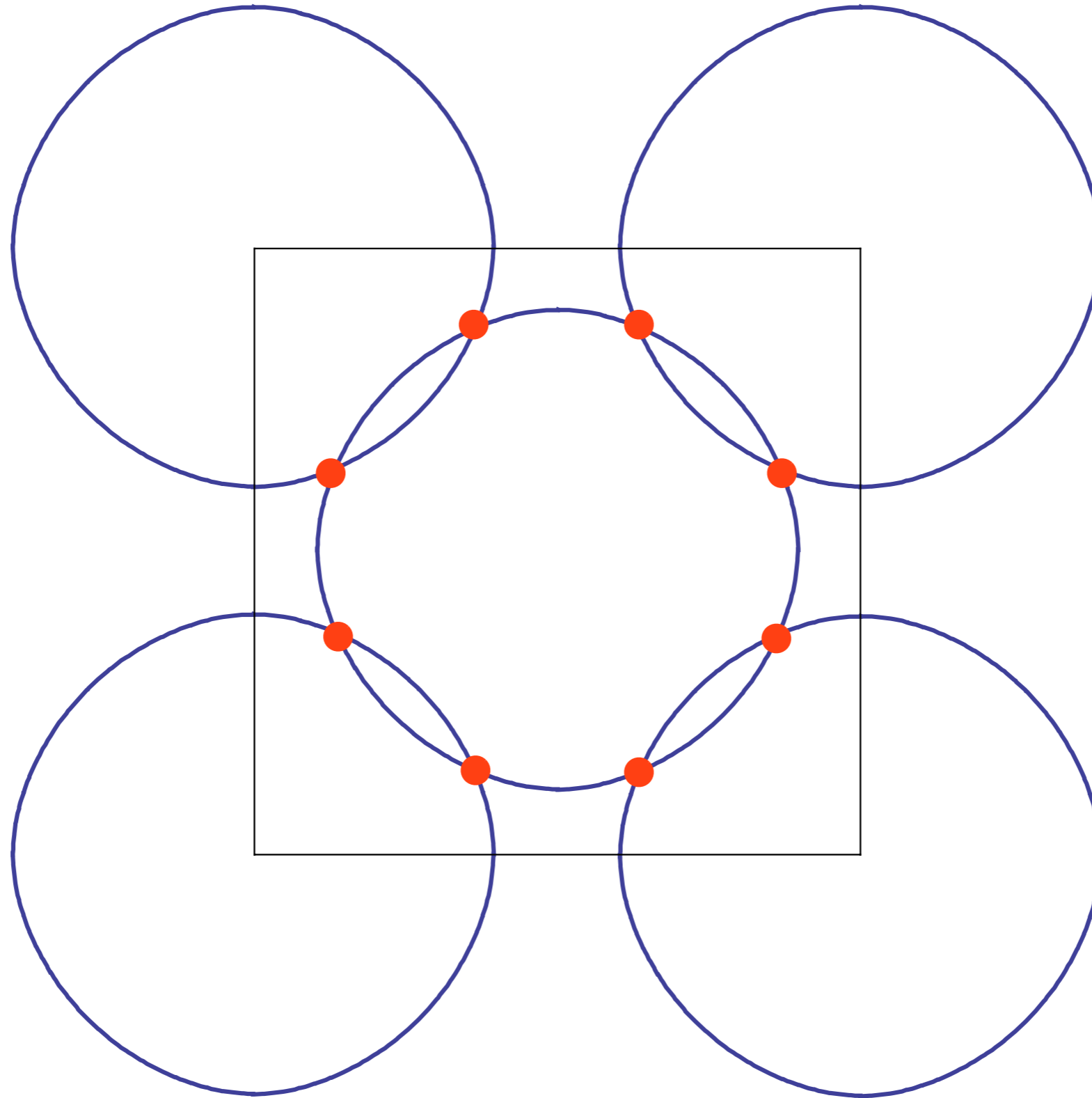
Metal with “large” Fermi surface

Fermi surface+antiferromagnetism



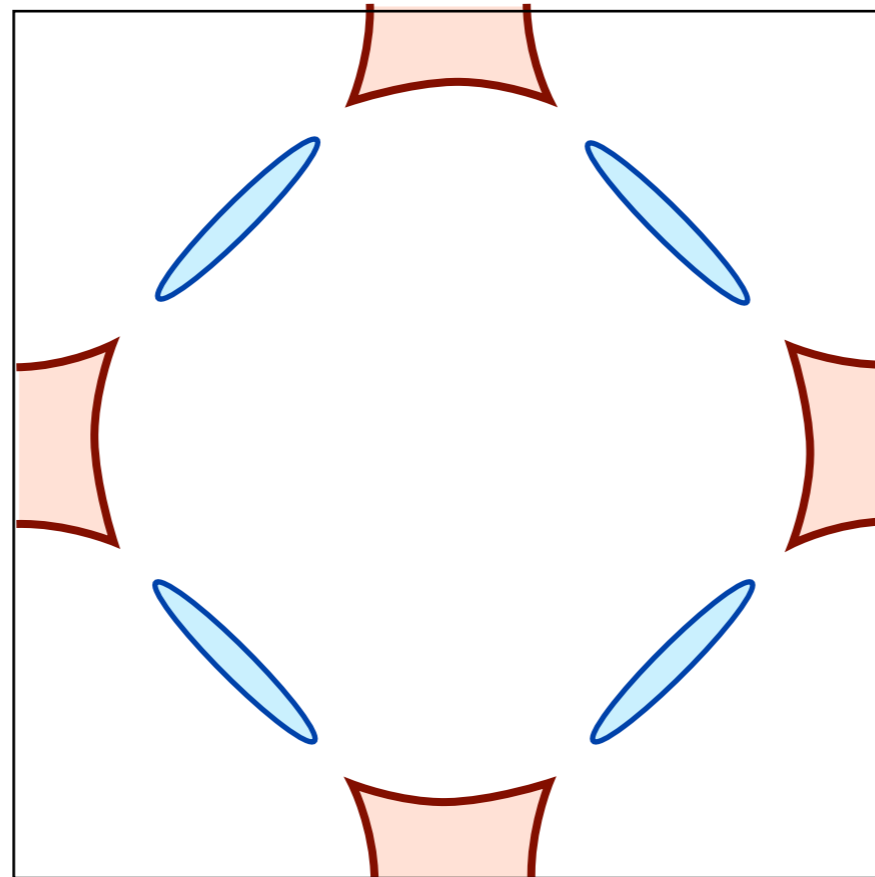
Fermi surfaces translated by $\mathbf{K} = (\pi, \pi)$.

Fermi surface+antiferromagnetism



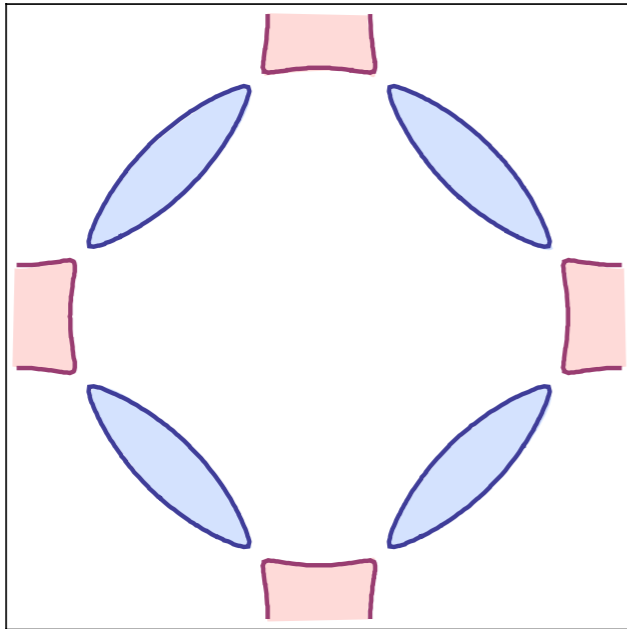
“Hot” spots

Fermi surface+antiferromagnetism



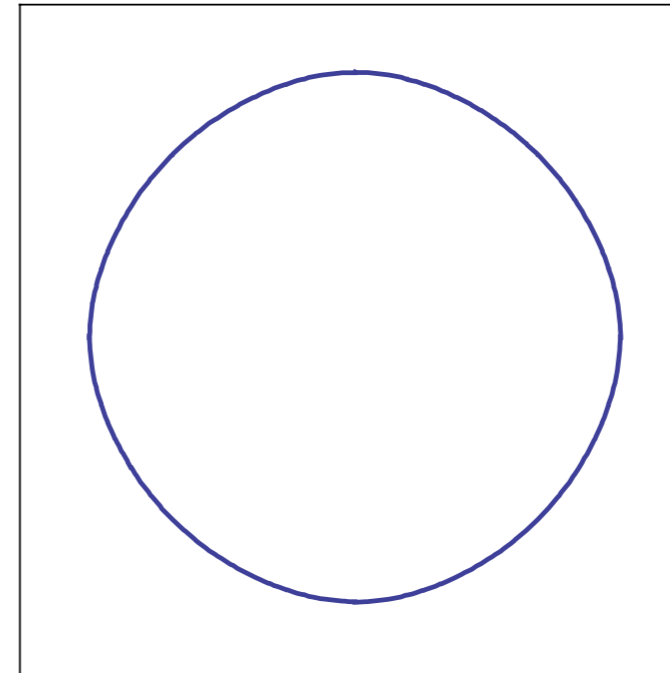
Electron and hole pockets in
antiferromagnetic phase with $\langle \vec{\varphi} \rangle \neq 0$

Fermi surface+antiferromagnetism



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

Metal with electron
and hole pockets



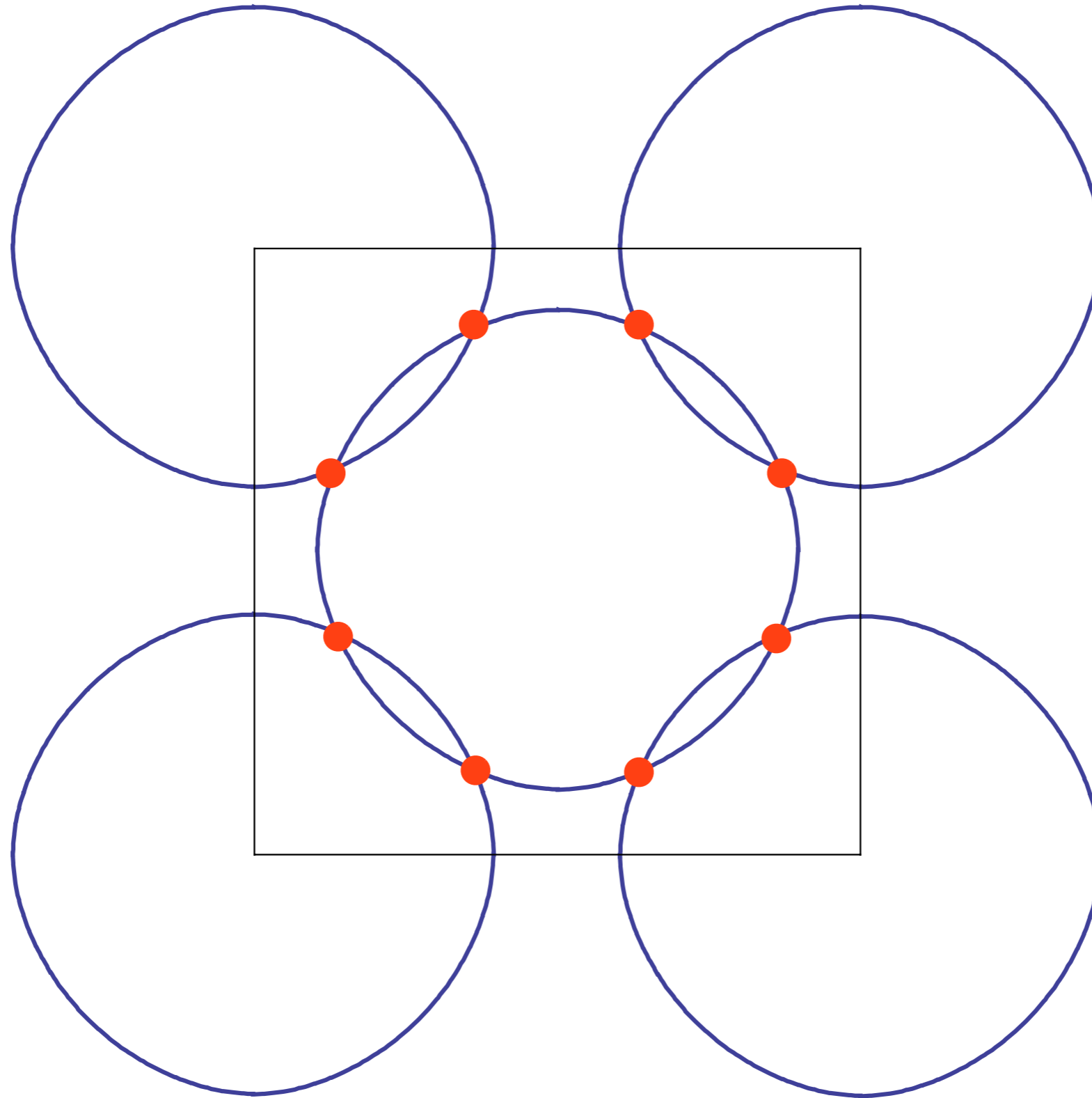
$$\langle \vec{\varphi} \rangle = 0$$

Metal with “large”
Fermi surface

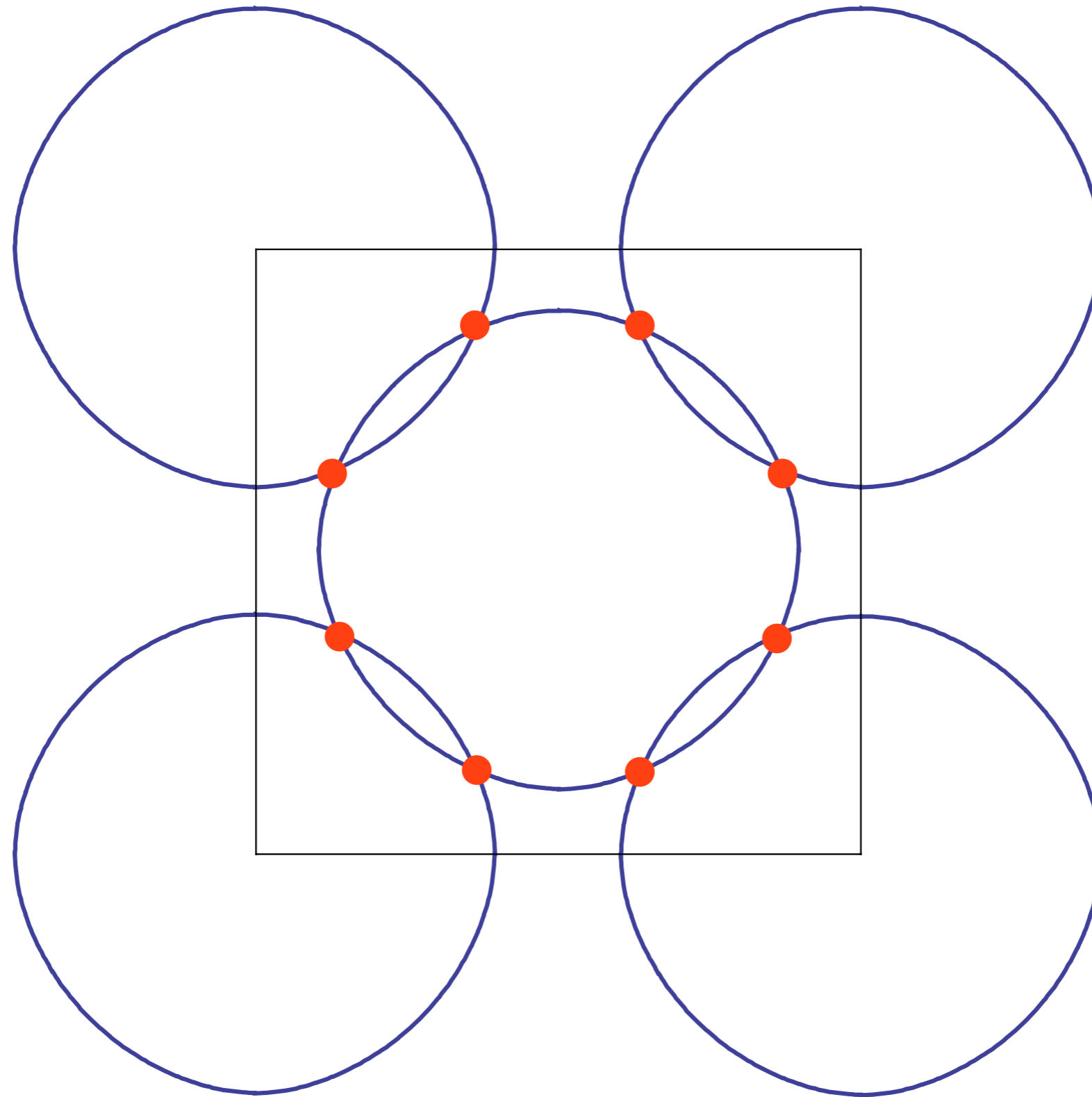
← Increasing interaction

S. Sachdev, A. V. Chubukov, and A. Sokol, *Phys. Rev. B* **51**, 14874 (1995).
A. V. Chubukov and D. K. Morr, *Physics Reports* **288**, 355 (1997).

