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

University of Maryland, College Park, March 14, 2013

Subir Sachdev

sachdev.physics.harvard.edu

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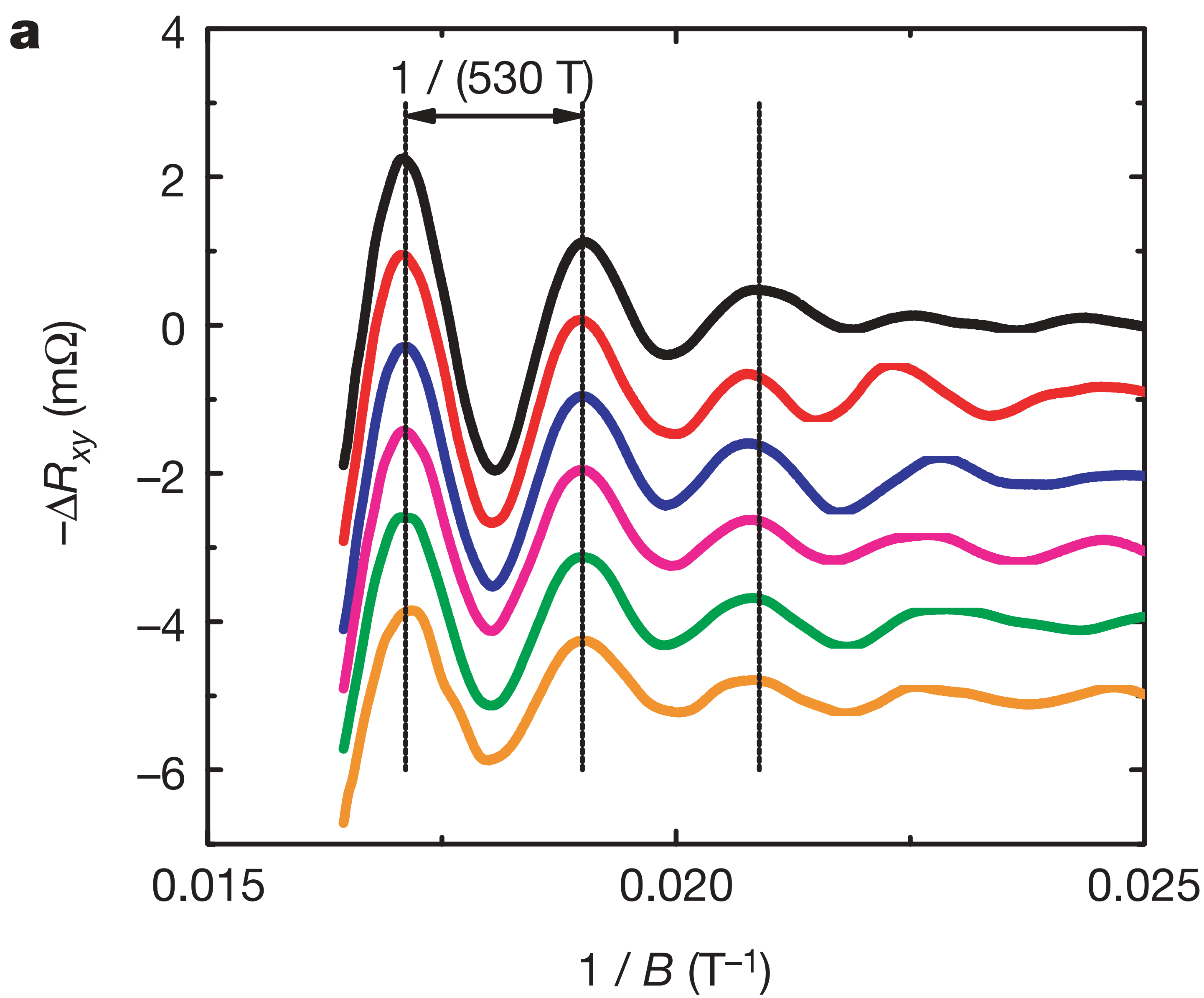
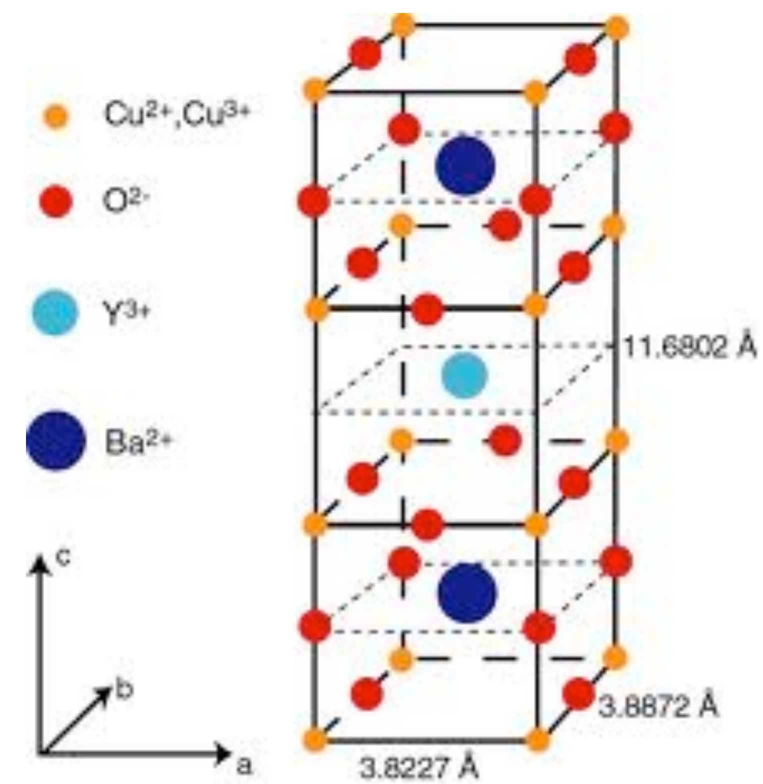
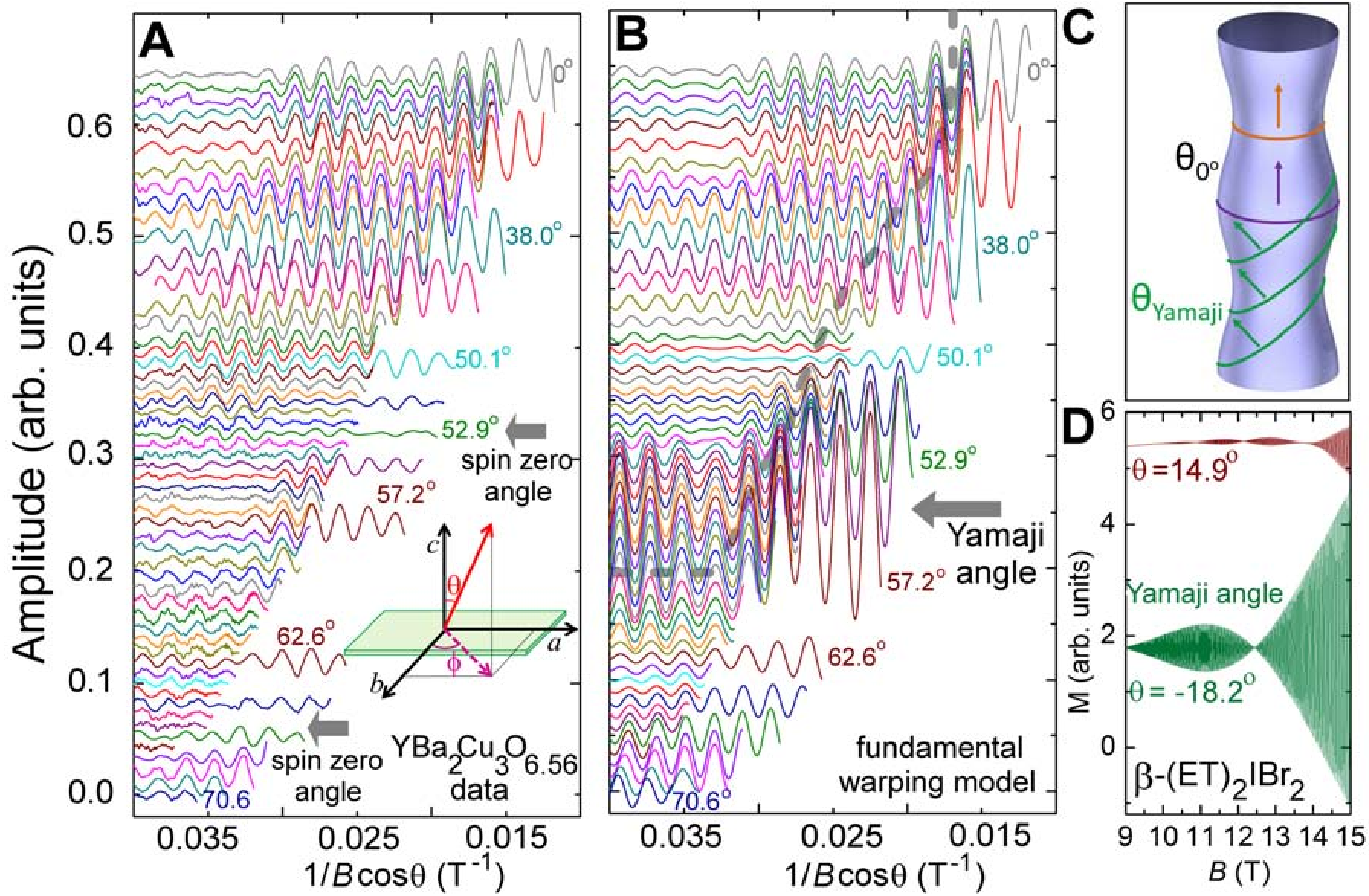
Quantum oscillations and the Fermi surface in an underdoped high-T_c superconductor