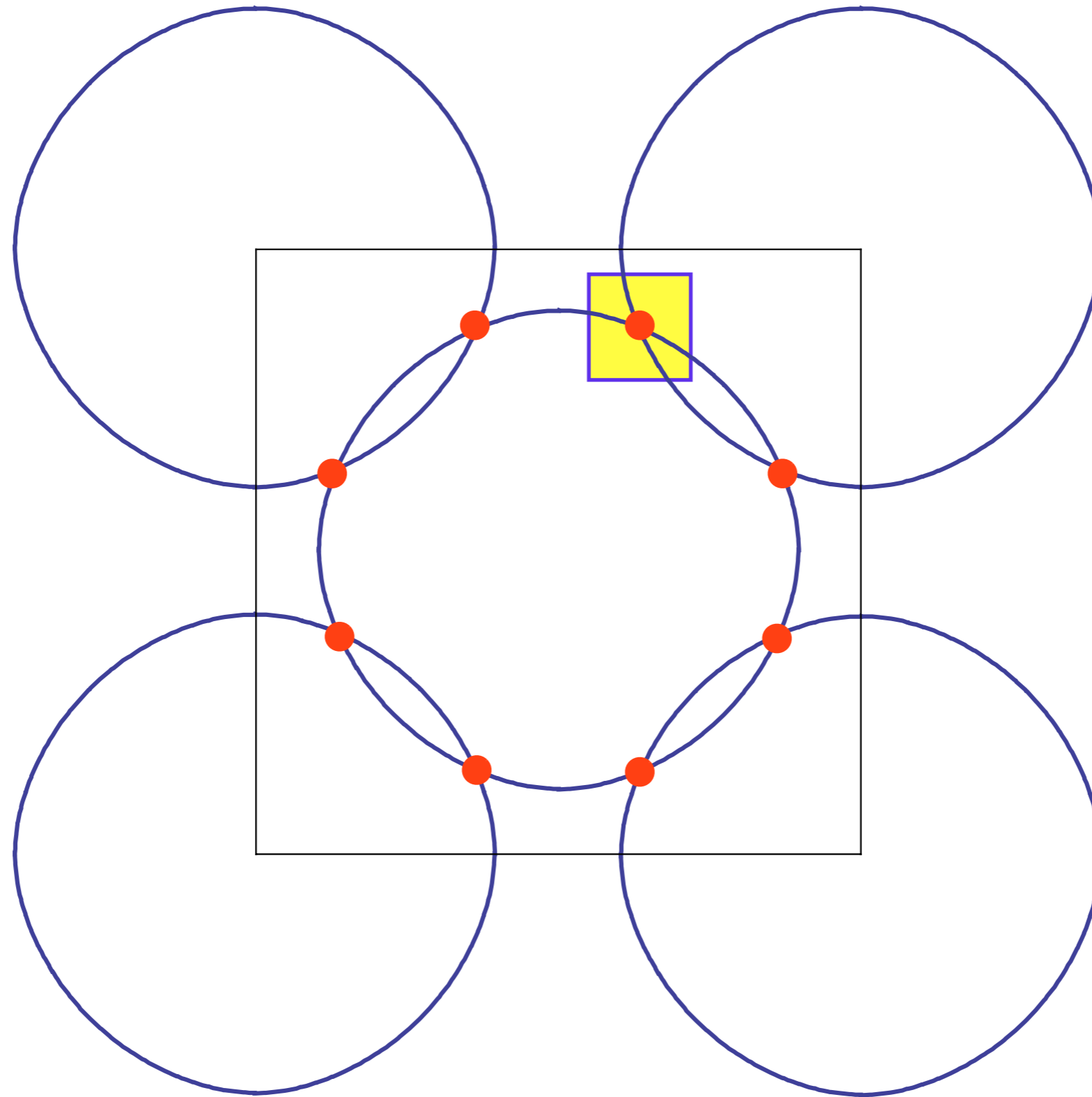
Fermi surface+antiferromagnetism



“Hot” spots

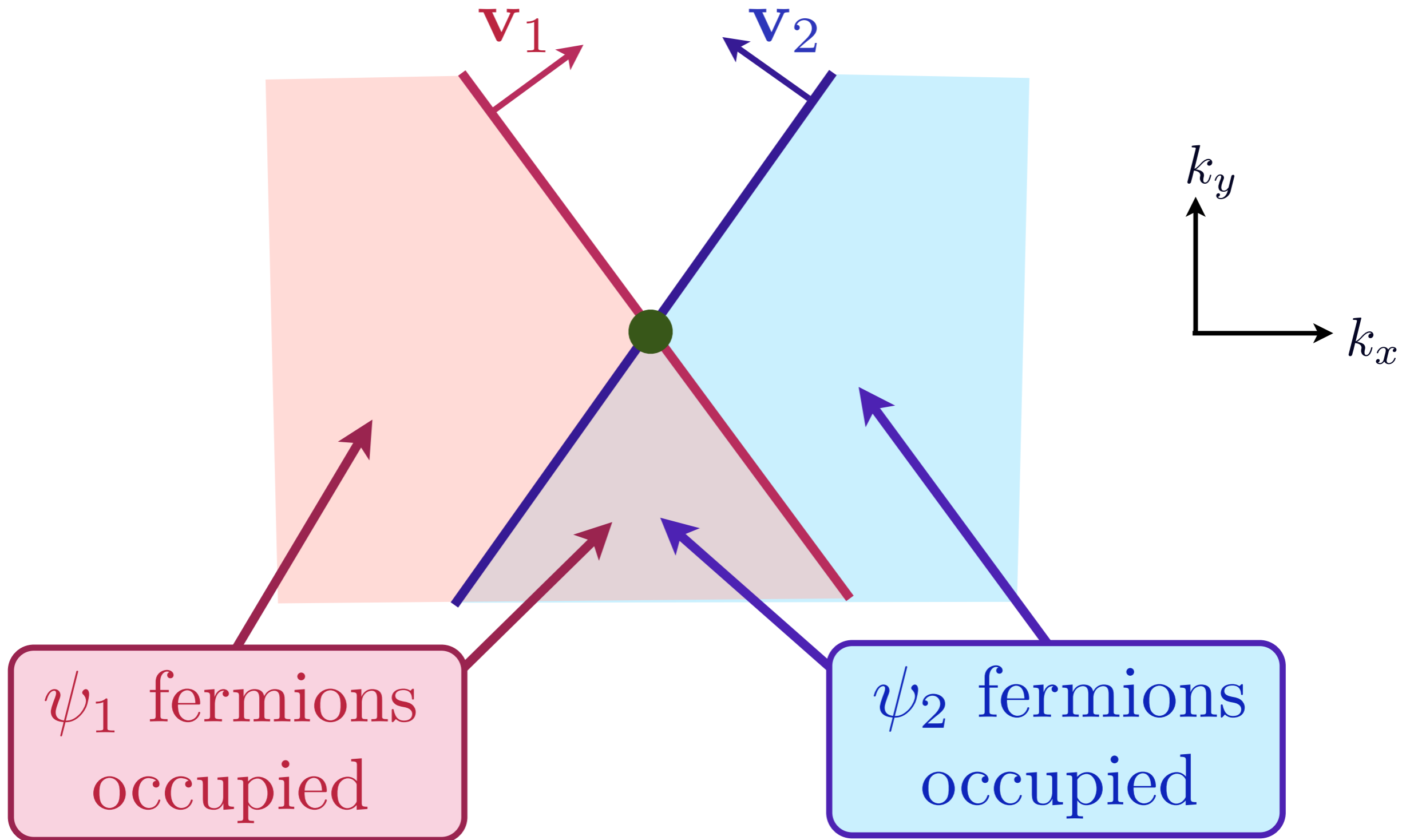


Low energy theory for critical point near hot spots



Low energy theory for critical point near hot spots

Theory has fermions $\psi_{1,2}$ (with Fermi velocities $\mathbf{v}_{1,2}$) and boson order parameter $\vec{\varphi}$, interacting with coupling λ



$$\mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i\mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i\mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha}$$

Order parameter: $\mathcal{L}_\varphi = \frac{1}{2} (\nabla_r \vec{\varphi})^2 + \frac{\tilde{\zeta}}{2} (\partial_\tau \vec{\varphi})^2 + \frac{s}{2} \vec{\varphi}^2 + \frac{u}{4} \vec{\varphi}^4$

“Yukawa” coupling: $\mathcal{L}_c = -\lambda \vec{\varphi} \cdot \left(\psi_{1\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{1\beta} \right)$

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Pairing by SDW fluctuation exchange

We now allow the SDW field $\vec{\varphi}$ to be dynamical, coupling to electrons as

$$H_{\text{sdw}} = - \sum_{\mathbf{k}, \mathbf{q}, \alpha, \beta} \vec{\varphi}_{\mathbf{q}} \cdot c_{\mathbf{k}, \alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{\mathbf{k}+\mathbf{K}+\mathbf{q}, \beta}.$$

Exchange of a $\vec{\varphi}$ quantum leads to the effective interaction

$$H_{ee} = -\frac{1}{2} \sum_{\mathbf{q}} \sum_{\mathbf{p}, \gamma, \delta} \sum_{\mathbf{k}, \alpha, \beta} V_{\alpha\beta, \gamma\delta}(\mathbf{q}) c_{\mathbf{k}, \alpha}^{\dagger} c_{\mathbf{k}+\mathbf{q}, \beta} c_{\mathbf{p}, \gamma}^{\dagger} c_{\mathbf{p}-\mathbf{q}, \delta},$$

where the pairing interaction is

$$V_{\alpha\beta, \gamma\delta}(\mathbf{q}) = \vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta} \frac{\chi_0}{\xi^{-2} + (\mathbf{q} - \mathbf{K})^2},$$

with $\chi_0 \xi^2$ the SDW susceptibility and ξ the SDW correlation length.

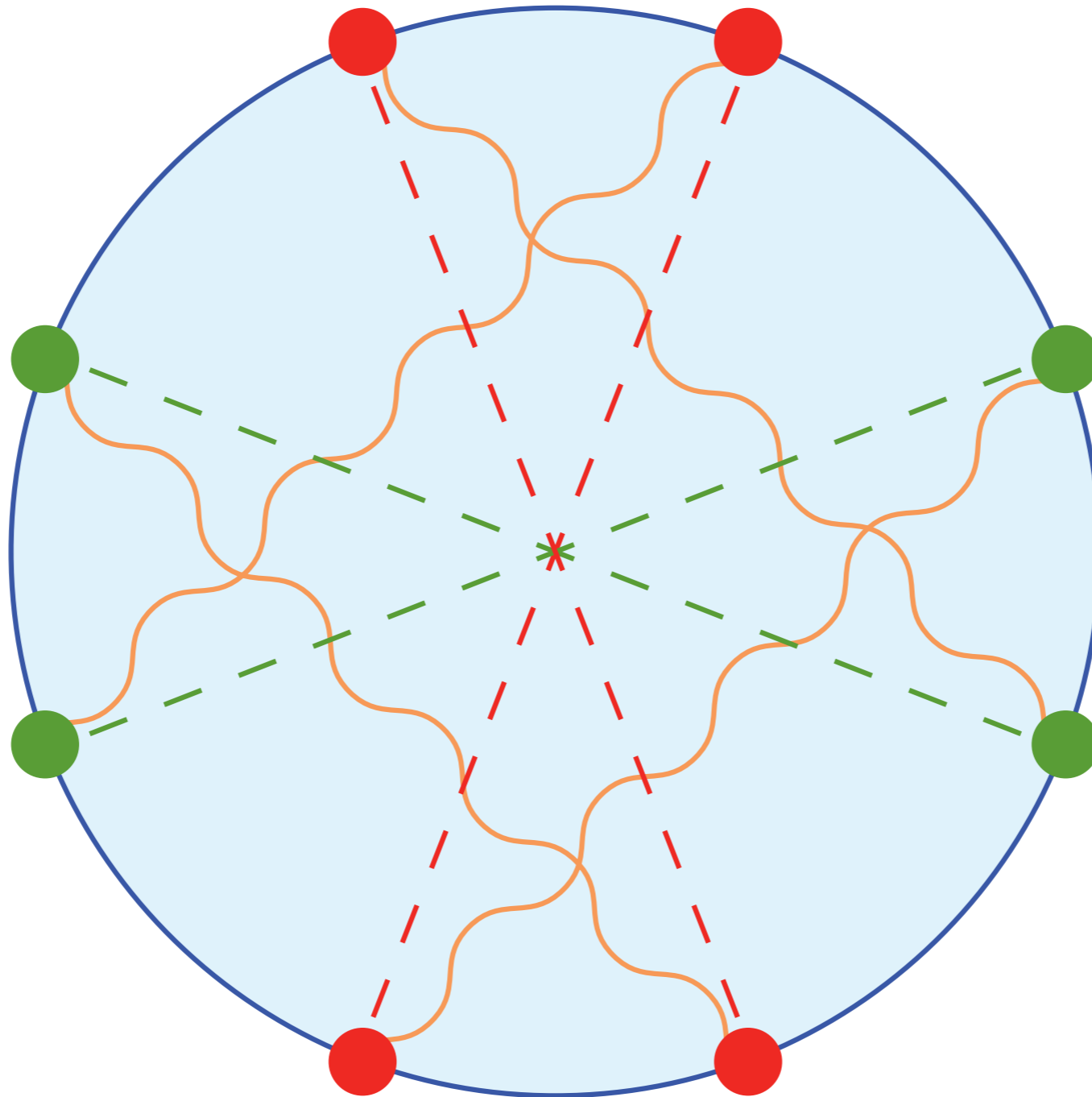
BCS Gap equation

In BCS theory, this interaction leads to the ‘gap equation’ for the pairing gap $\Delta_{\mathbf{k}} \propto \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$.

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{p}} \left(\frac{3\chi_0}{\xi^{-2} + (\mathbf{p} - \mathbf{k} - \mathbf{K})^2} \right) \frac{\Delta_{\mathbf{p}}}{2\sqrt{\varepsilon_{\mathbf{p}}^2 + \Delta_{\mathbf{p}}^2}}$$

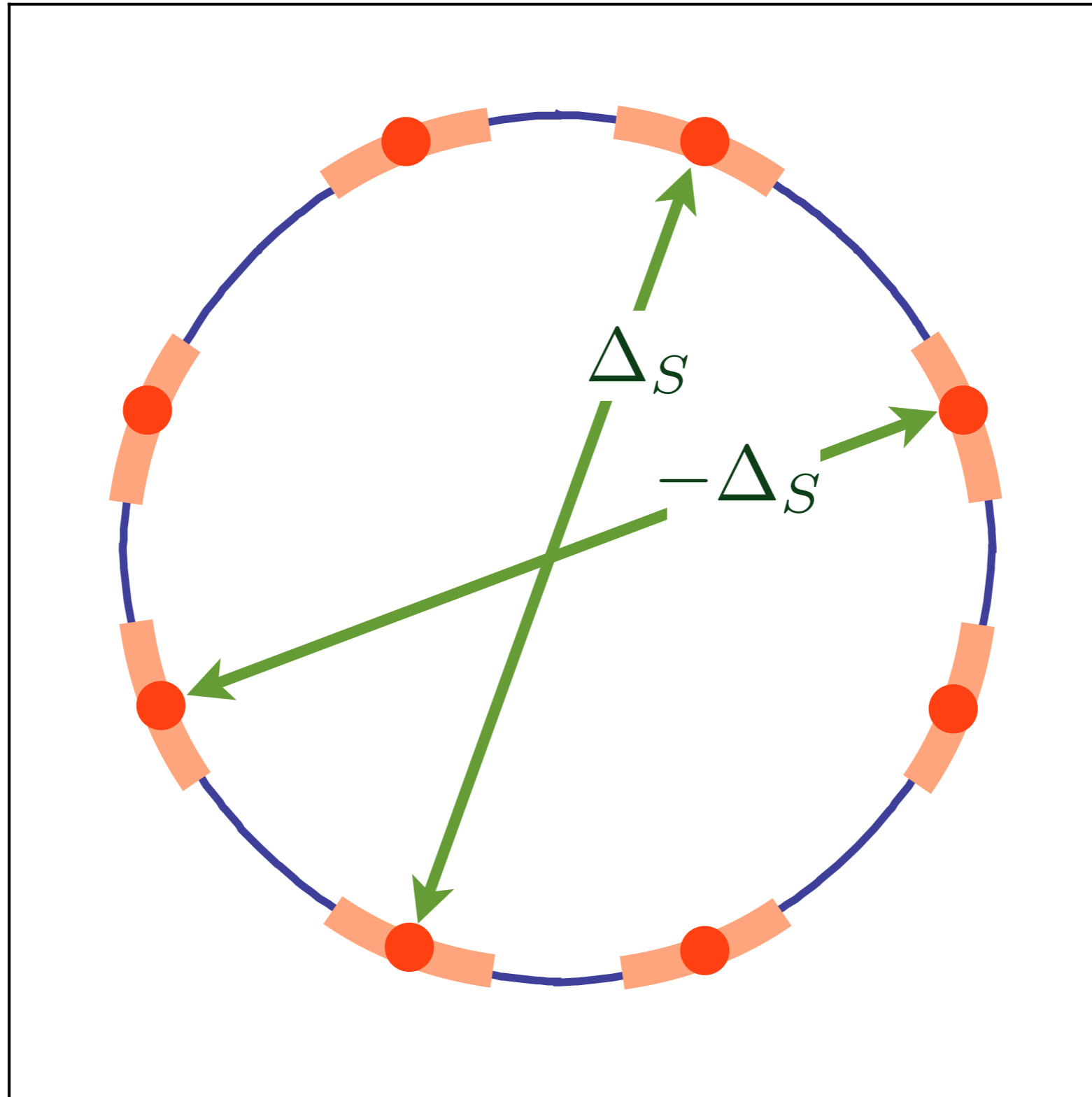
Non-zero solutions of this equation require that $\Delta_{\mathbf{k}}$ and $\Delta_{\mathbf{p}}$ have opposite signs when $\mathbf{p} - \mathbf{k} \approx \mathbf{K}$.

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)

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



Unconventional pairing at and near hot spots

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$$\mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i\mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i\mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha}$$

Order parameter: $\mathcal{L}_\varphi = \frac{1}{2} (\nabla_r \vec{\varphi})^2 + \frac{\tilde{\zeta}}{2} (\partial_\tau \vec{\varphi})^2 + \frac{s}{2} \vec{\varphi}^2 + \frac{u}{4} \vec{\varphi}^4$

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Emergent $[SU(2)]^4$ pseudospin symmetry

$$\mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i\mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i\mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha}$$

Order parameter:
$$\mathcal{L}_\varphi = \frac{1}{2} (\nabla_r \vec{\varphi})^2 + \frac{\tilde{\zeta}}{2} (\partial_\tau \vec{\varphi})^2 + \frac{s}{2} \vec{\varphi}^2 + \frac{u}{4} \vec{\varphi}^4$$

“Yukawa” coupling:
$$\mathcal{L}_c = -\lambda \vec{\varphi} \cdot \left(\psi_{1\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{1\beta} \right)$$

Introduce the spinors

$$\Psi_{1\alpha} = \begin{pmatrix} \psi_{1\alpha} \\ \epsilon_{\alpha\beta} \psi_{1\beta}^\dagger \end{pmatrix}, \quad \Psi_{2\alpha} = \begin{pmatrix} \psi_{2\alpha} \\ \epsilon_{\alpha\beta} \psi_{2\beta}^\dagger \end{pmatrix}$$

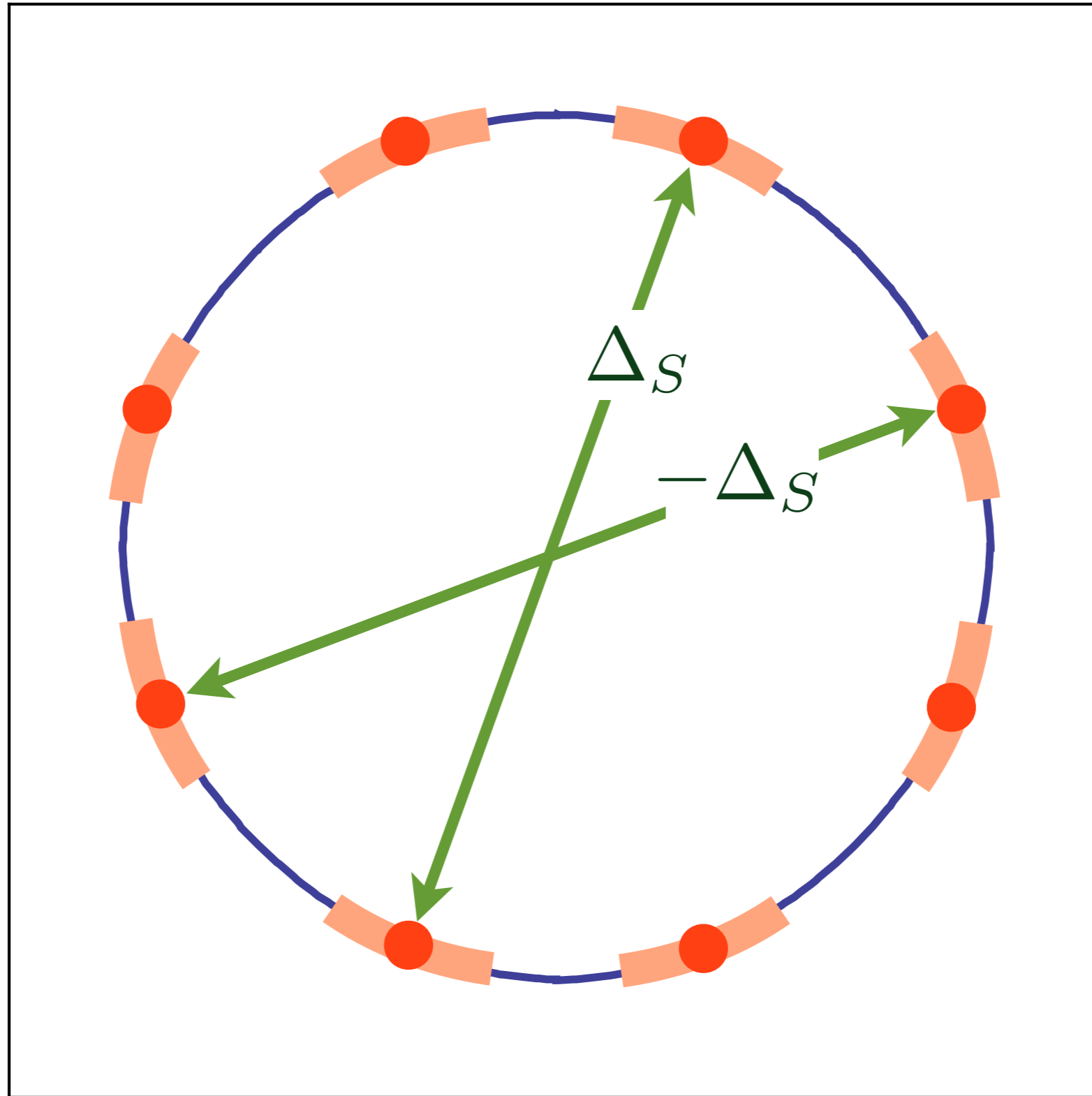
Then the Lagrangian is invariant under the $SU(2)$ transformation U with

$$\Psi_1 \rightarrow U \Psi_1, \quad \Psi_2 \rightarrow U \Psi_2$$

Note that U can be chosen *independently* at the 4 pairs of hotspots.