Nicolas Doiron-Leyraud[1], Cyril Proust[2], David LeBoeuf[1], Julien Levallois[2], Jean-Baptiste Bonnemaison[1], Ruixing Liang[3,4], D. A. Bonn[3,4], W. N. Hardy[3,4] & Louis Taillefer[1,4]

Nature **447**, 565 (2007)







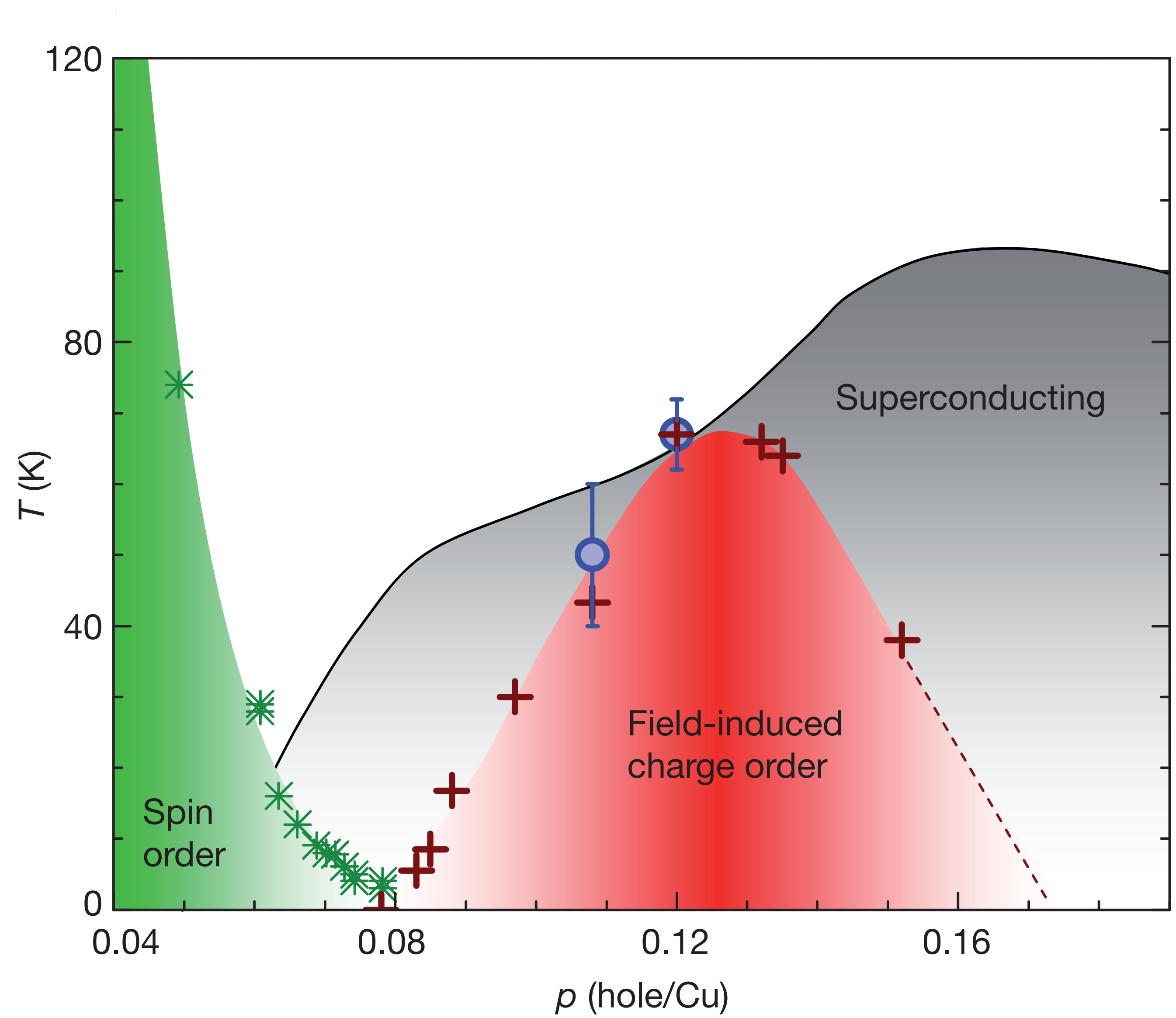
Twofold twisted Fermi surface from staggered order in an underdoped high T_c superconductor

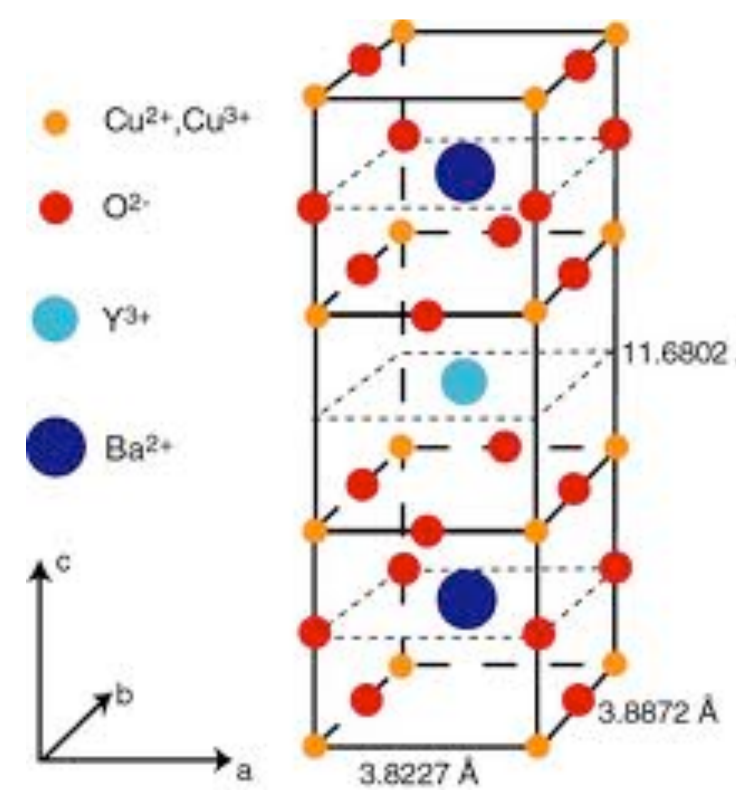
Suchitra E. Sebastian,[1*] N. Harrison,[2] F. F. Balakirev,[2] M. M. Altarawneh,[2,3]
Ruixing Liang,[4,5] D. A. Bonn,[4,5] W. N. Hardy,[4,5] G. G. Lonzarich,[1]