This symmetry relies on the linearization of the fermion dispersion about the hot spots.

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

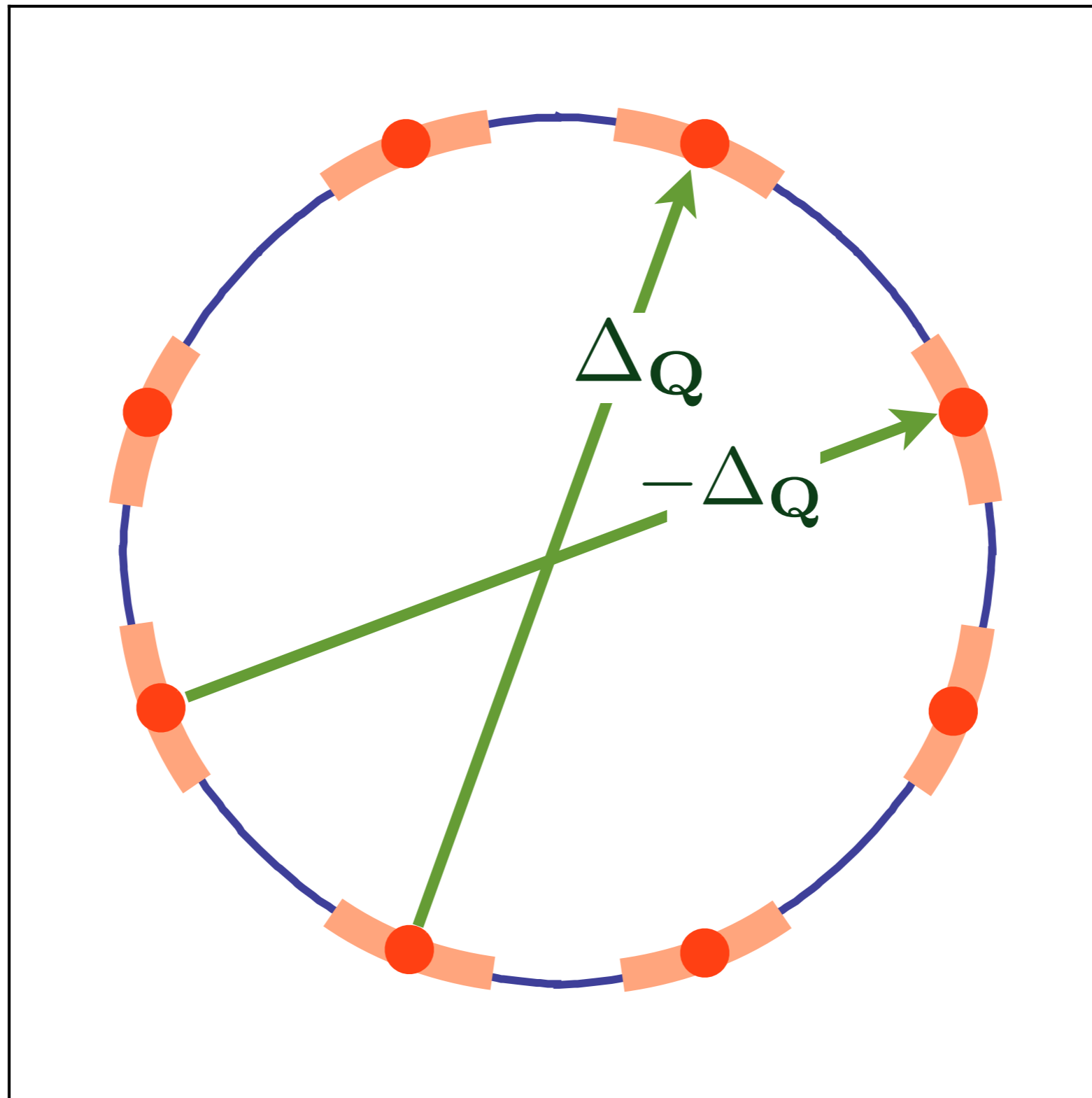


Unconventional pairing at and near hot spots

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

After
pseudospin
rotation

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



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

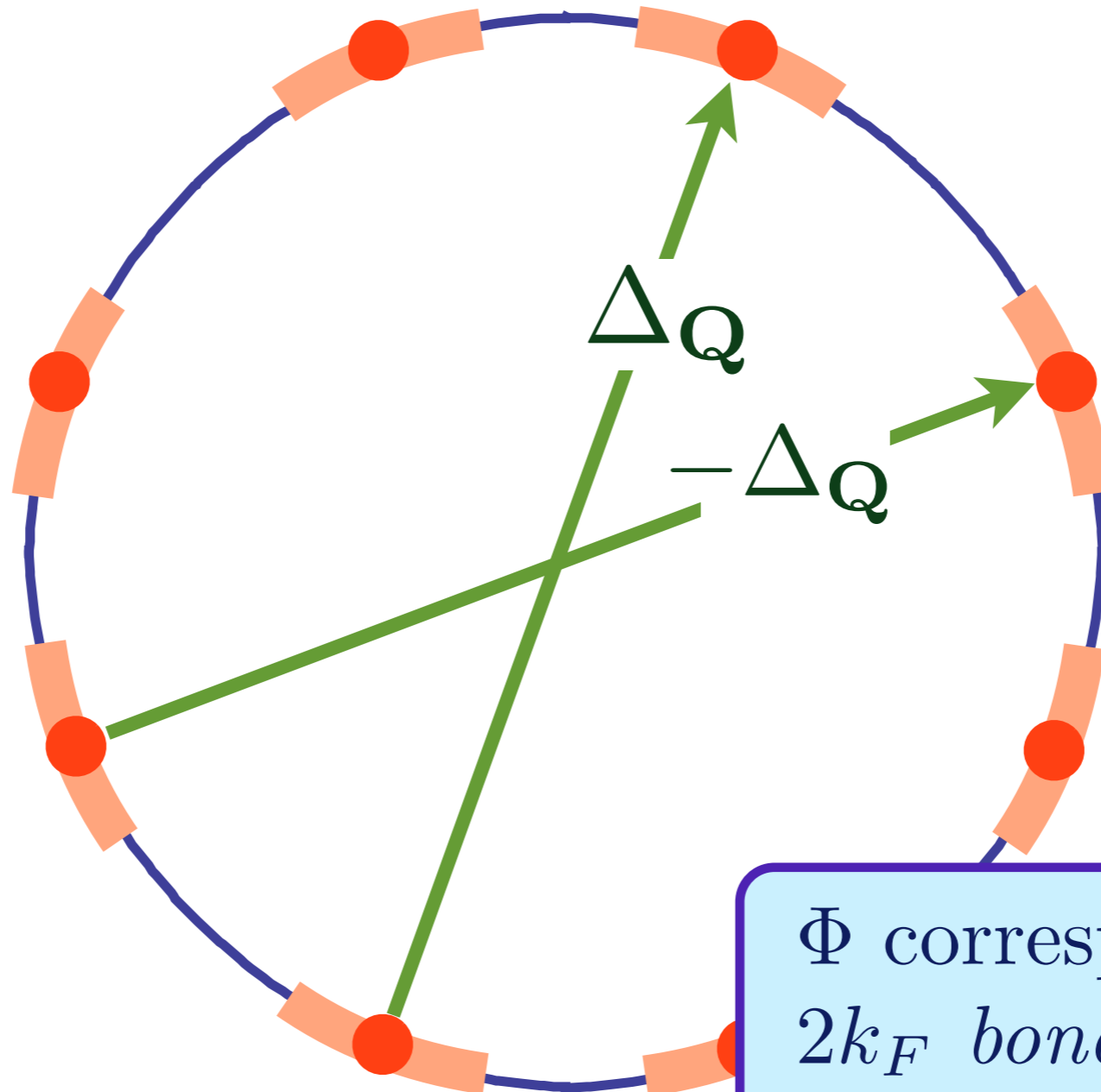
K. B. Efetov, H. Meier,
and C. Pepin,
arXiv:1210.3276

Unconventional particle-hole pairing at and near hot spots

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

After
pseudospin
rotation

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



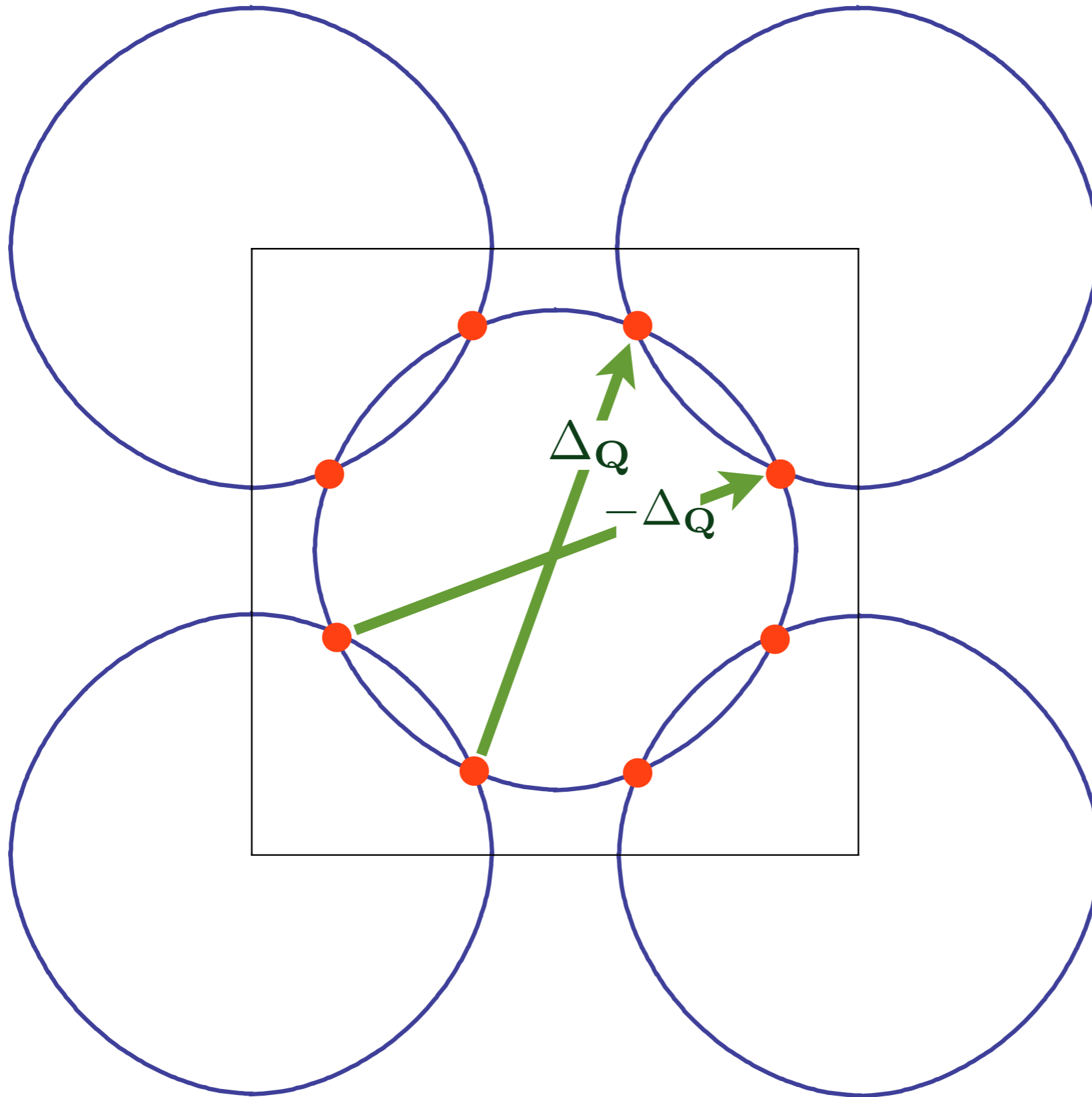
Φ corresponds to a
 $2k_F$ bond-nematic or a
quadrupole density wave

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

K. B. Efetov, H. Meier,
and C. Pepin,
arXiv:1210.3276

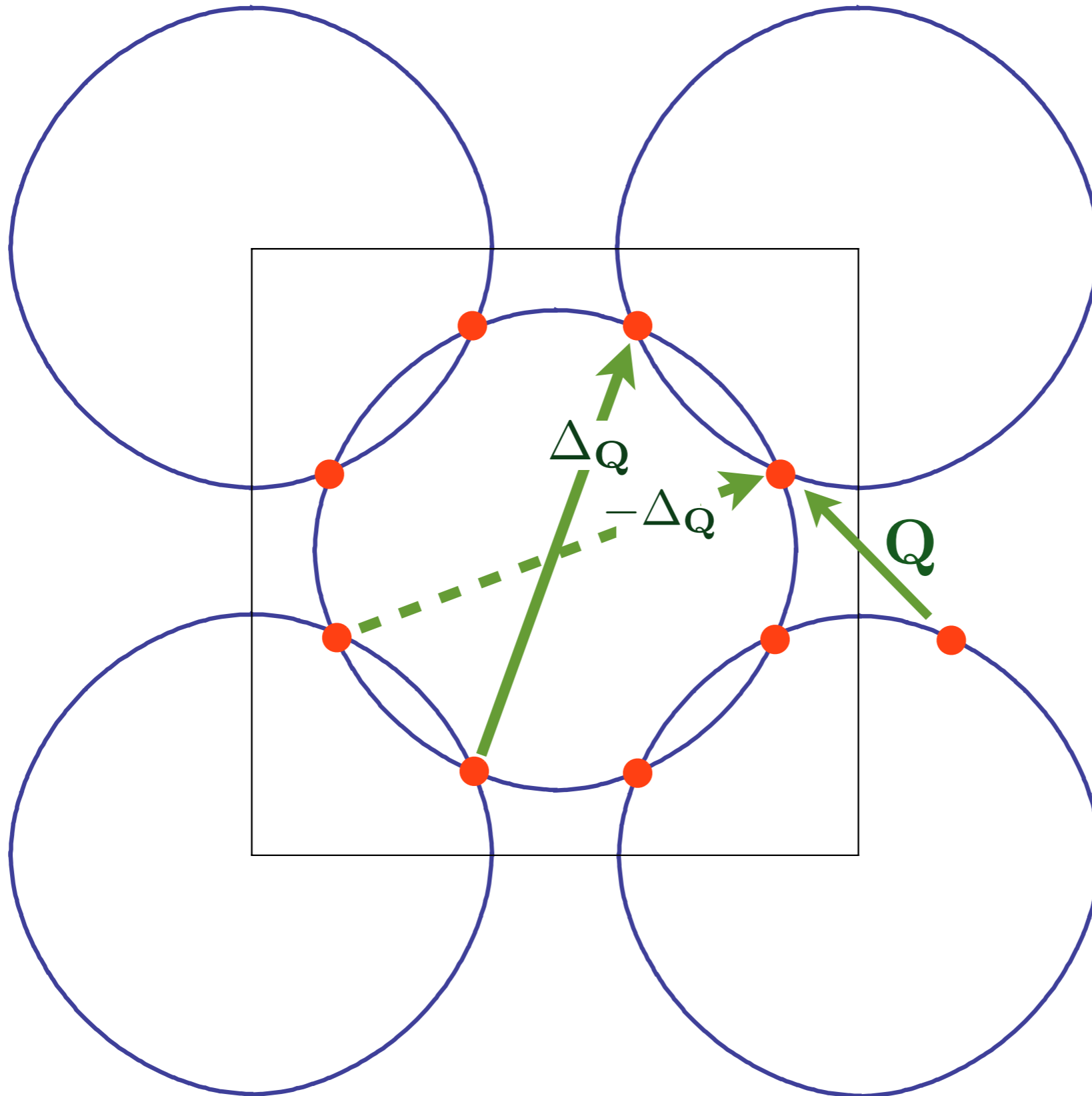
Unconventional particle-hole pairing at and near hot spots

Incommensurate bond order



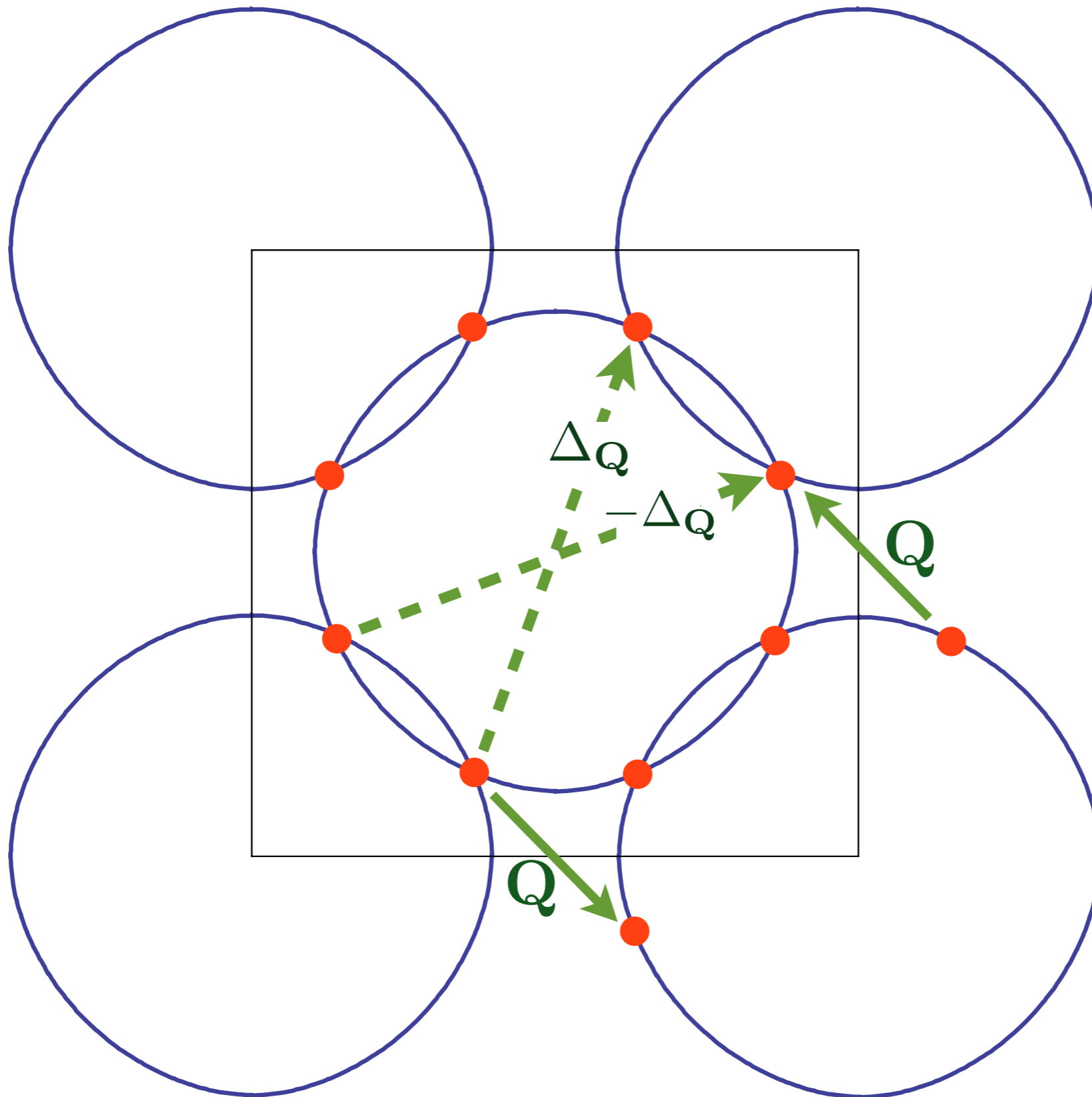
$$\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \rangle = \Delta_Q (\cos k_x - \cos k_y)$$