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

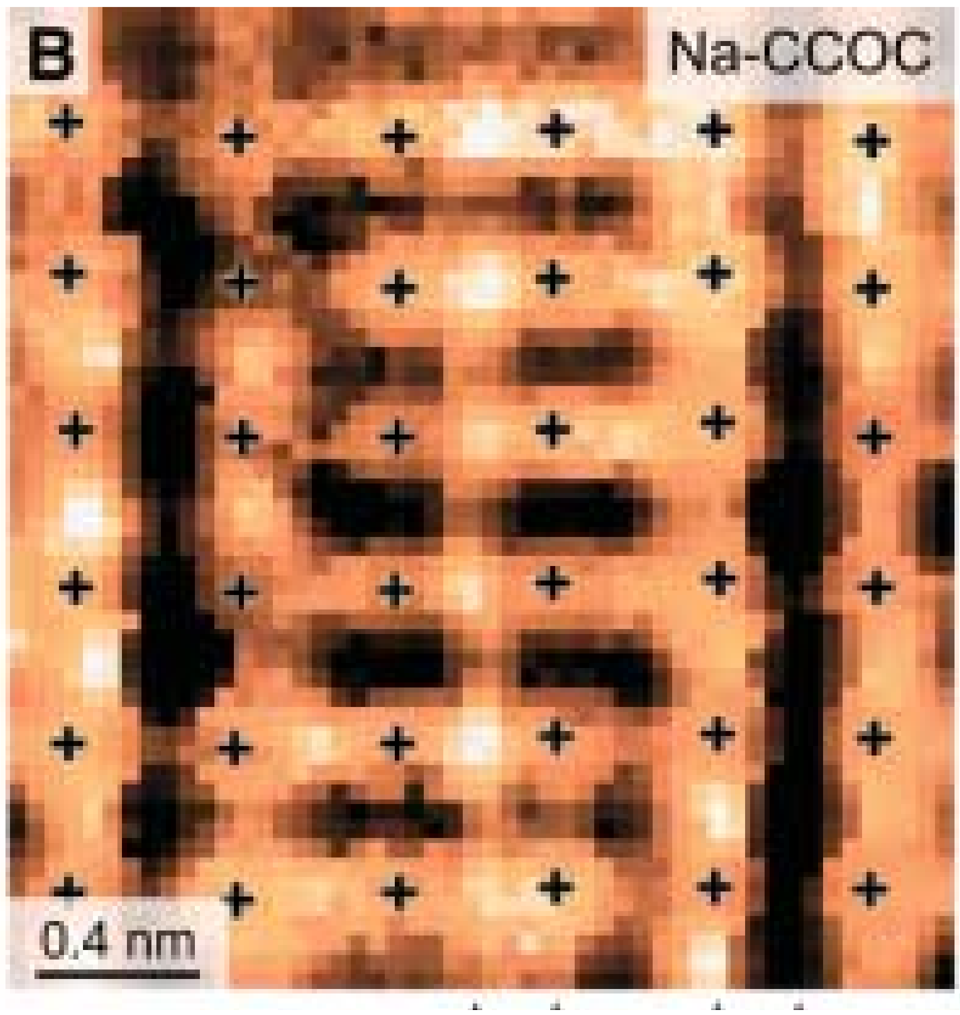




An Intrinsic Bond-Centered Electronic Glass with Unidirectional Domains in Underdoped Cuprates