Incommensurate bond order



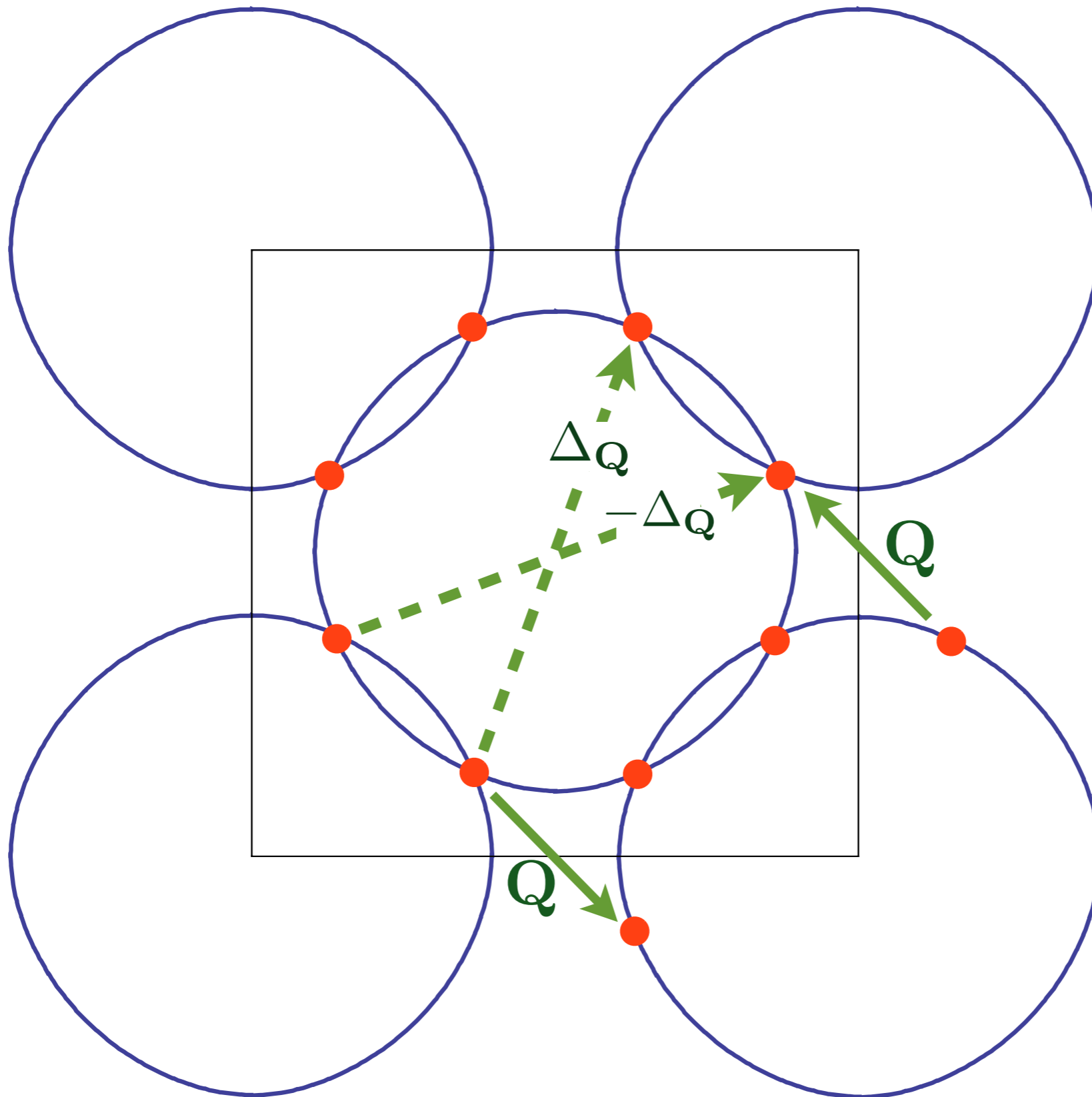
$$\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \rangle = \Delta\mathbf{Q}(\cos k_x - \cos k_y)$$

Incommensurate bond order



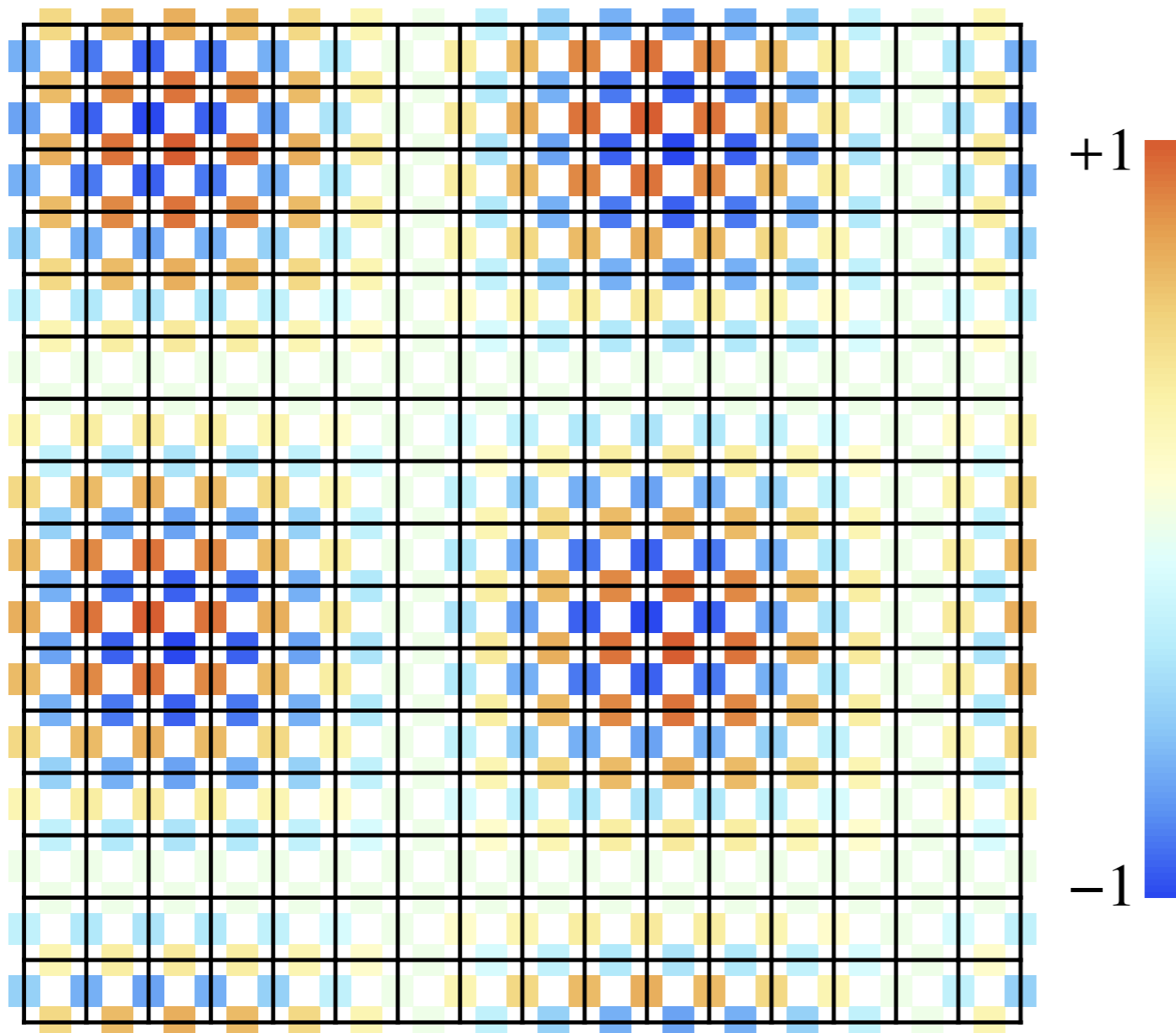
$$\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \rangle = \Delta\mathbf{Q}(\cos k_x - \cos k_y)$$

Incommensurate bond order



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

Incommensurate bond order



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

No modulations on sites, $\langle c_{\mathbf{r}\alpha}^\dagger c_{\mathbf{s}\alpha} \rangle$ is modulated
only for $\mathbf{r} \neq \mathbf{s}$.

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

Hartree-Fock computation on lattice model

$$H = \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) c_{\mathbf{k},\alpha}^\dagger c_{\mathbf{k},\alpha} - \frac{1}{2V} \sum_{\mathbf{q}} \chi(\mathbf{q}) \vec{S}(-\mathbf{q}) \cdot \vec{S}(\mathbf{q}).$$

$$\vec{S}(\mathbf{q}) = \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q},\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{\mathbf{k},\beta}$$

Hartree-Fock computation on lattice model

$$H = \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) c_{\mathbf{k},\alpha}^\dagger c_{\mathbf{k},\alpha} - \frac{1}{2V} \sum_{\mathbf{q}} \chi(\mathbf{q}) \vec{S}(-\mathbf{q}) \cdot \vec{S}(\mathbf{q}).$$

$$\vec{S}(\mathbf{q}) = \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q},\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{\mathbf{k},\beta}$$

$$H_{MF} = \sum_{\mathbf{k}} \left[\varepsilon(\mathbf{k}) c_{\mathbf{k},\alpha}^\dagger c_{\mathbf{k},\alpha} + \Delta_S(\mathbf{k}) \epsilon_{\alpha\beta} c_{\mathbf{k},\alpha} c_{-\mathbf{k}\beta} + \text{H.c.} \right. \\ \left. + \sum_{\mathbf{Q}} \Delta_{\mathbf{Q}}(\mathbf{k}) c_{\mathbf{k}+\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}-\mathbf{Q}/2,\alpha} \right],$$

$$F \leq F_{MF} + \langle H - H_{MF} \rangle_{MF}$$

Hartree-Fock computation on lattice model

$$F = 2 \sum_{\mathbf{k}, \mathbf{k}'} \Delta_S^*(\mathbf{k}) \sqrt{\Pi_S(\mathbf{k})} \mathcal{M}_S(\mathbf{k}, \mathbf{k}') \sqrt{\Pi_S(\mathbf{k}')} \Delta_S(\mathbf{k}') \\ + \sum_{\mathbf{k}, \mathbf{k}', \mathbf{Q}} \Delta_Q^*(\mathbf{k}) \sqrt{\Pi_Q(\mathbf{k})} \mathcal{M}_Q(\mathbf{k}, \mathbf{k}') \sqrt{\Pi_Q(\mathbf{k}')} \Delta_Q(\mathbf{k}') +$$

$$\mathcal{M}_S(\mathbf{k}, \mathbf{k}') = \delta_{\mathbf{k}, \mathbf{k}'} + \frac{3}{V} \chi(\mathbf{k} - \mathbf{k}') \sqrt{\Pi_S(\mathbf{k}) \Pi_S(\mathbf{k}')}$$

$$\mathcal{M}_Q(\mathbf{k}, \mathbf{k}') = \delta_{\mathbf{k}, \mathbf{k}'} + \frac{3}{V} \chi(\mathbf{k} - \mathbf{k}') \sqrt{\Pi_Q(\mathbf{k}') \Pi_Q(\mathbf{k})}$$

$$\Pi_S(\mathbf{k}) = \frac{1 - 2f(\varepsilon(\mathbf{k}))}{2\varepsilon(\mathbf{k})}$$

$$\Pi_Q(\mathbf{k}) = \frac{f(\varepsilon(\mathbf{k} + \mathbf{Q}/2)) - f(\varepsilon(\mathbf{k} - \mathbf{Q}/2))}{\varepsilon(\mathbf{k} - \mathbf{Q}/2) - \varepsilon(\mathbf{k} + \mathbf{Q}/2)}$$

Hartree-Fock computation on lattice model

$$F = 2 \sum_{\mathbf{k}, \mathbf{k}'} \Delta_S^*(\mathbf{k}) \sqrt{\Pi_S(\mathbf{k})} \mathcal{M}_S(\mathbf{k}, \mathbf{k}') \sqrt{\Pi_S(\mathbf{k}')} \Delta_S(\mathbf{k}') \\ + \sum_{\mathbf{k}, \mathbf{k}', \mathbf{Q}} \Delta_Q^*(\mathbf{k}) \sqrt{\Pi_Q(\mathbf{k})} \mathcal{M}_Q(\mathbf{k}, \mathbf{k}') \sqrt{\Pi_Q(\mathbf{k}')} \Delta_Q(\mathbf{k}') +$$

$$\mathcal{M}_S(\mathbf{k}, \mathbf{k}') = \delta_{\mathbf{k}, \mathbf{k}'} + \frac{3}{V} \chi(\mathbf{k} - \mathbf{k}') \sqrt{\Pi_S(\mathbf{k}) \Pi_S(\mathbf{k}')}$$

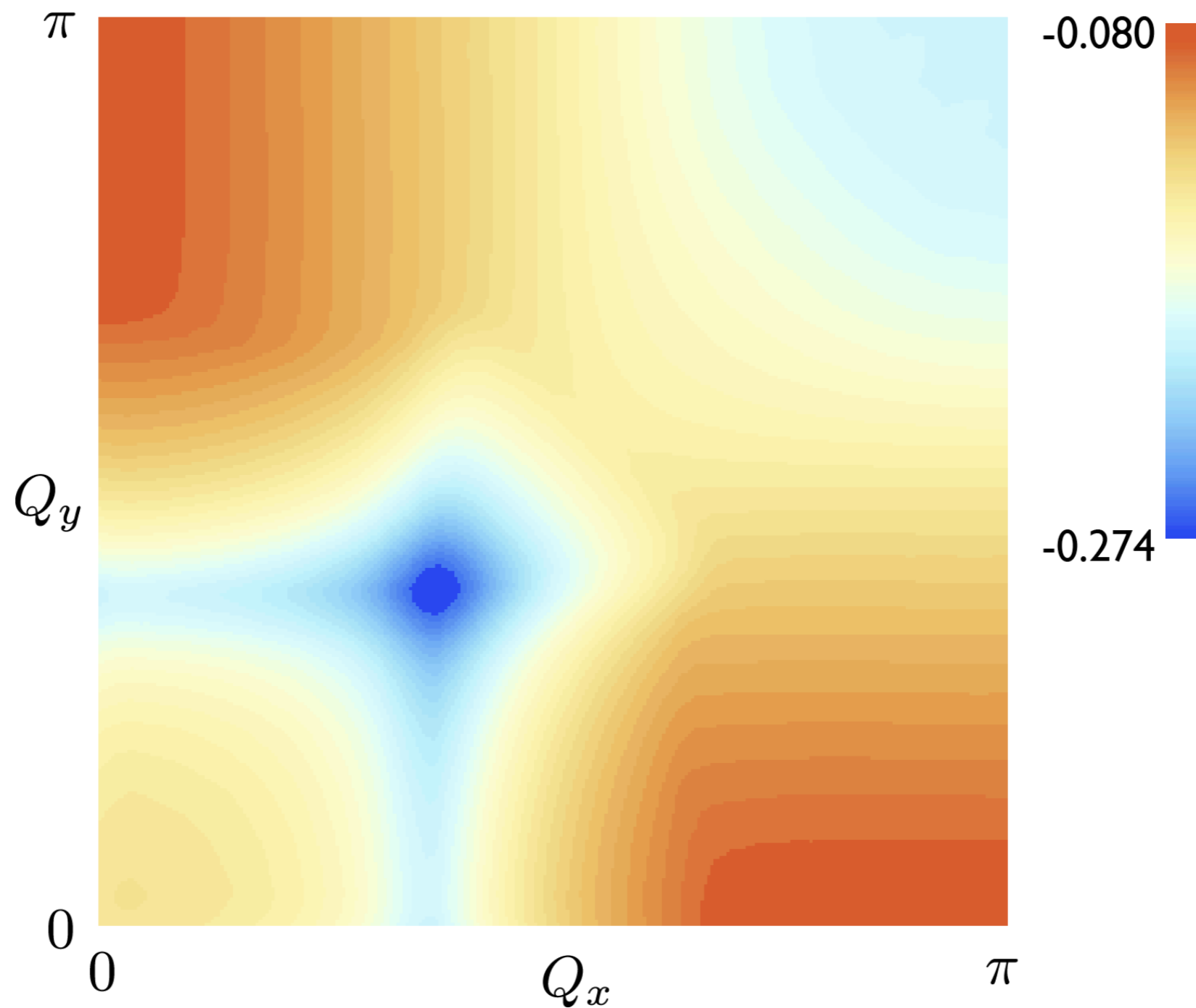
$$\mathcal{M}_Q(\mathbf{k}, \mathbf{k}') = \delta_{\mathbf{k}, \mathbf{k}'} + \frac{3}{V} \chi(\mathbf{k} - \mathbf{k}') \sqrt{\Pi_Q(\mathbf{k}') \Pi_Q(\mathbf{k})}$$

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$$\frac{3}{V} \sum_{\mathbf{k}'} \sqrt{\Pi_{S,Q}(\mathbf{k})} \chi(\mathbf{k} - \mathbf{k}') \sqrt{\Pi_{S,Q}(\mathbf{k}')} \phi_{S,Q}(\mathbf{k}') = \lambda_{S,Q} \phi_{S,Q}(\mathbf{k})$$

Hartree-Fock computation on lattice model



Charge-ordering eigenvalue

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

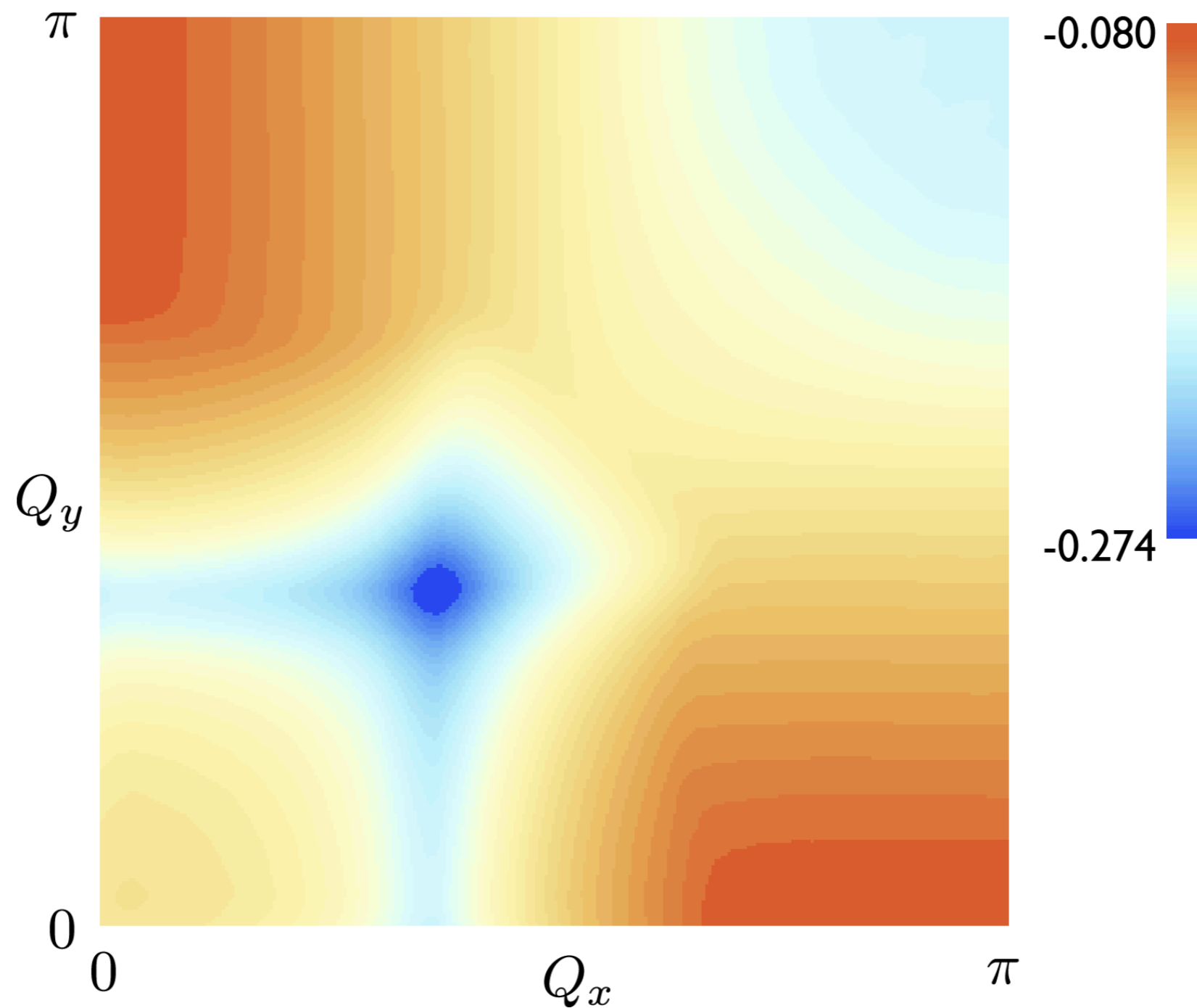
Hartree-Fock computation on lattice model

$$\Delta_Q(\mathbf{k}) = \sum_{\gamma} c_{Q,\gamma} \psi_{\gamma}(\mathbf{k})$$

γ	$\psi_{\gamma}(\mathbf{k})$	$Q =$ (1.15,1.15)	$Q =$ (1.15, 0)	$Q =$ (0,0)	$Q =$ (π, π)	$\Delta_S(\mathbf{k})$
s	1	0	-0.231	0	0	0
s'	$\cos k_x + \cos k_y$	0	0.044	0	0	0
s''	$\cos(2k_x) + \cos(2k_y)$	0	-0.046	0	0	0
d	$\cos k_x - \cos k_y$	0.993	0.963	0.997	0	0.997
d'	$\cos(2k_x) - \cos(2k_y)$	-0.069	-0.067	-0.057	0	-0.056
d''	$2 \sin k_x \sin k_y$	0	0	0	0	0
p_x	$\sqrt{2} \sin k_x$	0	0	0	0.706	0
p_y	$\sqrt{2} \sin k_y$	0	0	0	-0.706	0
g	$(\cos k_x - \cos k_y)$ $\times \sqrt{8} \sin k_x \sin k_y$	-0.009	0	0	0	0

Charge-ordering eigenvector

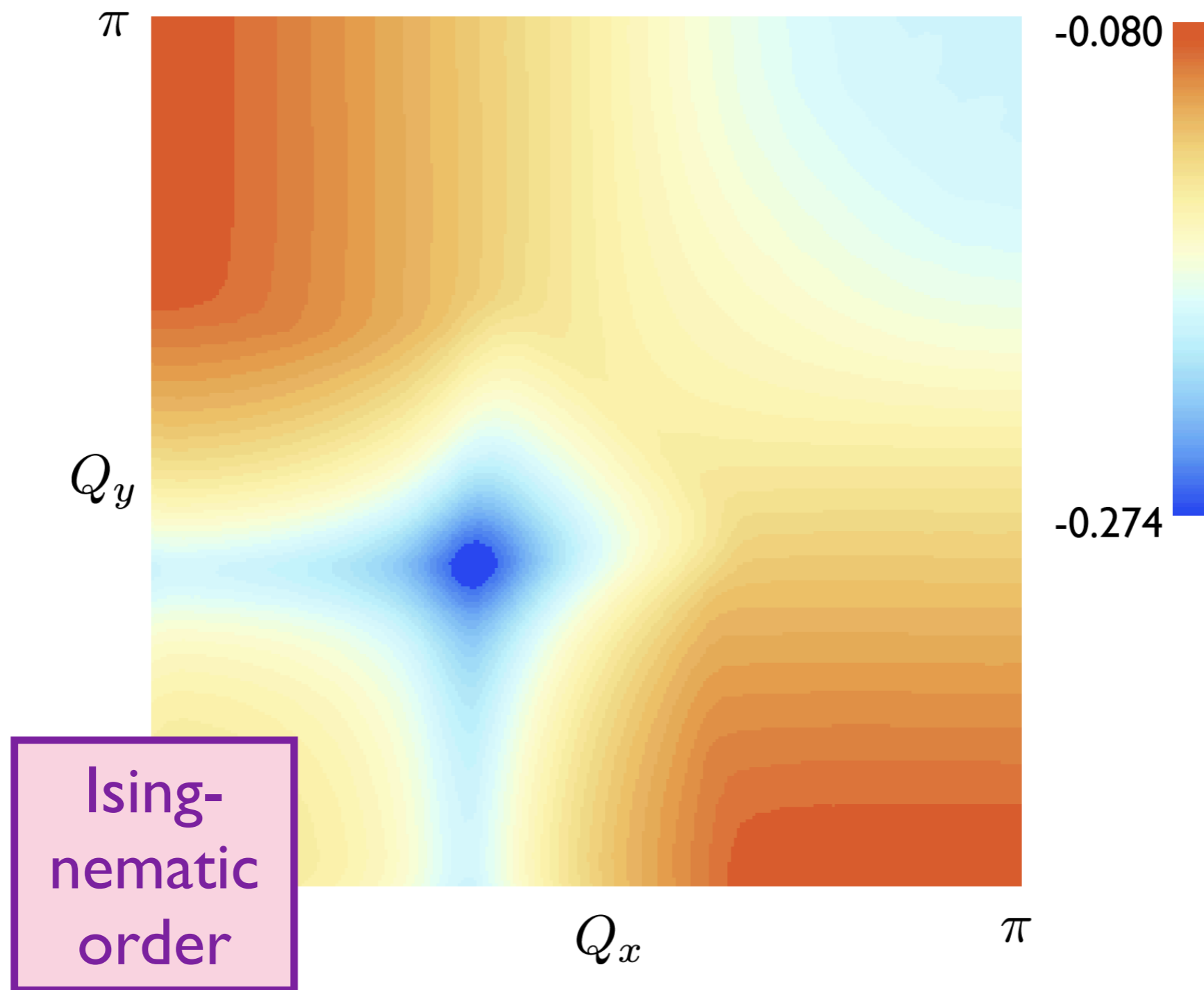
Hartree-Fock computation on lattice model



Charge-ordering eigenvalue

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

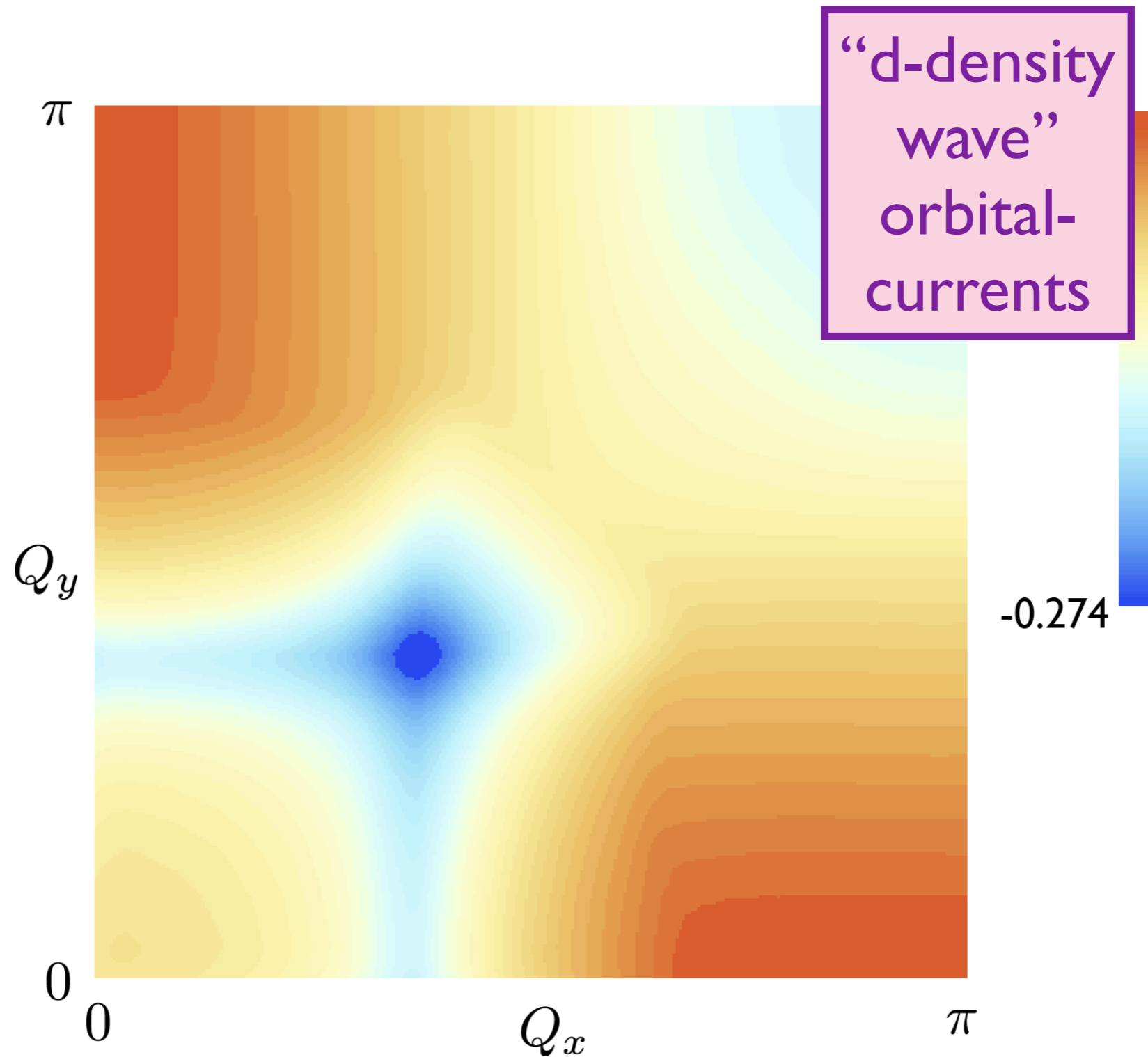
Hartree-Fock computation on lattice model



Charge-ordering eigenvalue

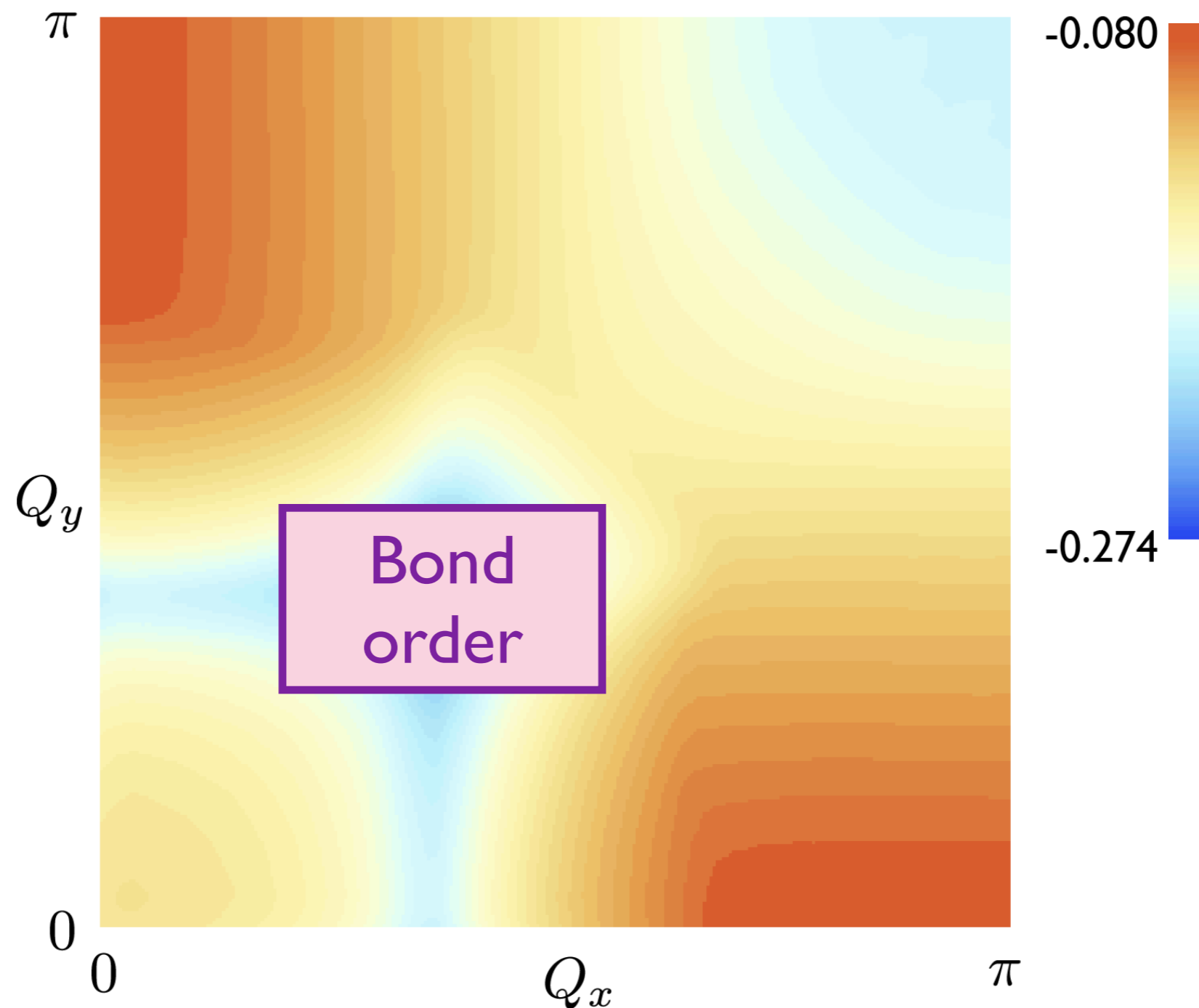
S. Sachdev and R. La Placa, arXiv:1303.2114

Hartree-Fock computation on lattice model



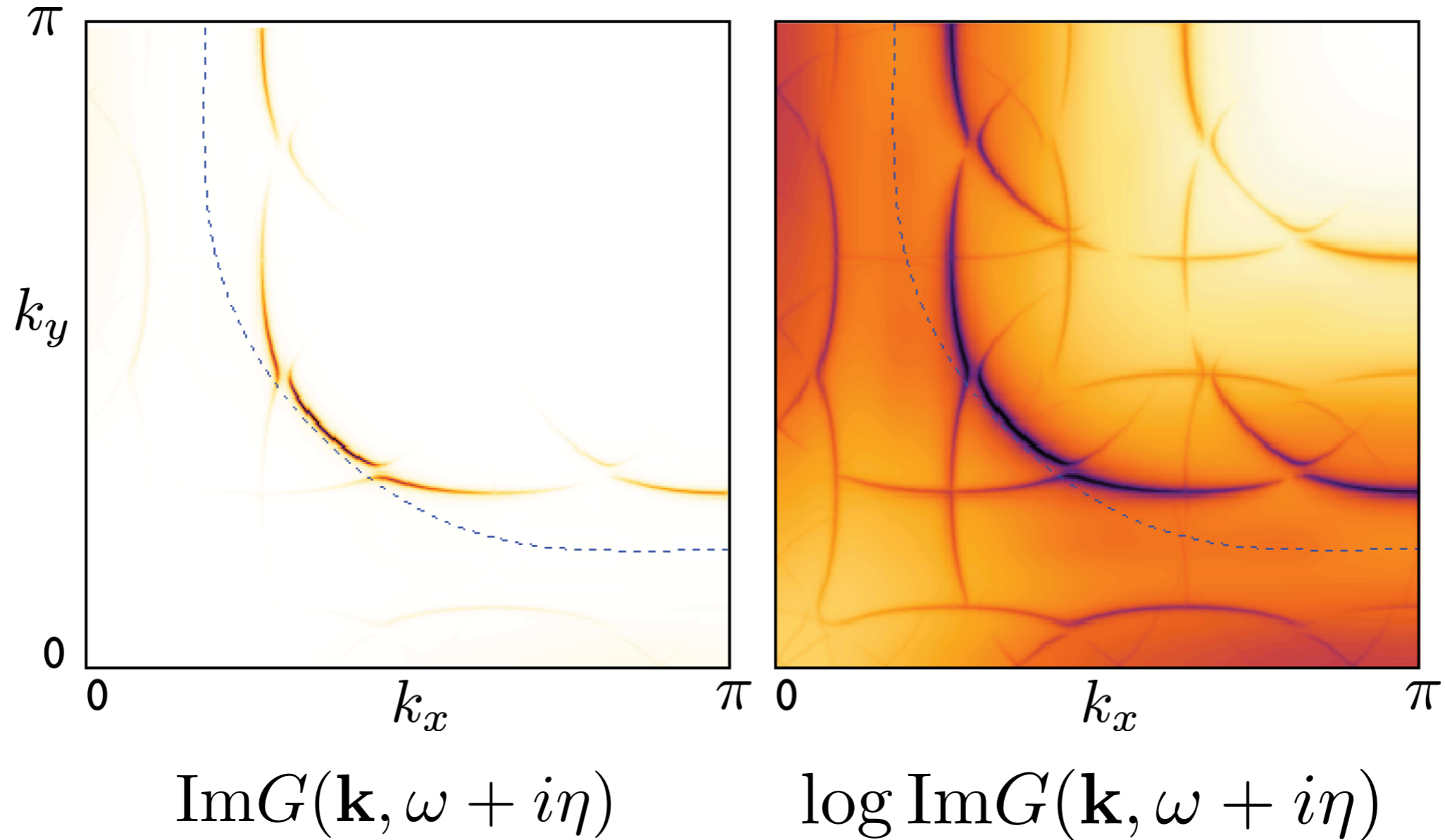
Charge-ordering eigenvalue

Hartree-Fock computation on lattice model



Charge-ordering eigenvalue

Hartree-Fock computation on lattice model



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

$$\text{with } \Delta_s/\Delta_d = -0.234.$$

Outline

1. Antiferromagnetism in metals:
low energy theory
2. d-wave superconductivity
3. Emergent pseudospin symmetry,
and bond order
4. Quantum Monte Carlo
without the sign problem