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]*

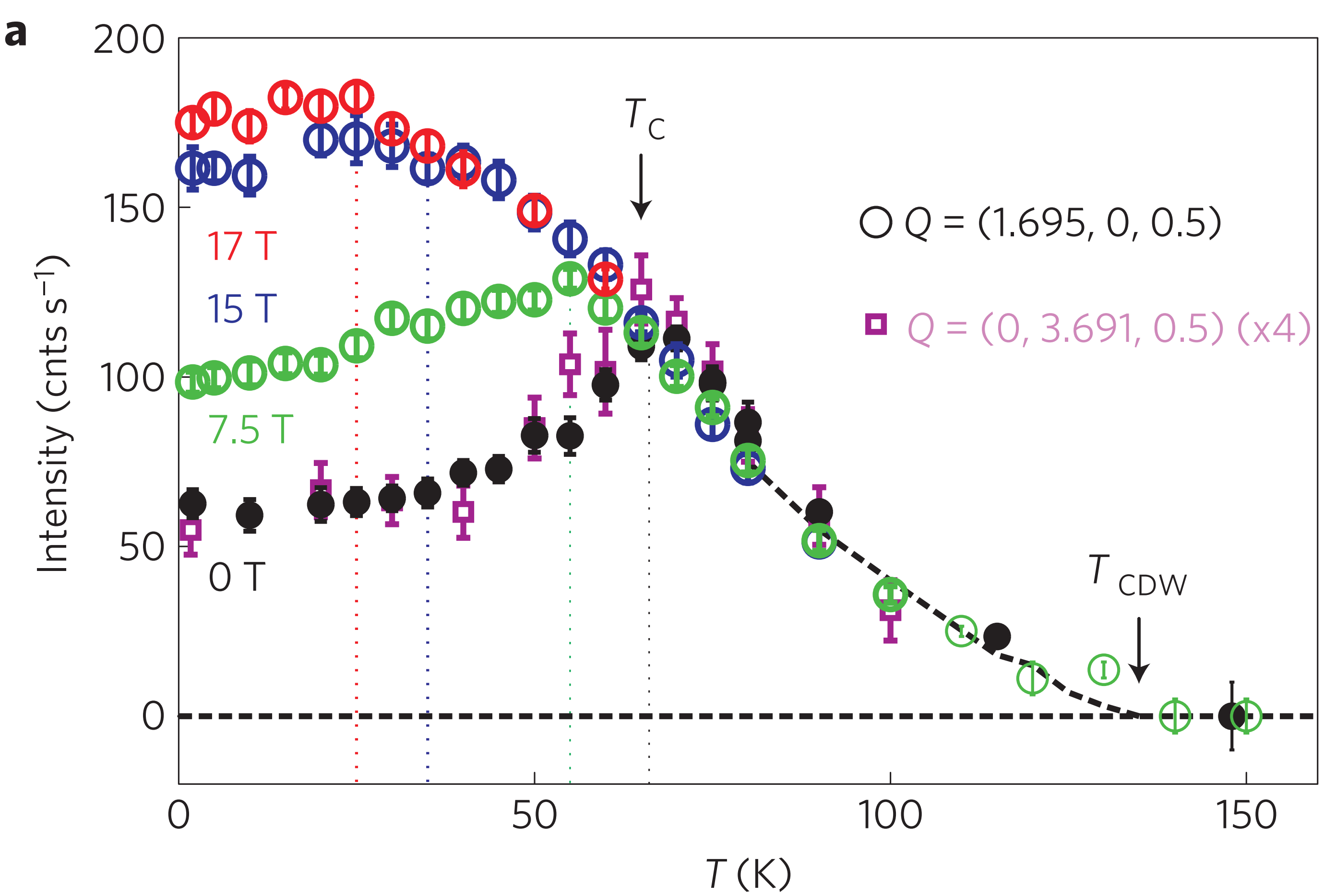
9 MARCH 2007 VOL 315 **SCIENCE**

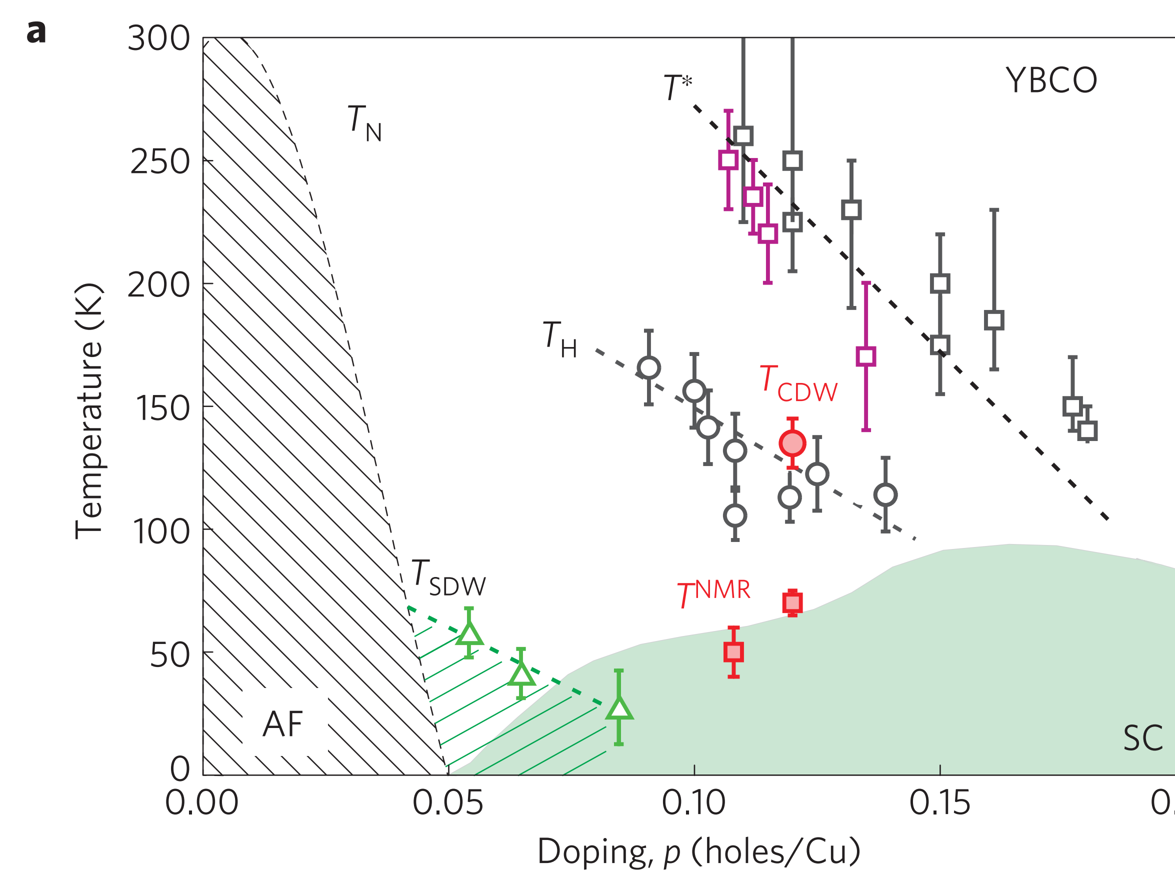


Direct observation of competition between superconductivity and charge density wave order in $YBa_2Cu_3O_{6.67}$

J. Chang[1,2]★, E. Blackburn[3], A. T. Holmes[3], N. B. Christensen[4], J. Larsen[4,5], J. Mesot[1,2], Ruixing Liang[6,7], D. A. Bonn[6,7], W. N. Hardy[6,7], A. Watenphul[8], M. v. Zimmermann[8], E. M. Forgan[3] and S. M. Hayden[9]

NATURE PHYSICS | VOL 8 | DECEMBER 2012 |



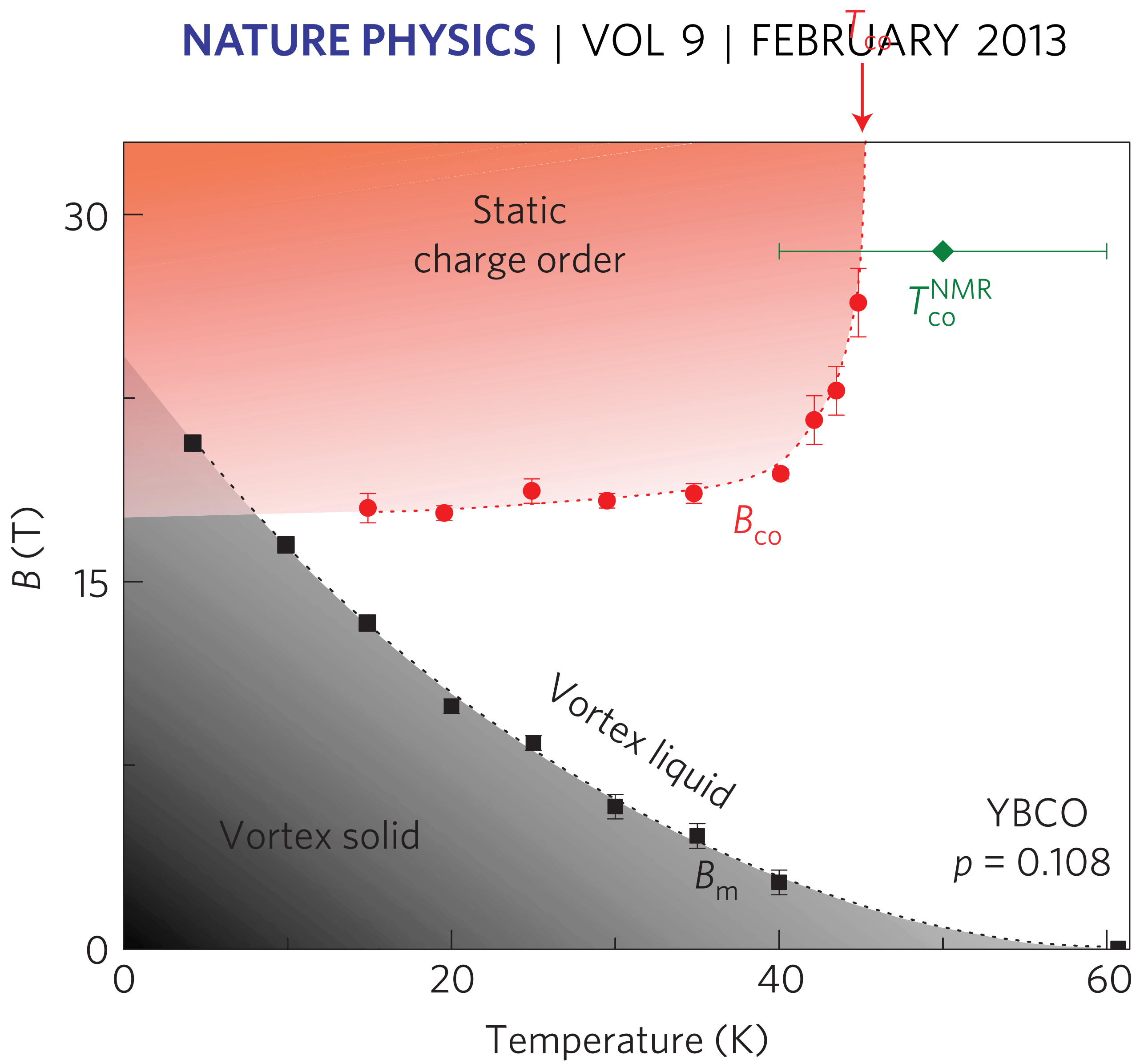


Saturday, March 16, 13

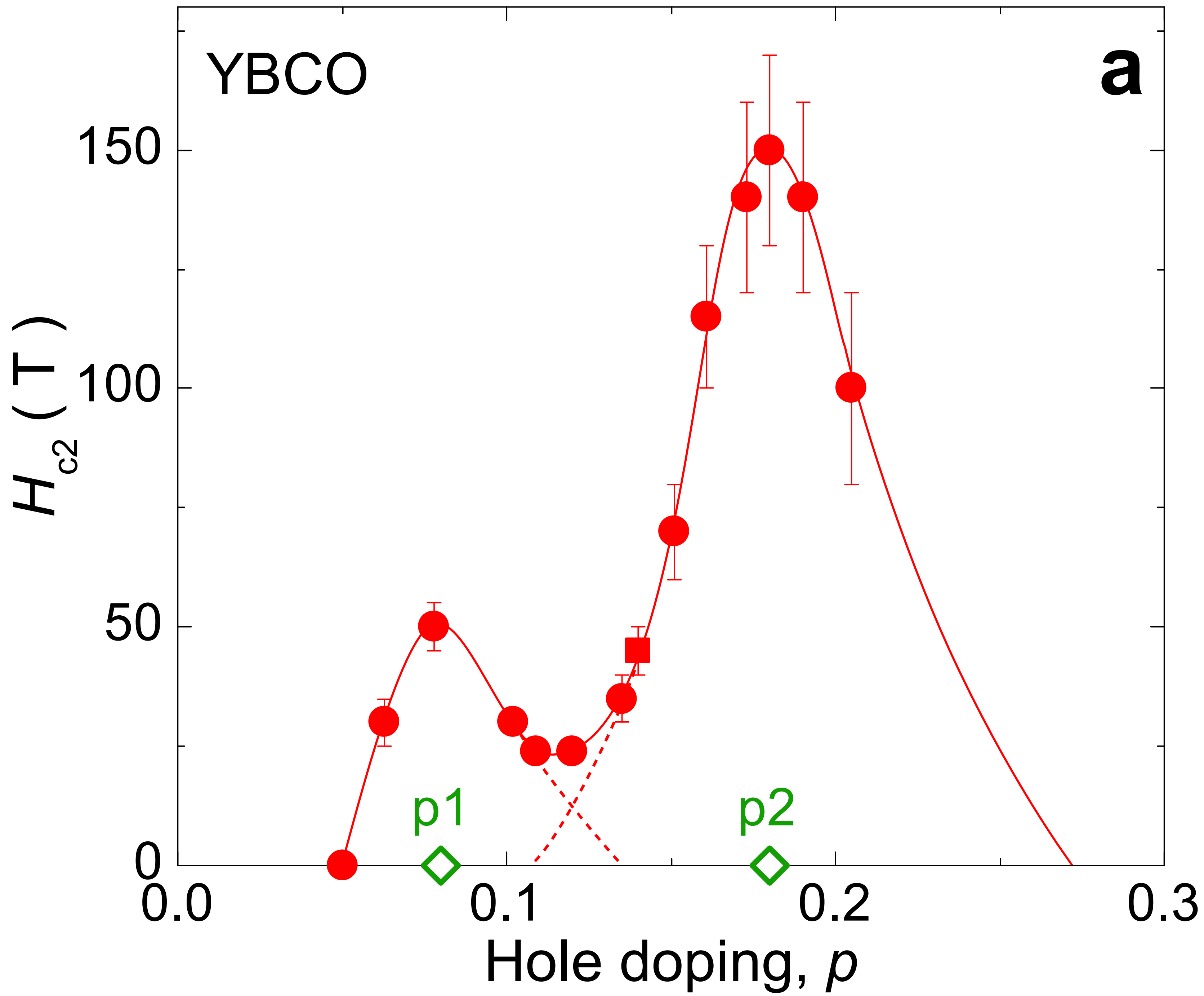
Thermodynamic phase diagram of static charge order in underdoped $YBa_2Cu_3O_y$