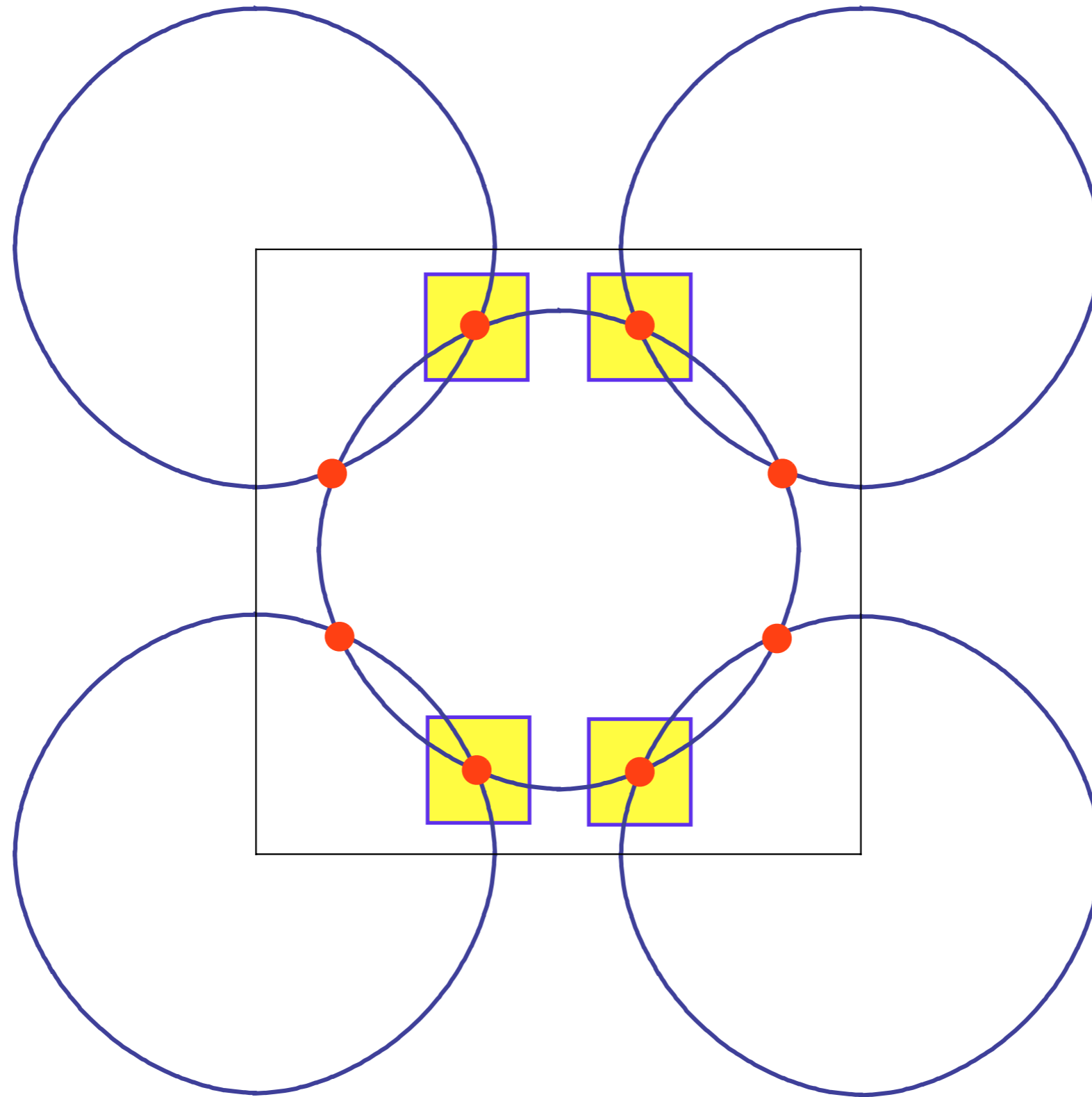
Outline

1. Antiferromagnetism in metals:
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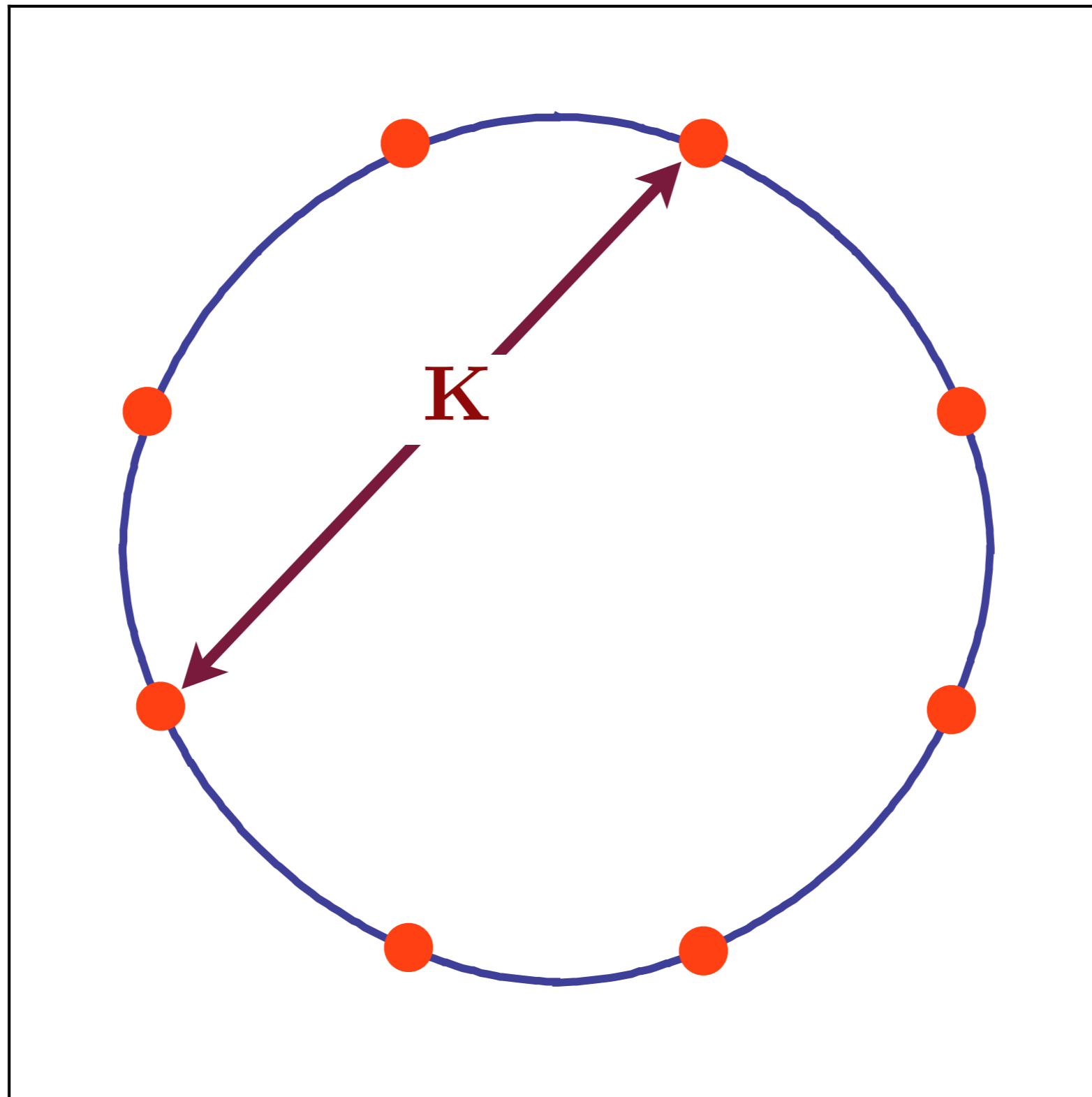
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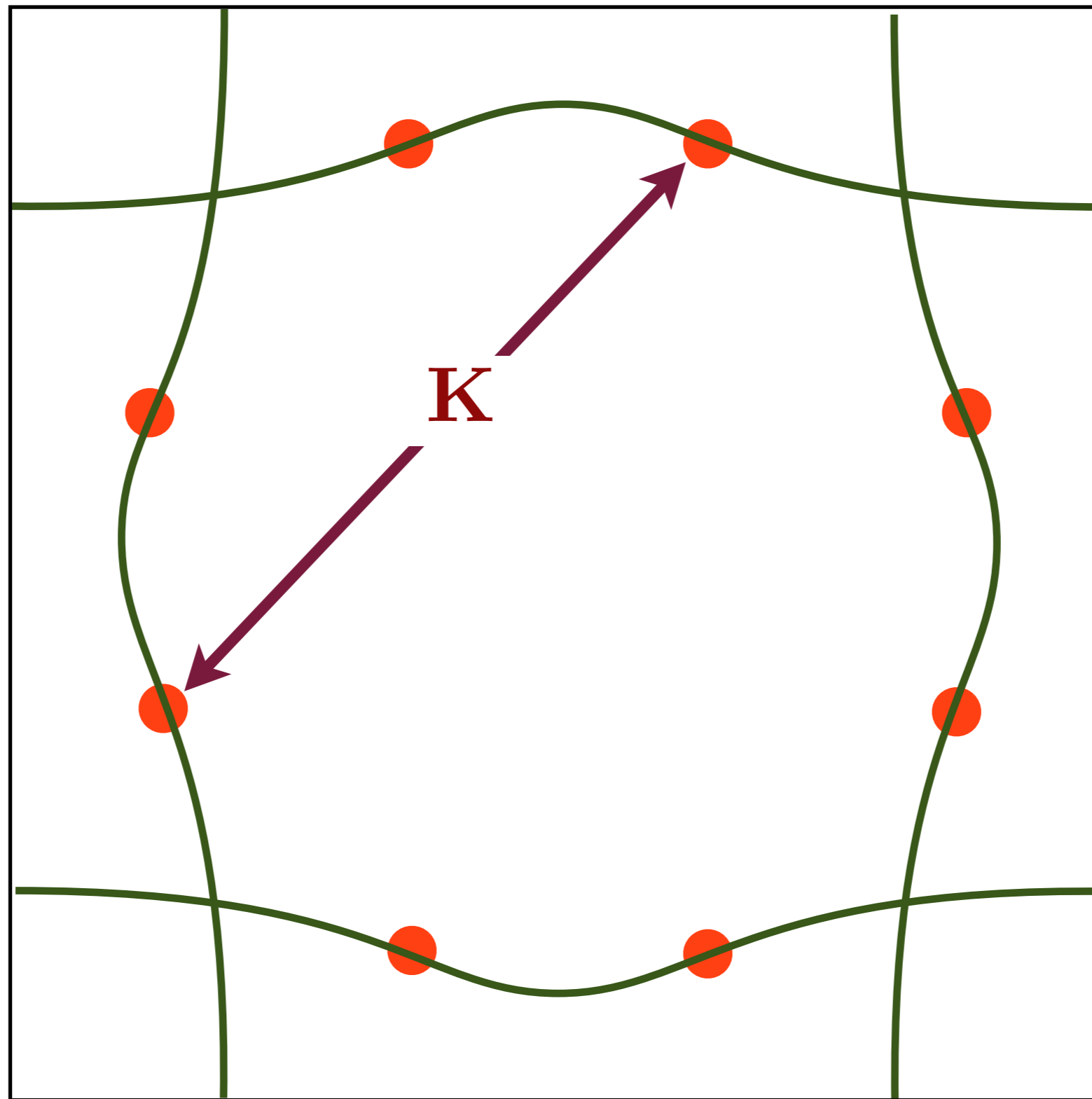
Low energy theory for critical point near hot spots

QMC for the onset of antiferromagnetism



Hot spots in a single band model

QMC for the onset of antiferromagnetism

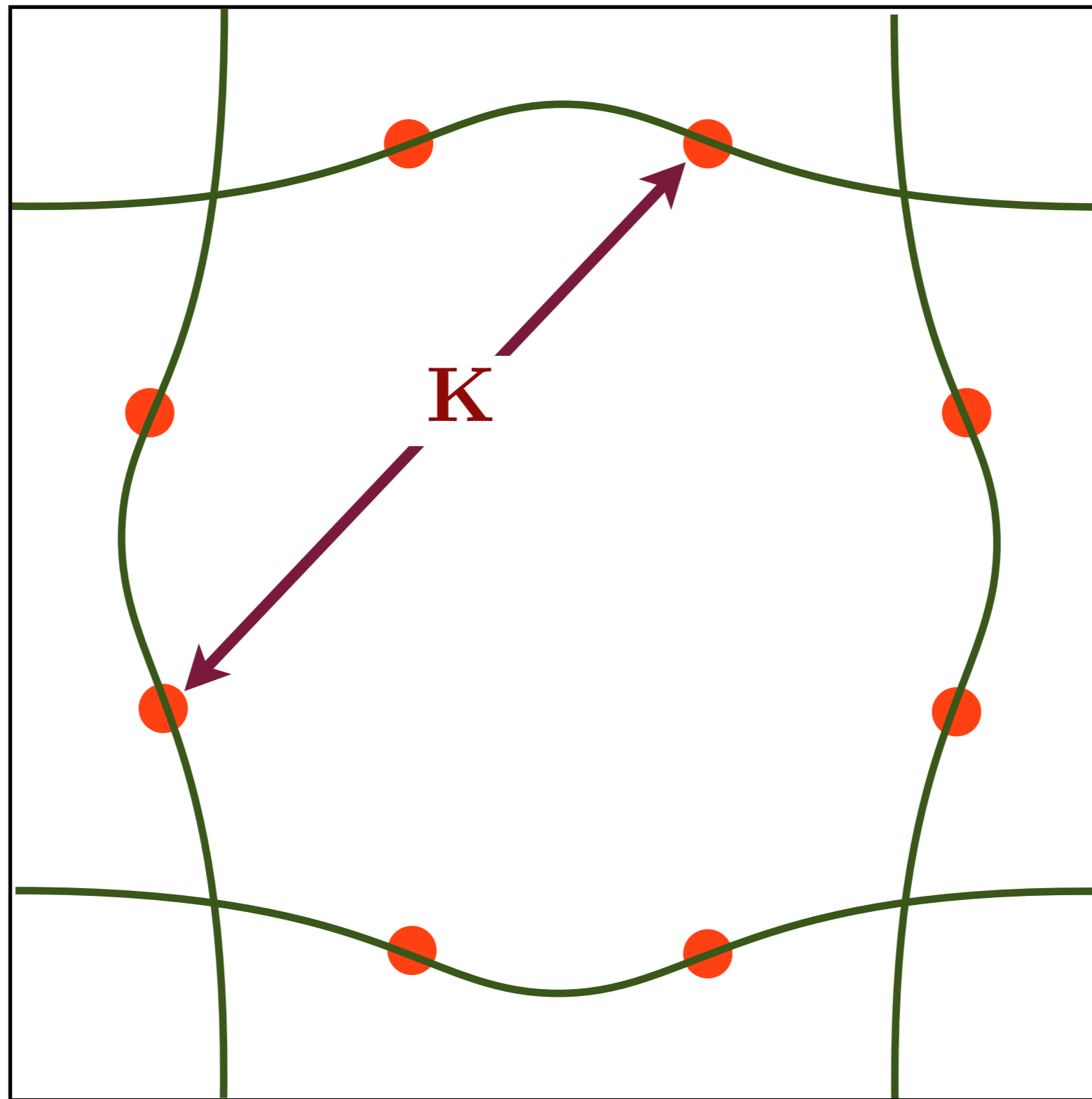


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Science **338**, 1606
(2012).

Hot spots in a two band model

QMC for the onset of antiferromagnetism

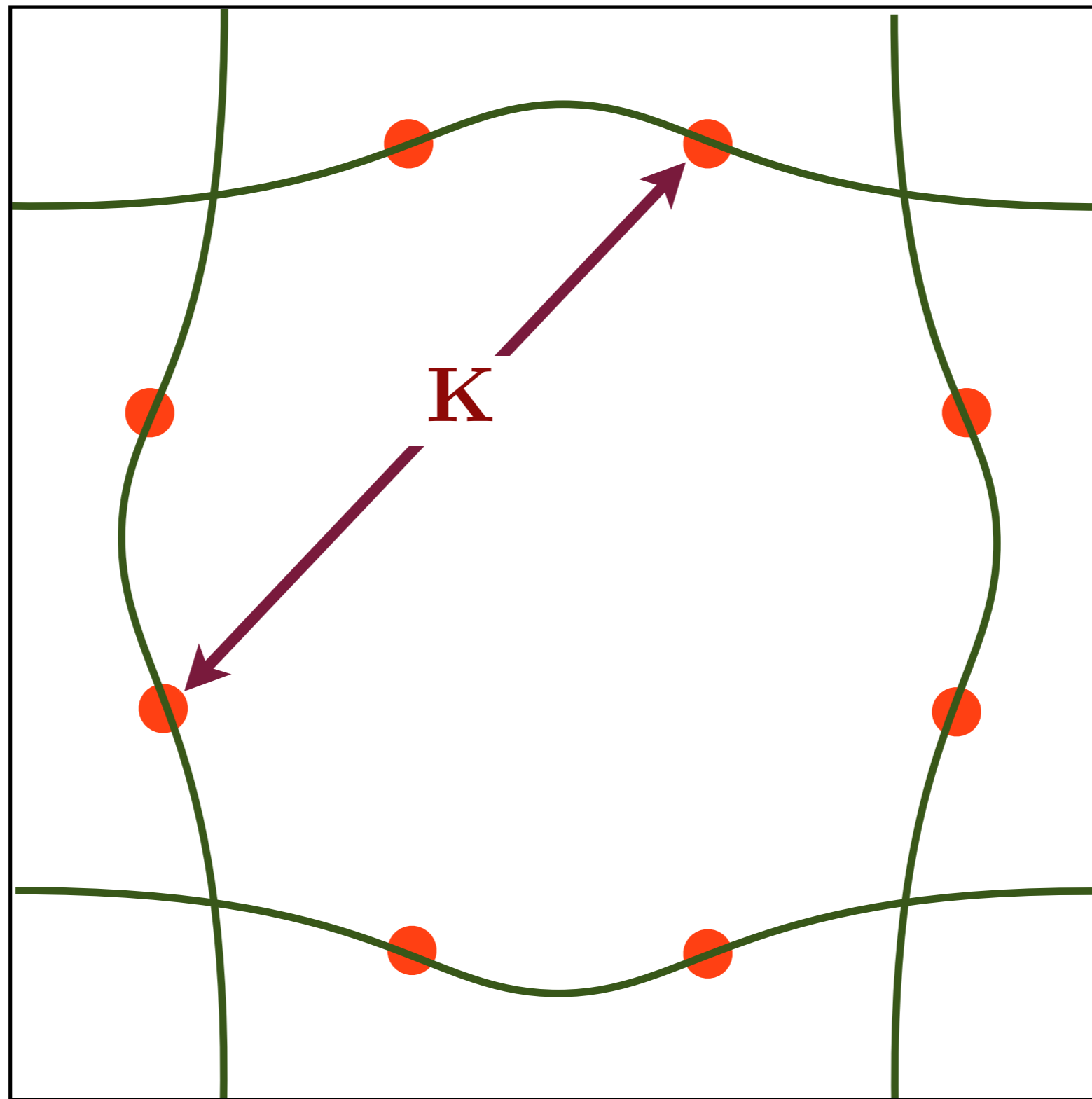
Faithful realization of the *generic* universal low energy theory for the onset of antiferromagnetism.



Hot spots in a two band model

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QMC for the onset of antiferromagnetism

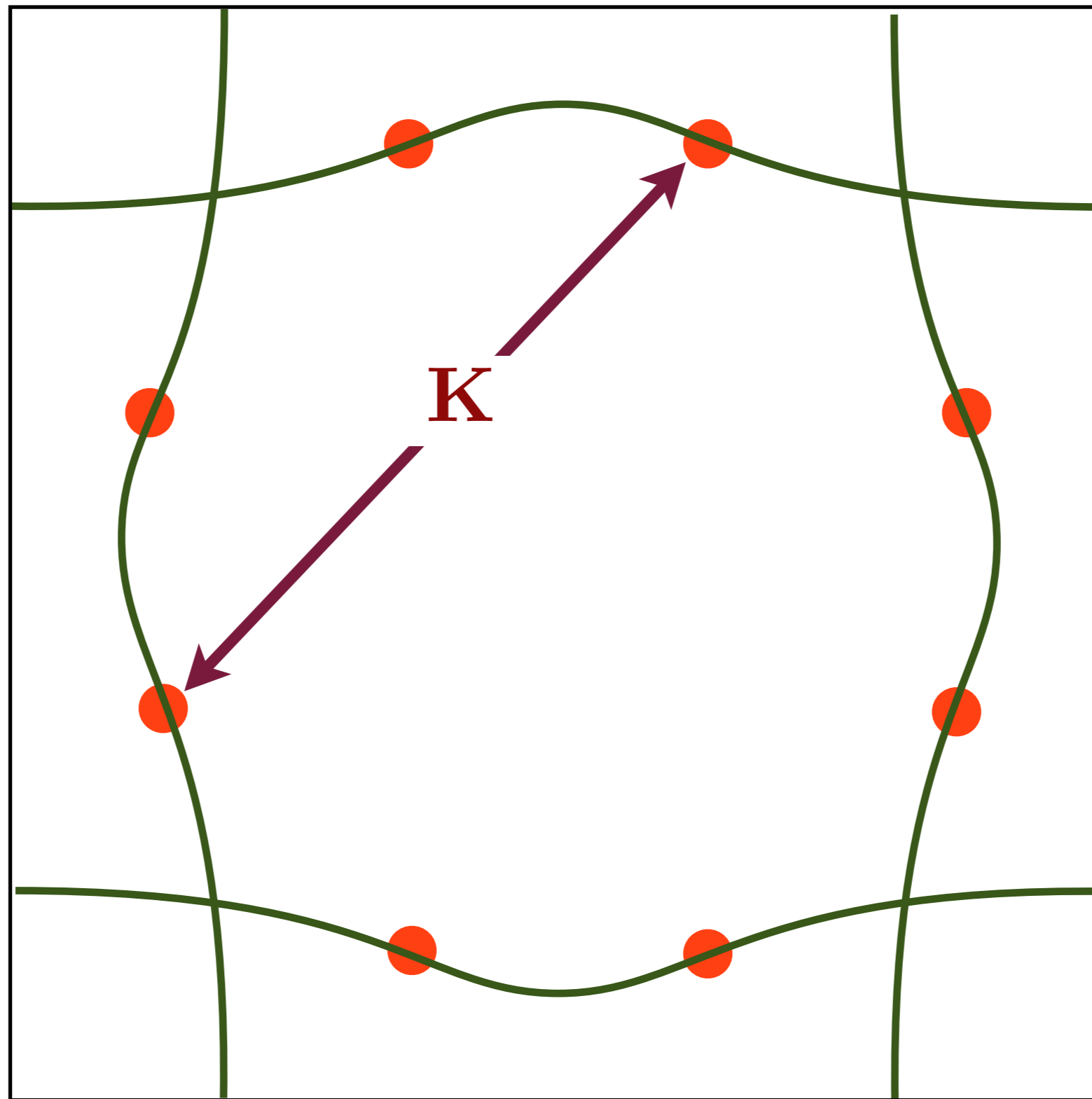


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Hot spots in a two band model

QMC for the onset of antiferromagnetism

Sign problem is absent as long as K connects hotspots in distinct bands

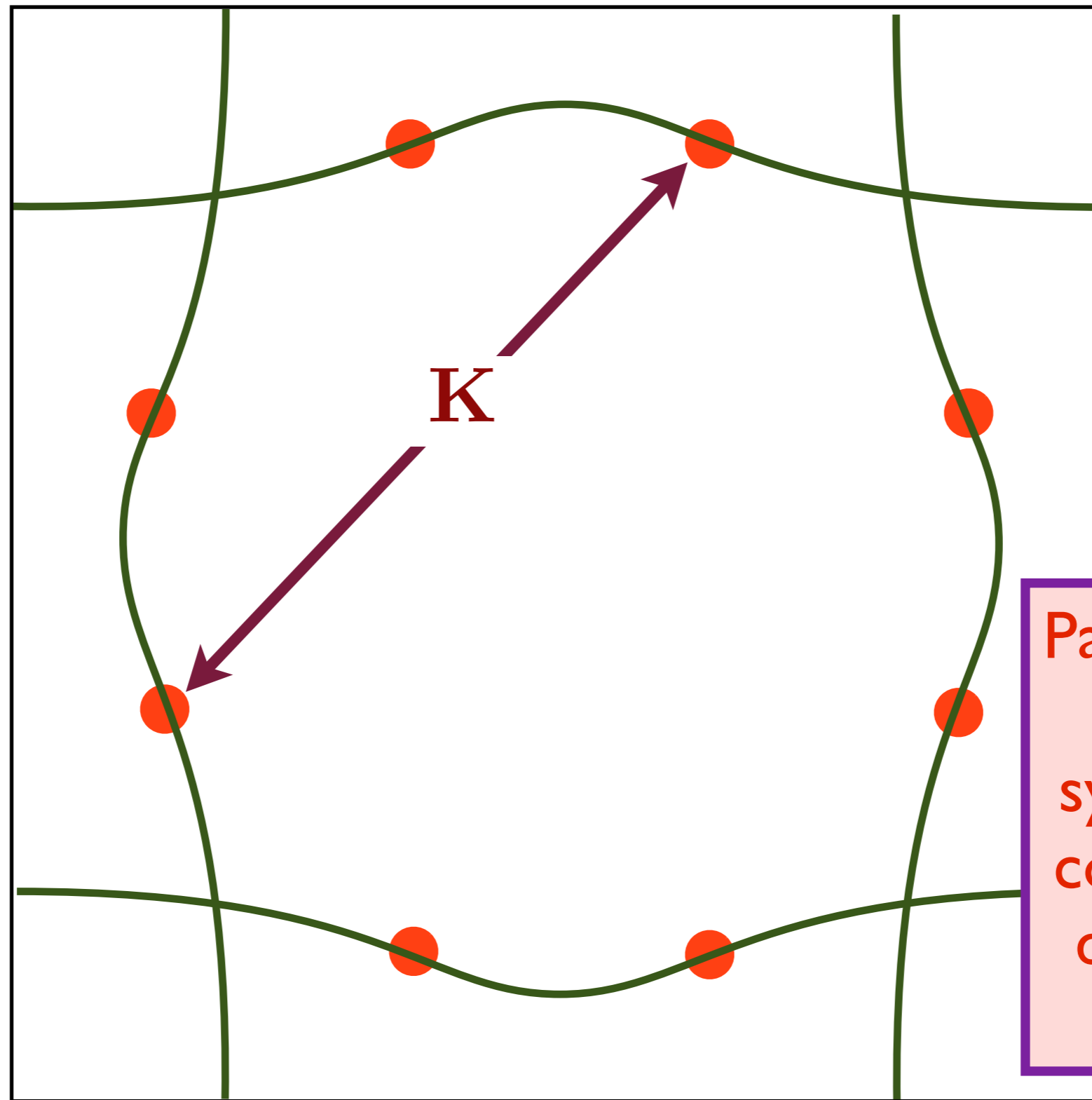


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Hot spots in a two band model

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Particle-hole or point-group symmetries or commensurate densities **not** required!

Hot spots in a two band model

QMC for the onset of antiferromagnetism

Electrons with dispersion $\varepsilon_{\mathbf{k}}$
interacting with fluctuations of the
antiferromagnetic order parameter $\vec{\varphi}$.

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}c_{\alpha} \mathcal{D}\vec{\varphi} \exp(-\mathcal{S}) \\ \mathcal{S} &= \int d\tau \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^{\dagger} \left(\frac{\partial}{\partial \tau} - \varepsilon_{\mathbf{k}} \right) c_{\mathbf{k}\alpha} \\ &+ \int d\tau d^2x \left[\frac{1}{2} (\nabla_x \vec{\varphi})^2 + \frac{r}{2} \vec{\varphi}^2 + \dots \right] \\ &- \lambda \int d\tau \sum_i \vec{\varphi}_i \cdot (-1)^{\mathbf{x}_i} c_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta} \end{aligned}$$

QMC for the onset of antiferromagnetism

Electrons with dispersions $\varepsilon_{\mathbf{k}}^{(x)}$ and $\varepsilon_{\mathbf{k}}^{(y)}$ interacting with fluctuations of the antiferromagnetic order parameter $\vec{\varphi}$.

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QMC for the onset of antiferromagnetism

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No sign problem !

QMC for the onset of antiferromagnetism

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Applies without changes to the microscopic band structure in the iron-based superconductors

QMC for the onset of antiferromagnetism

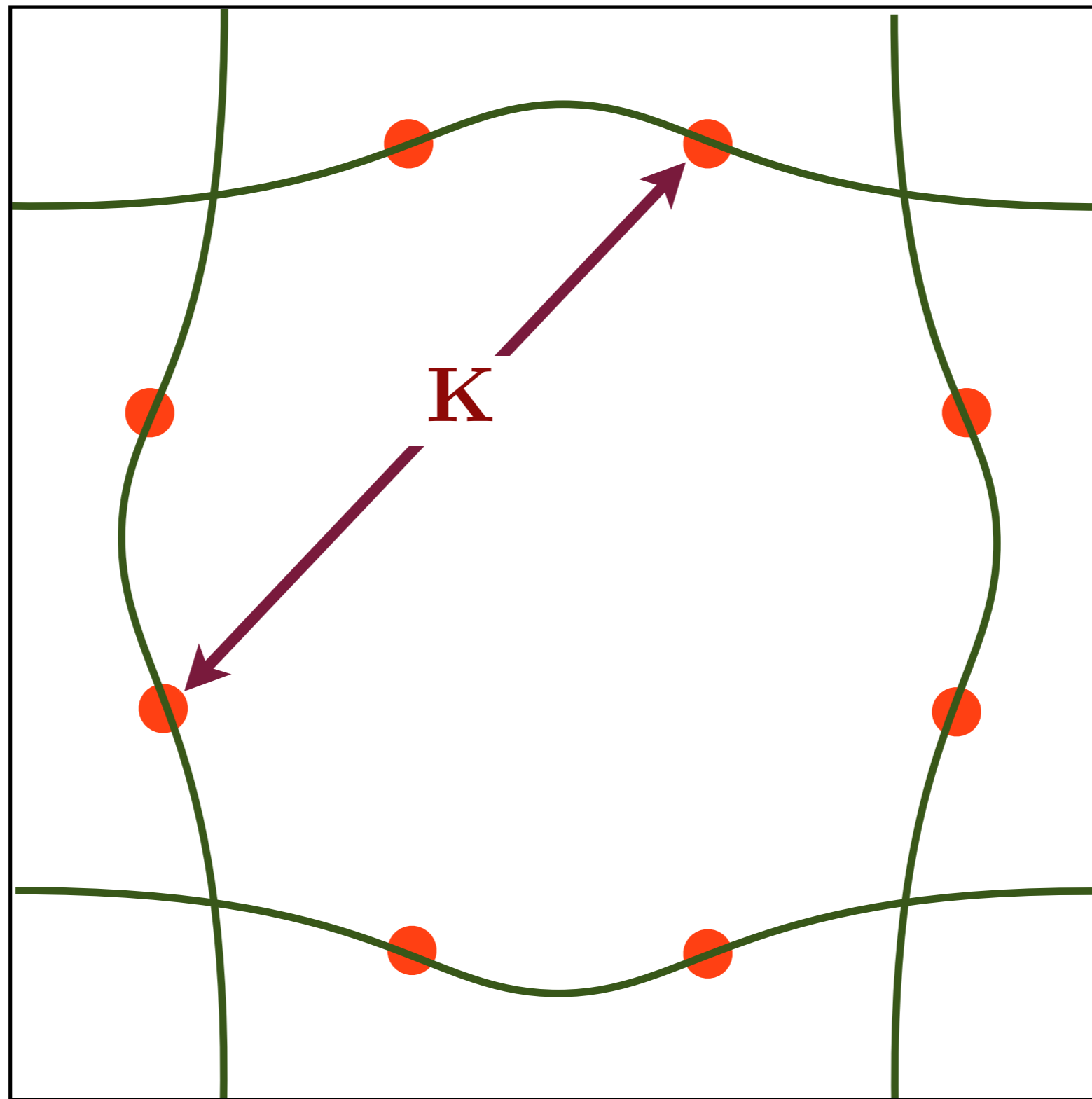
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Can integrate out $\vec{\varphi}$ to obtain an extended Hubbard model. The interactions in this model only couple electrons in separate bands.

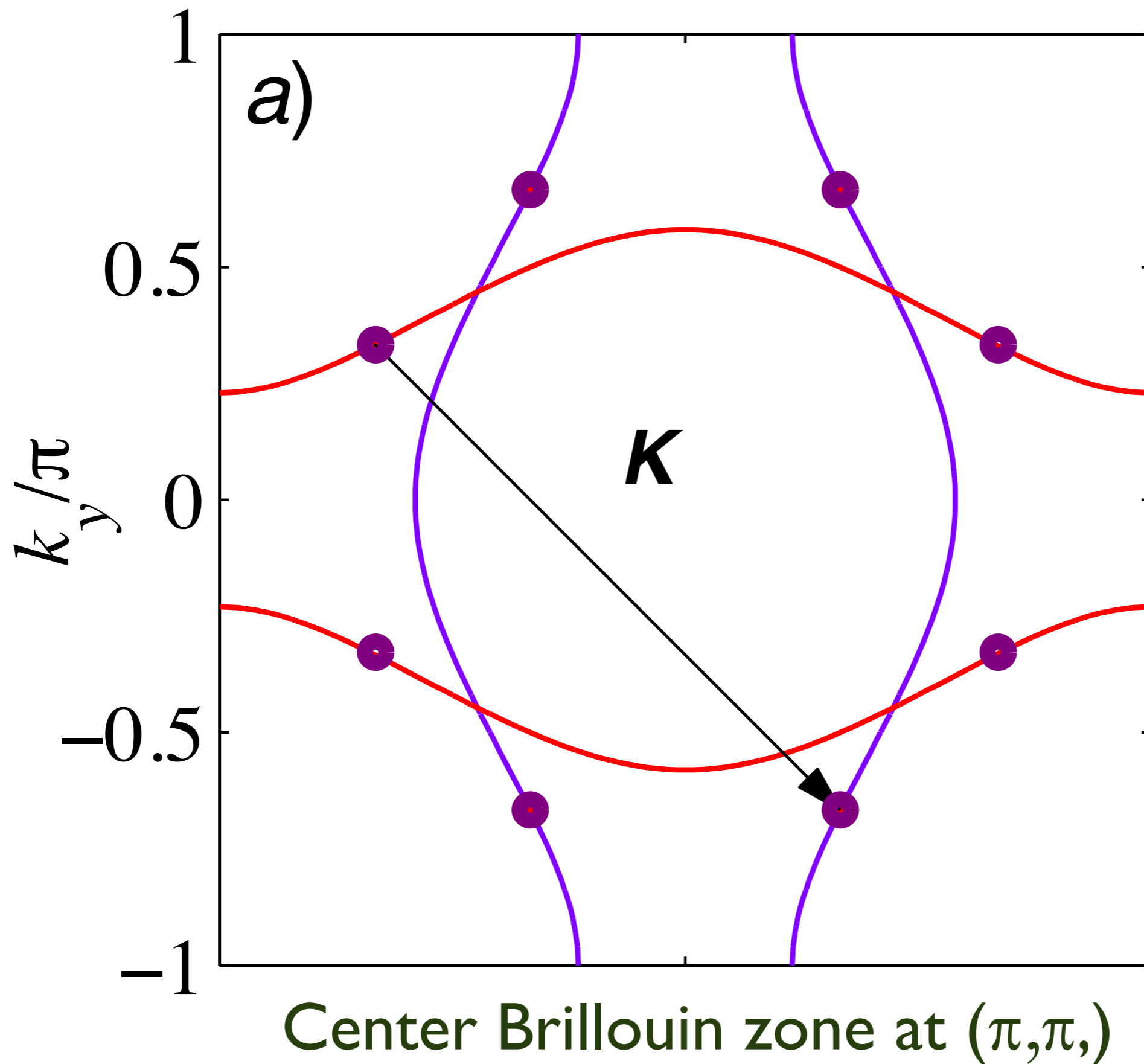
QMC for the onset of antiferromagnetism



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Hot spots in a two band model