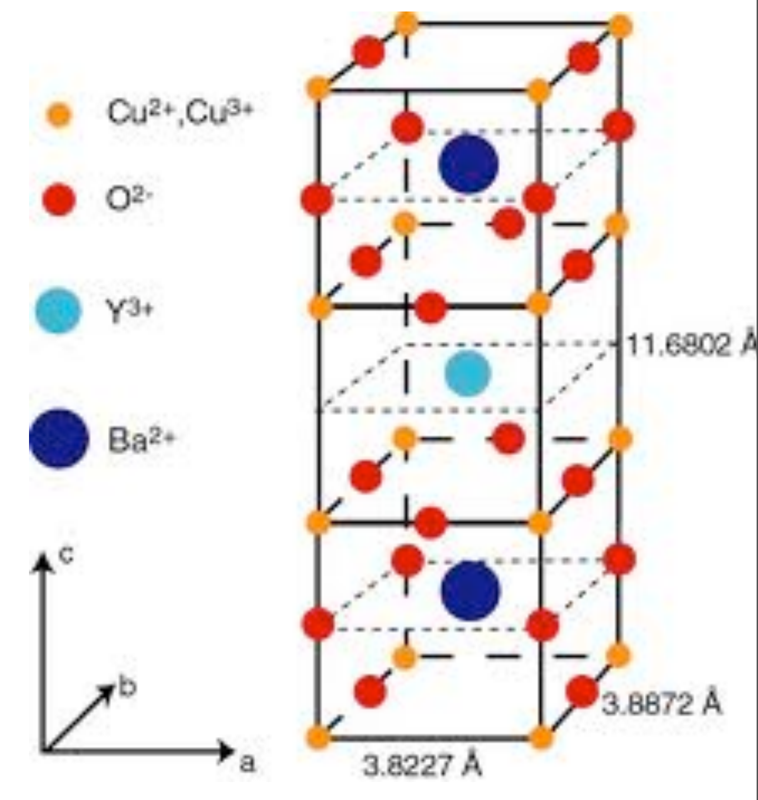
David LeBoeuf[1]★, S. Krämer[2], W. N. Hardy[3,4], Ruixing Liang[3,4], D. A. Bonn[3,4] and Cyril Proust[1,4]★