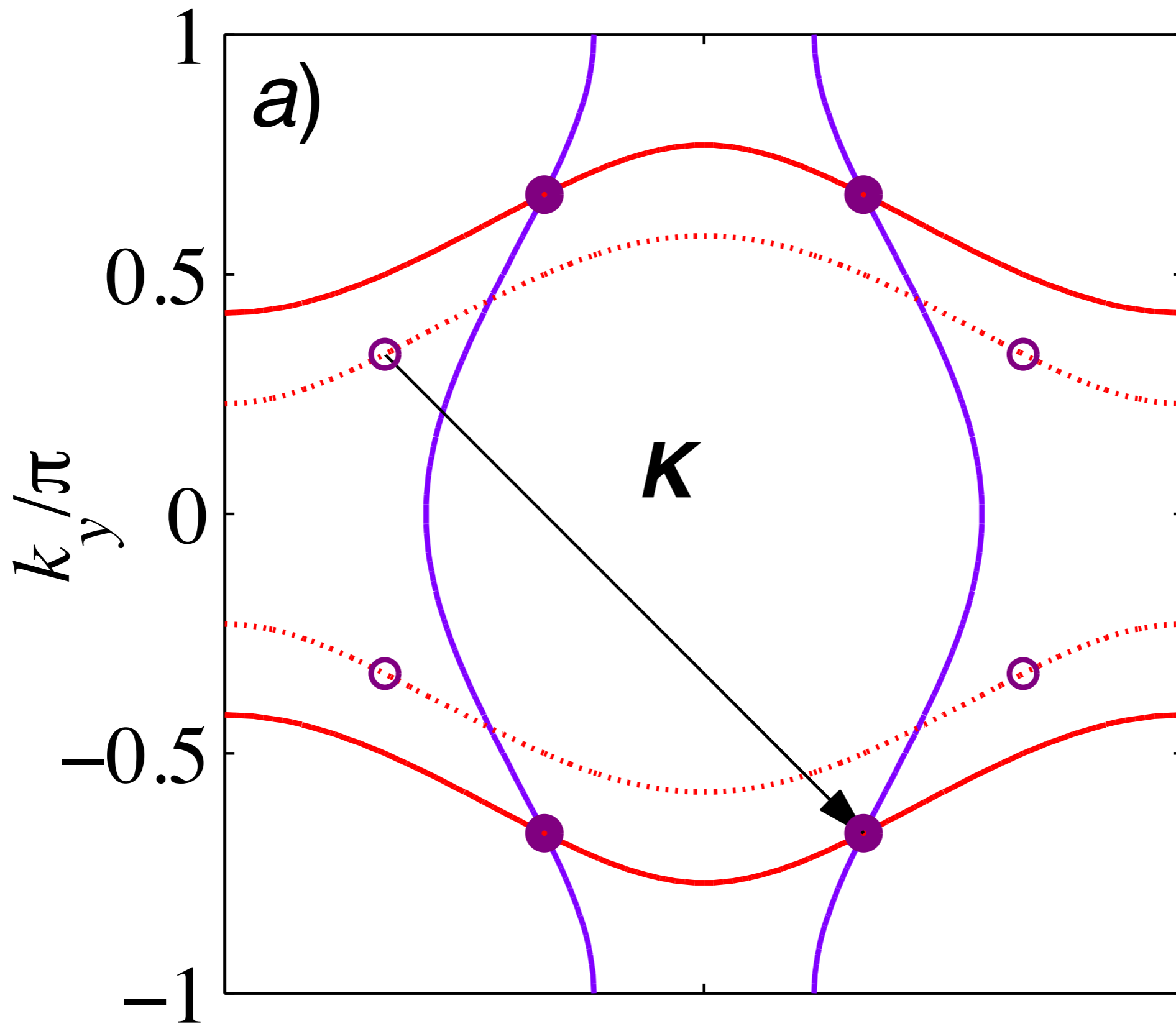
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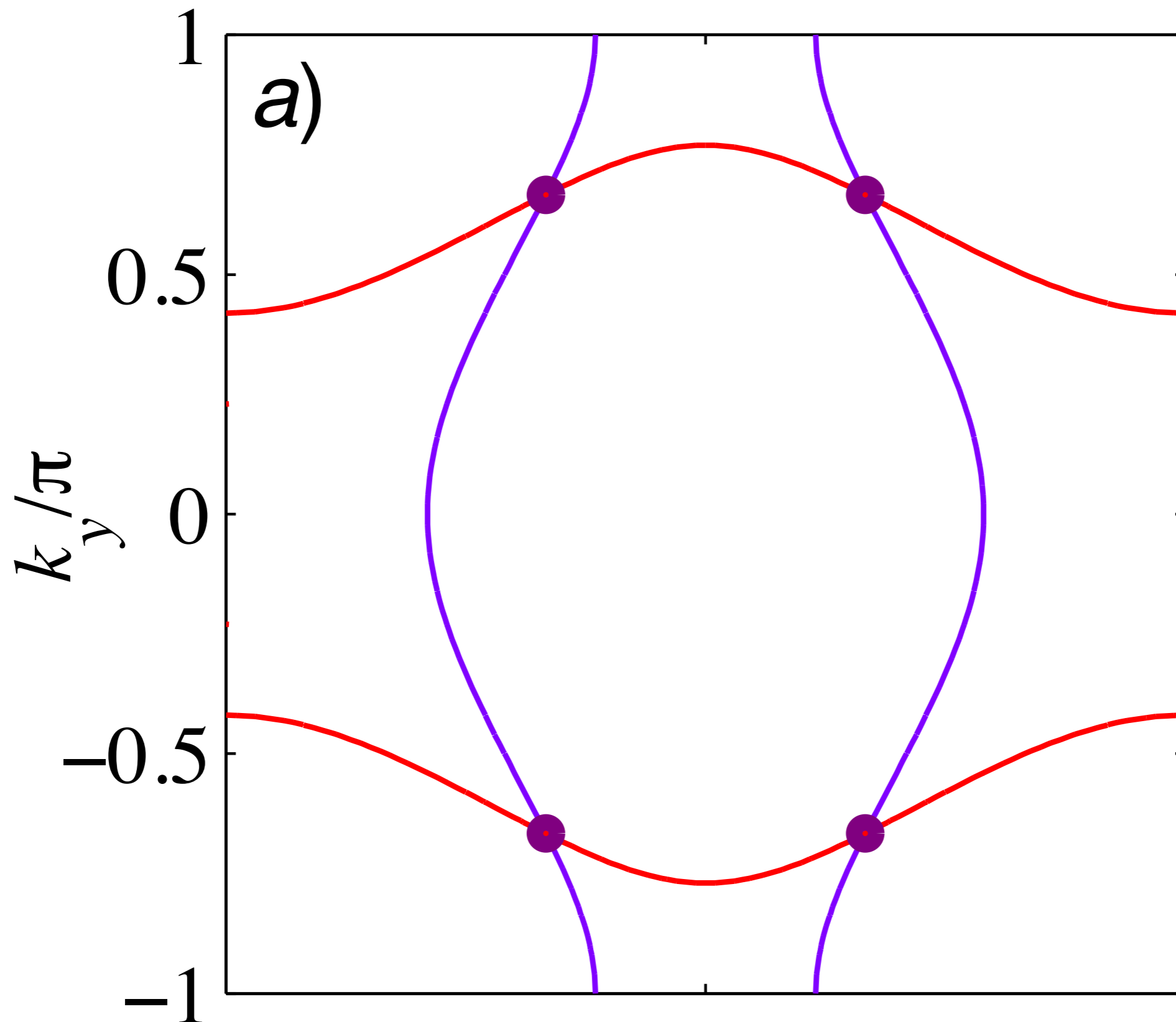
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Move one of the Fermi surface by (π, π)

QMC for the onset of antiferromagnetism

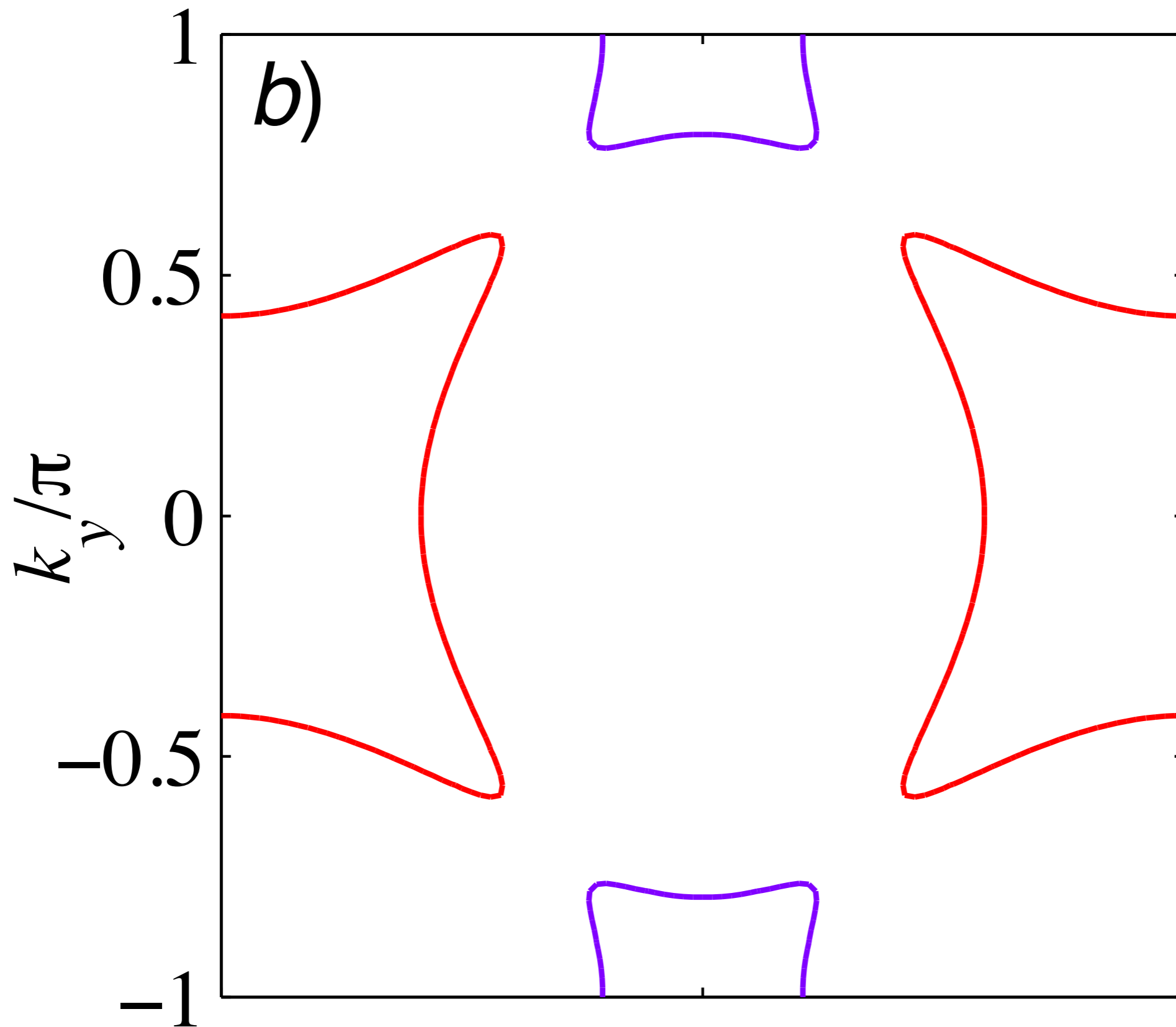


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Now hot spots are at Fermi surface intersections

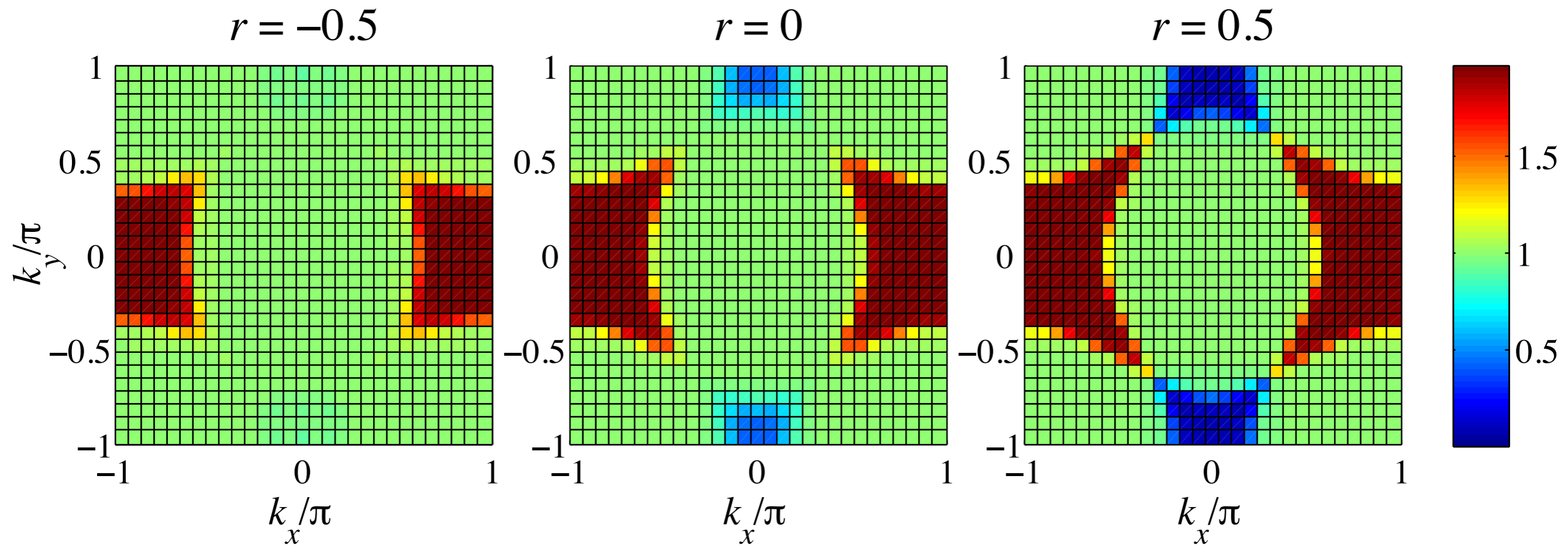
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Expected Fermi surfaces in the AFM ordered phase

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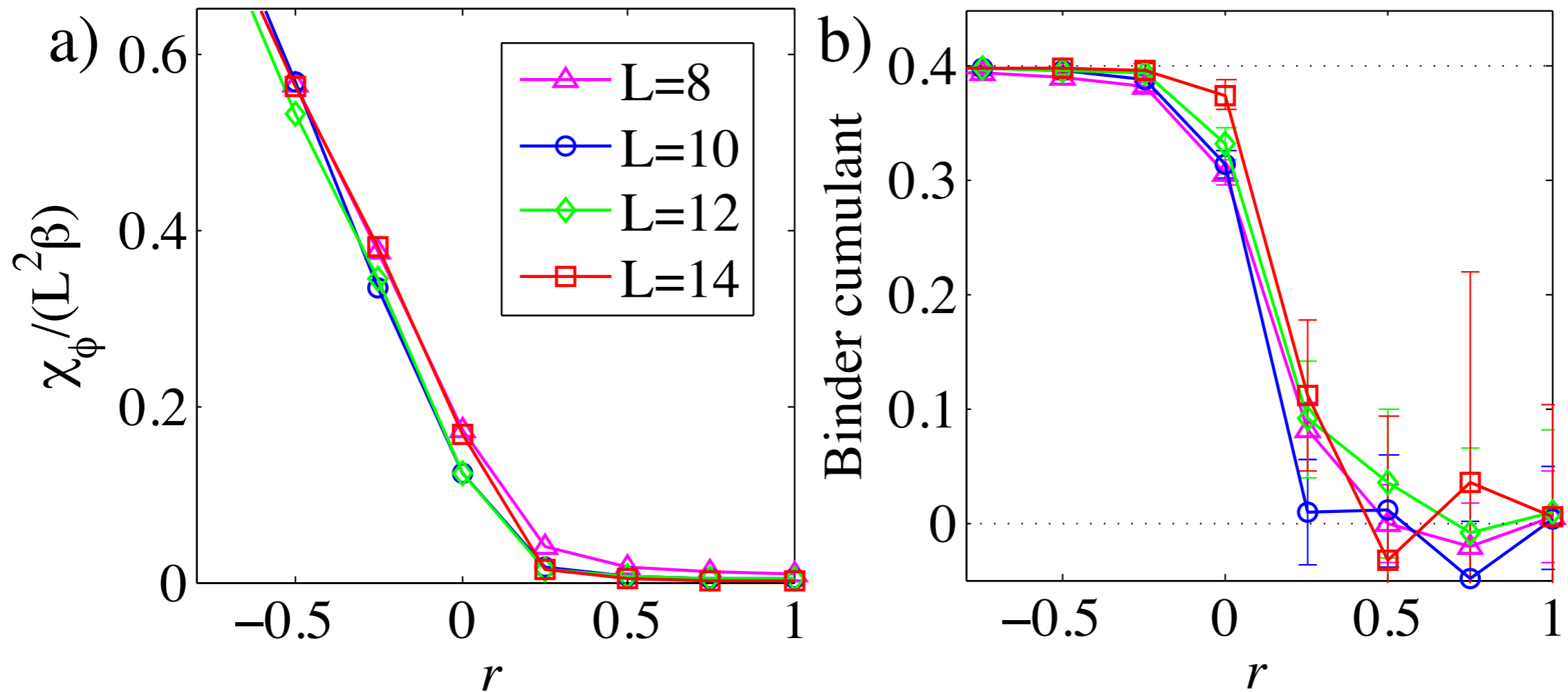


Electron occupation number $n_{\mathbf{k}}$
as a function of the tuning parameter r

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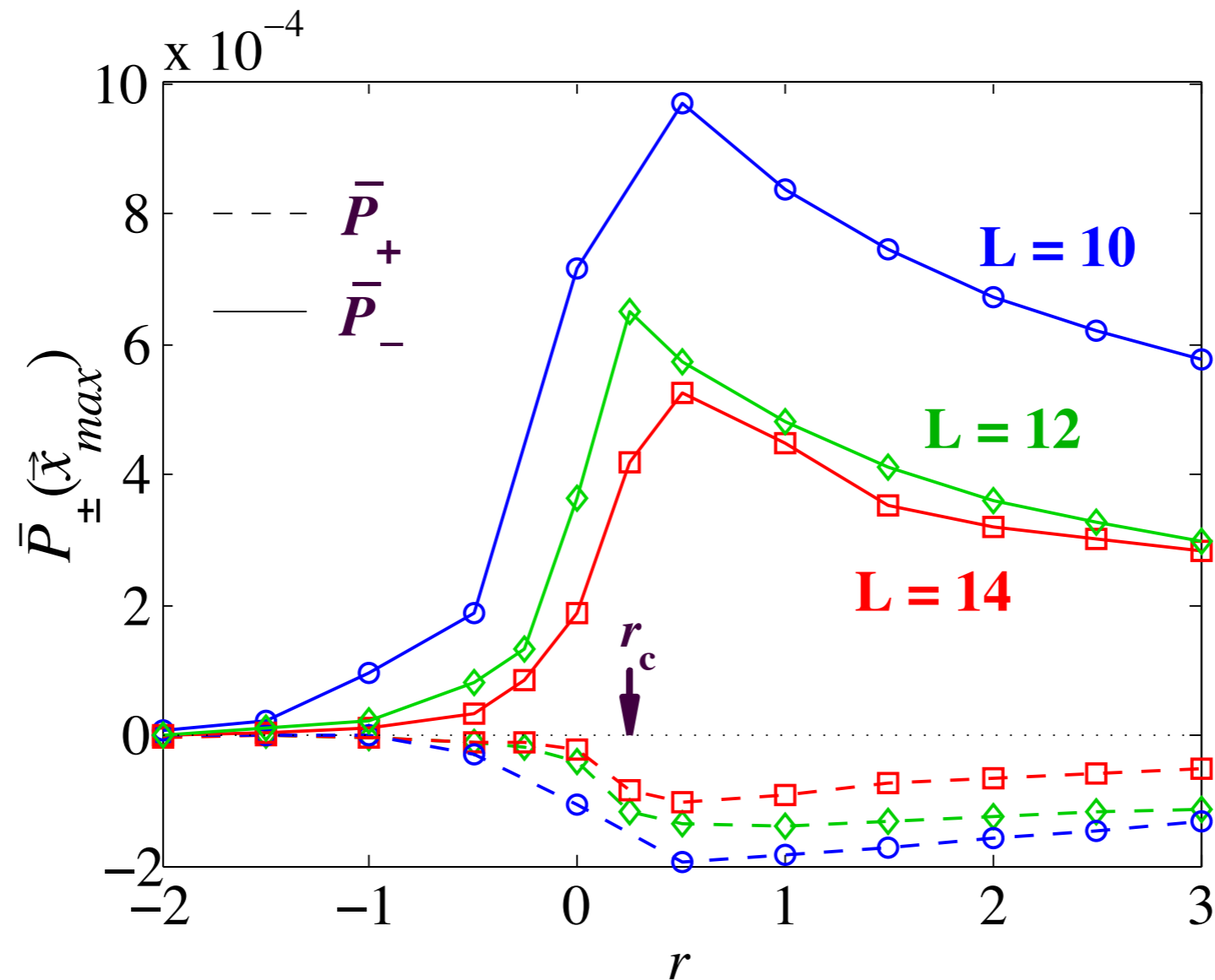


AF susceptibility, χ_ϕ , and Binder cumulant
as a function of the tuning parameter r

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QMC for the onset of antiferromagnetism



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

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Conclusions

- 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.

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Conclusions

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- New sign-problem-free quantum Monte Carlo for studying such metals. Obtained (*first ?*) convincing evidence for unconventional superconductivity at strong coupling.
- Good prospects for studying competing charge orders, and non-Fermi liquid physics at non-zero temperature.