NATURE PHYSICS | VOL 9 | FEBRUARY 2013

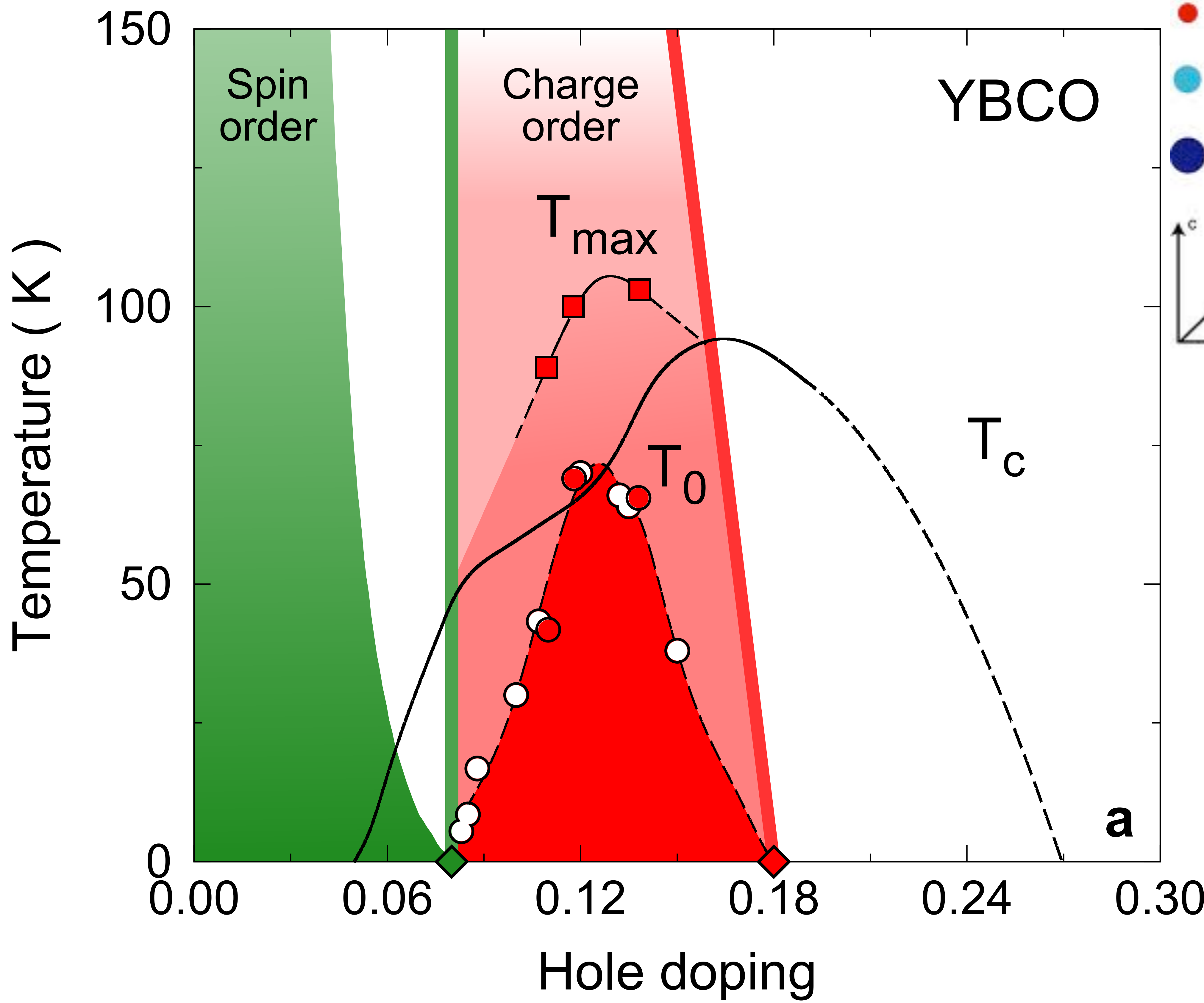


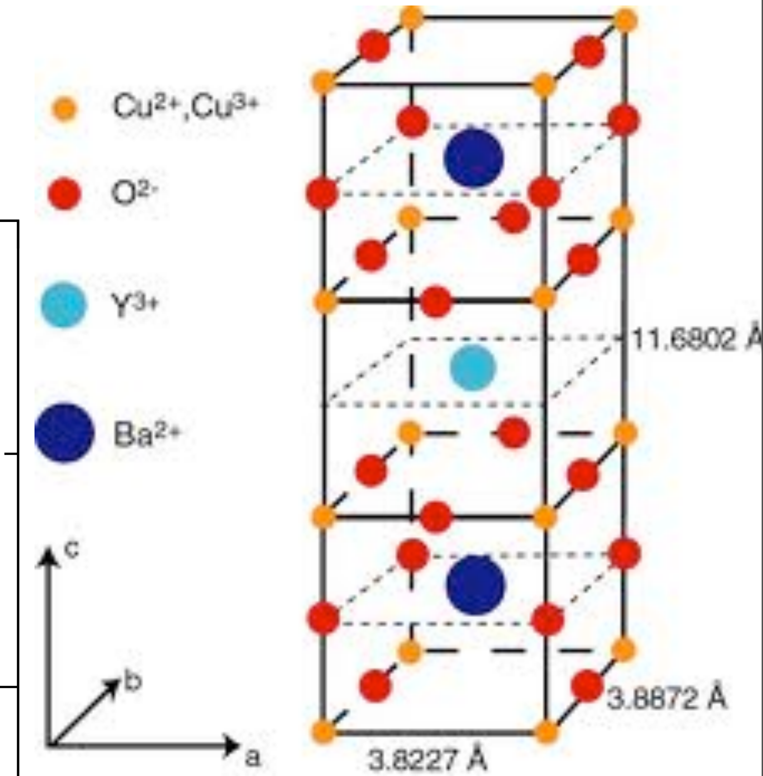
The comparison of different acoustic modes indicates that the charge modulation is biaxial, which differs from a uniaxial stripe charge order.





G. Grissonnanche et al., preprint





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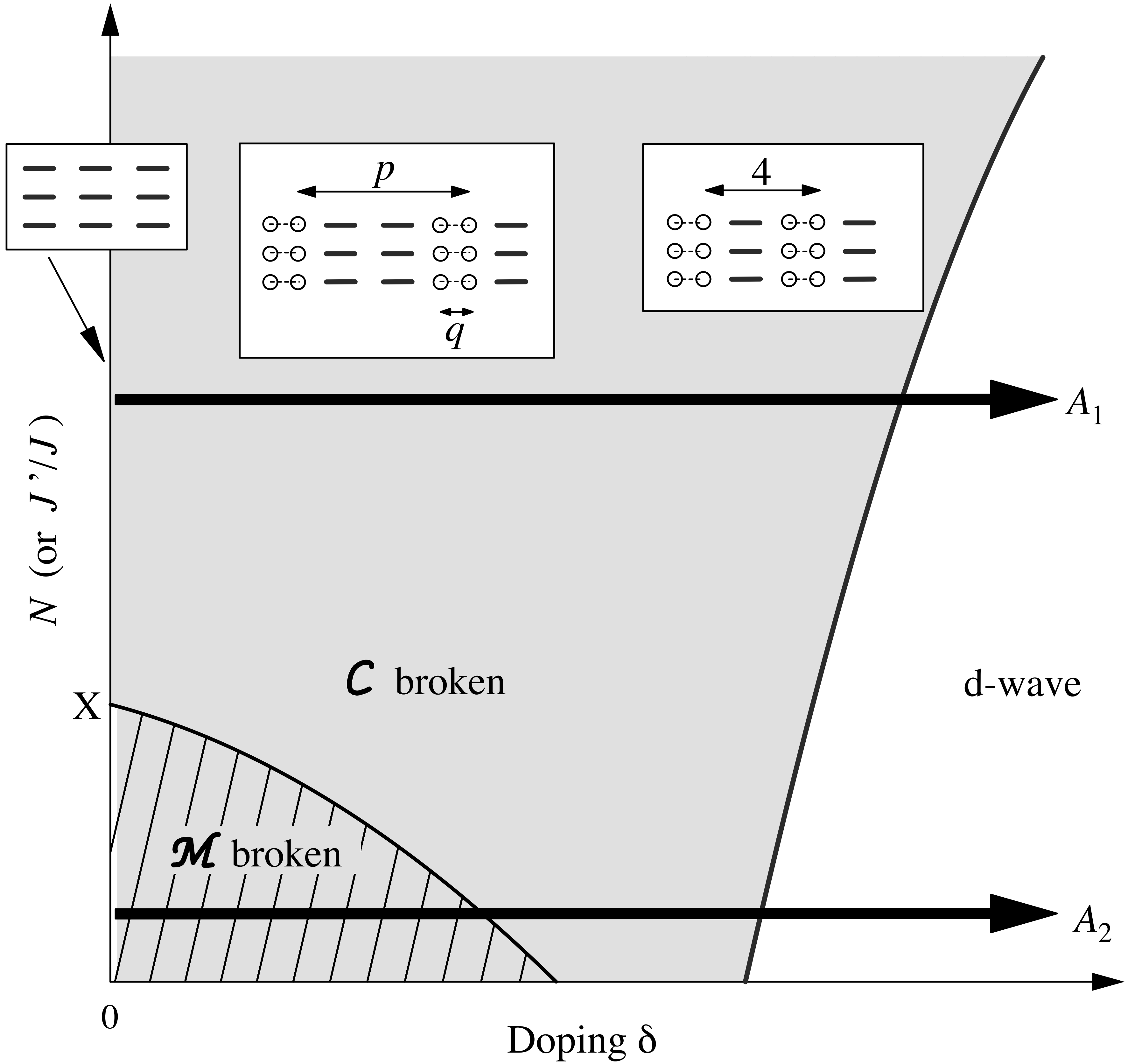

M. Vojta and S. Sachdev, Physical Review Letters **83**, 3916 (1999)

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

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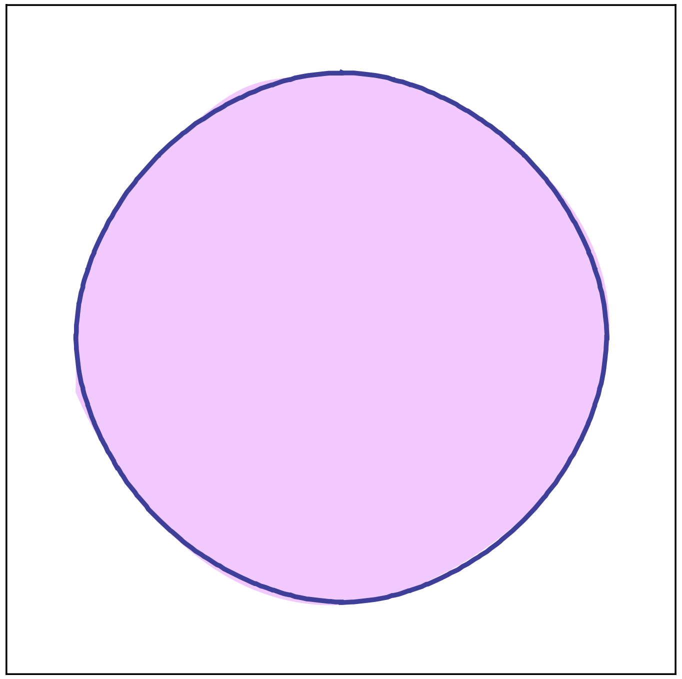
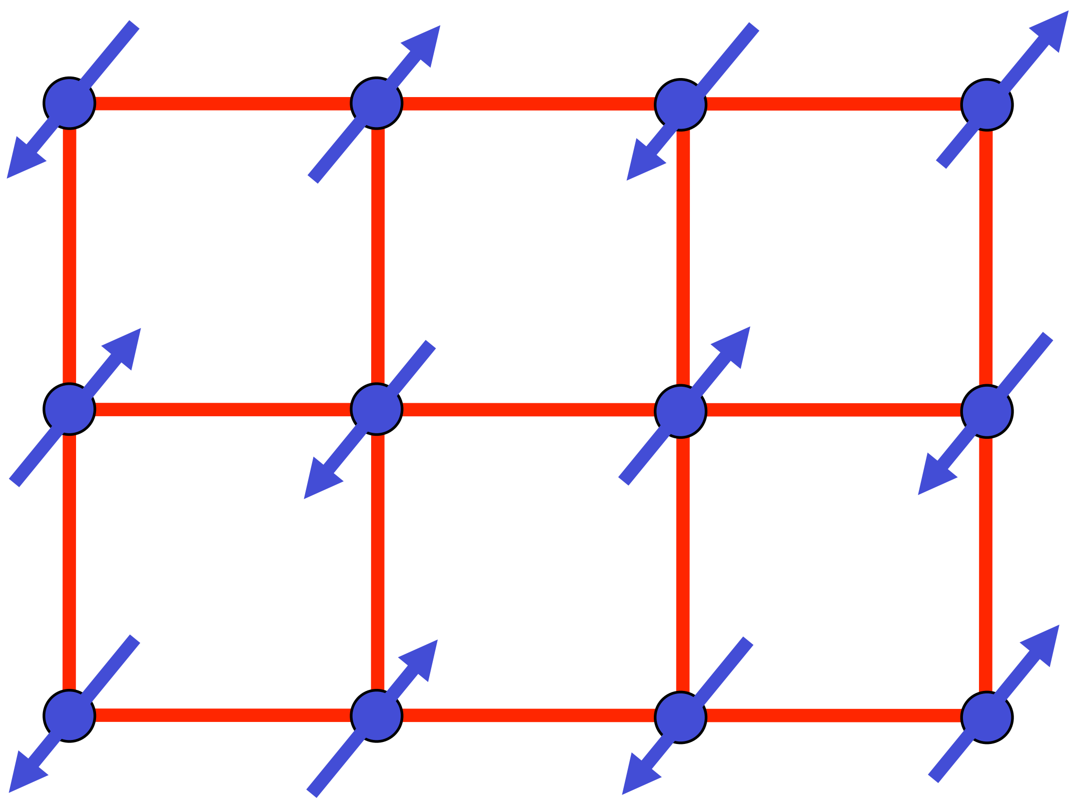
Fermi surface+antiferromagnetism

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.

The Hubbard Model

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

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

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

$$n_{i\alpha} = c^\dagger_{i\alpha} c_{i\alpha}$$

$$c^\dagger_{i\alpha} c_{j\beta} + c_{j\beta} c^\dagger_{i\alpha} = \delta_{ij}\delta_{\alpha\beta}$$
$$c_{i\alpha} c_{j\beta} + c_{j\beta} c_{i\alpha} = 0$$

The Hubbard Model

Decouple *U* term by a Hubbard-Stratanovich transformation

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

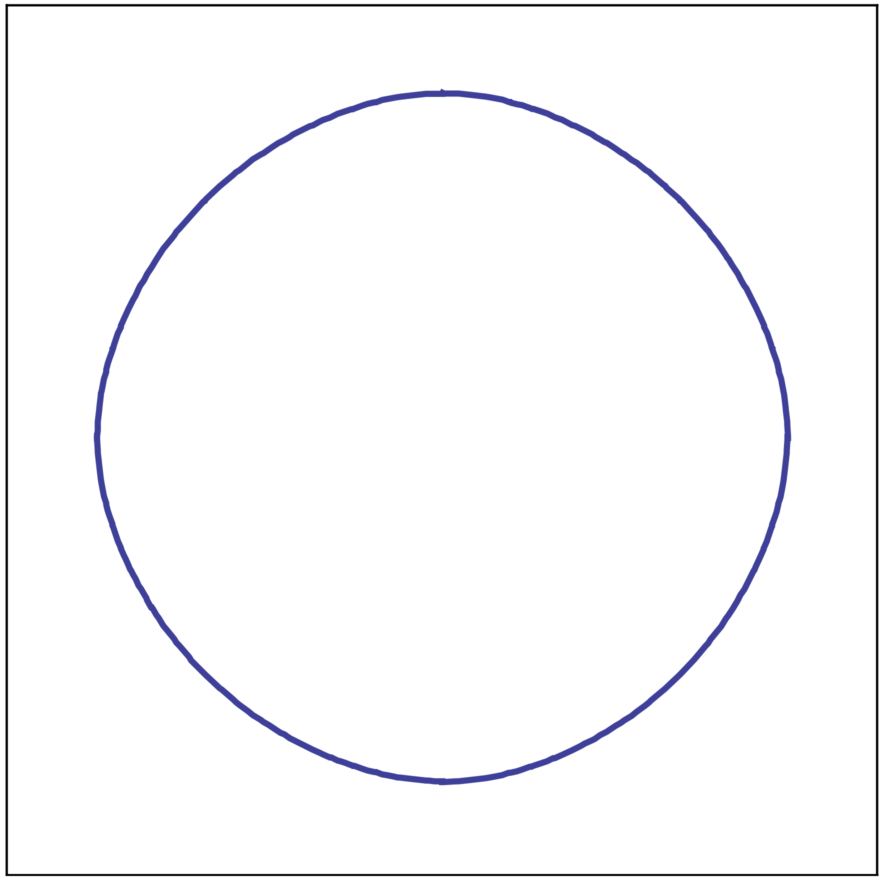
$$\mathcal{L}_c = c_a^\dagger \varepsilon(-i\boldsymbol{\nabla}) c_a$$

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

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

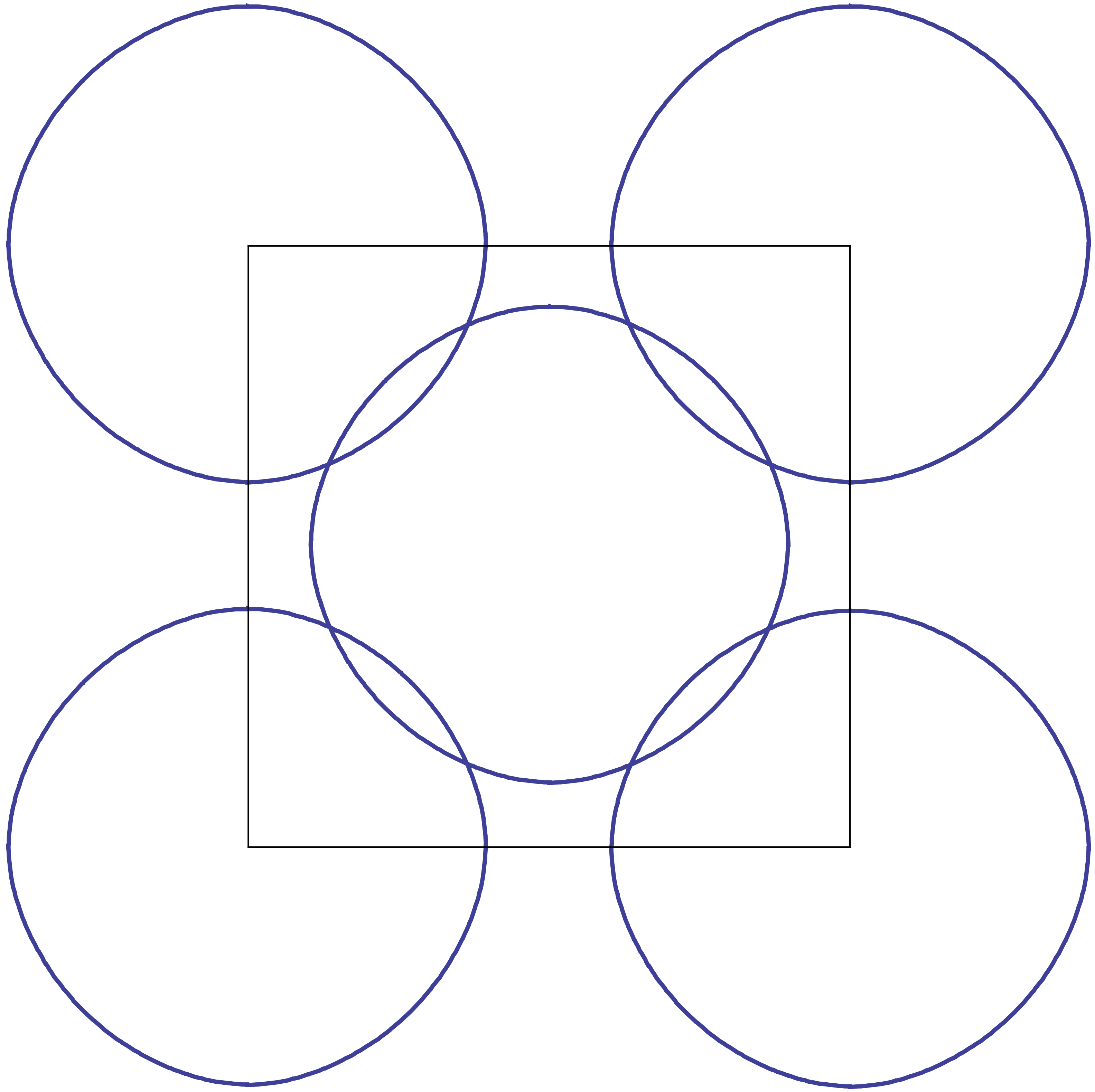
"Yukawa" coupling between fermions and antiferromagnetic order:
$\lambda^2 \sim U$, the Hubbard repulsion

Fermi surface+antiferromagnetism



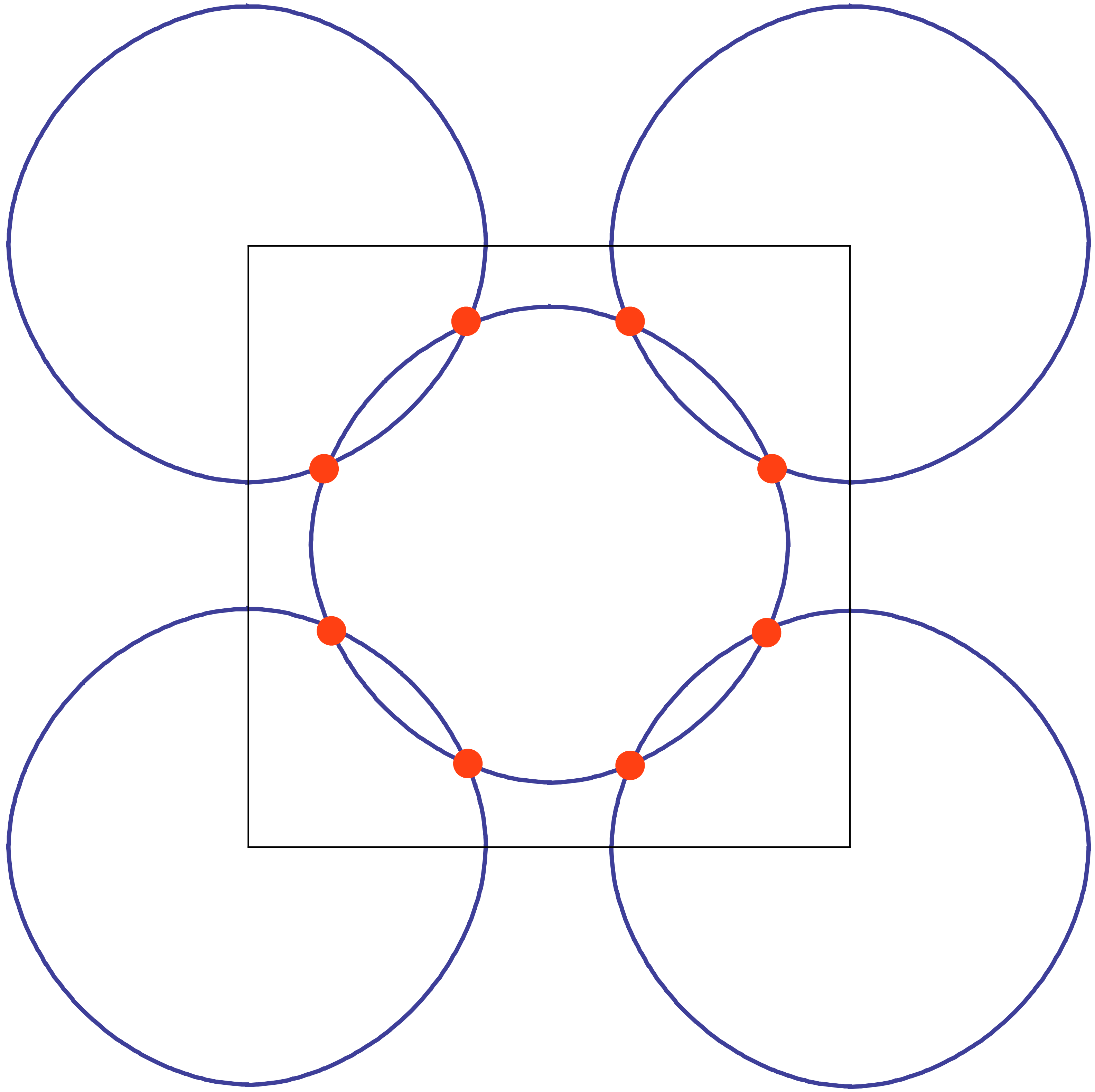
Metal with "large" Fermi surface

Fermi surface+antiferromagnetism



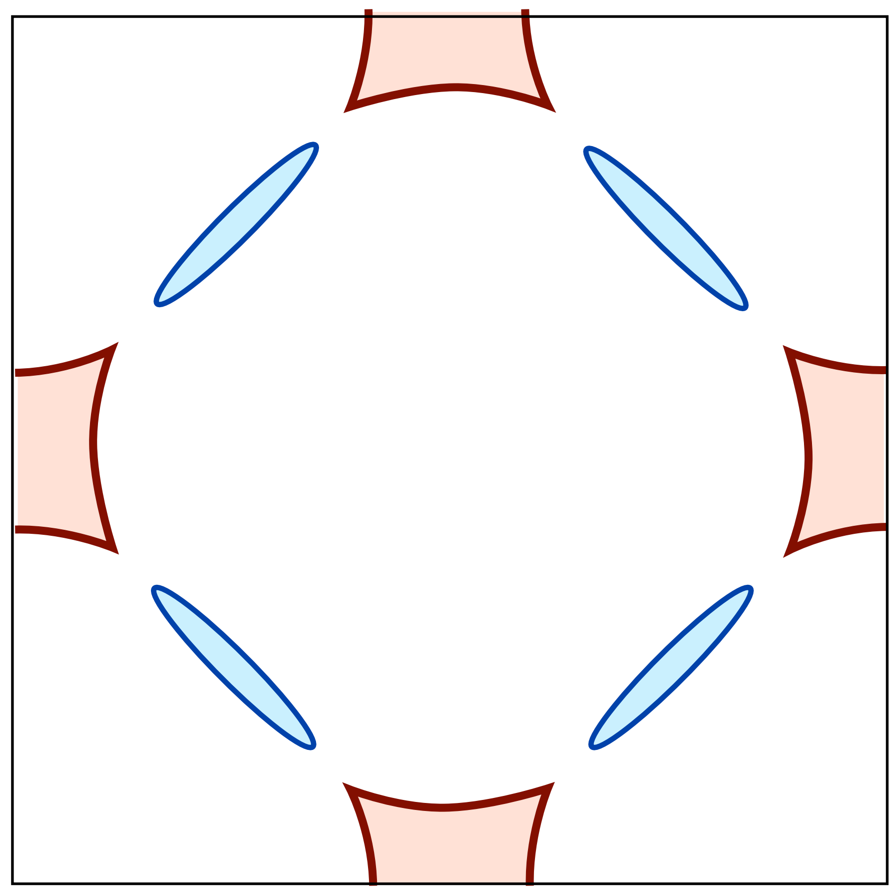
Fermi surfaces translated by $\mathbf{K} = (\pi, \pi)$.

Fermi surface+antiferromagnetism



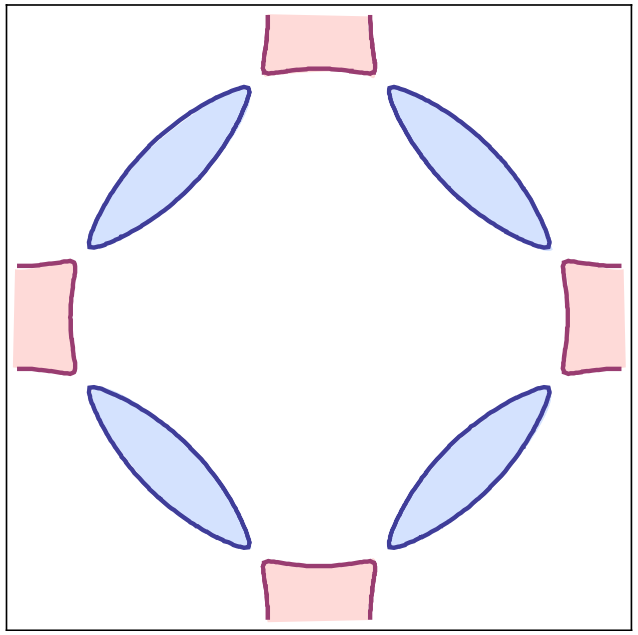
“Hot” spots

Fermi surface+antiferromagnetism



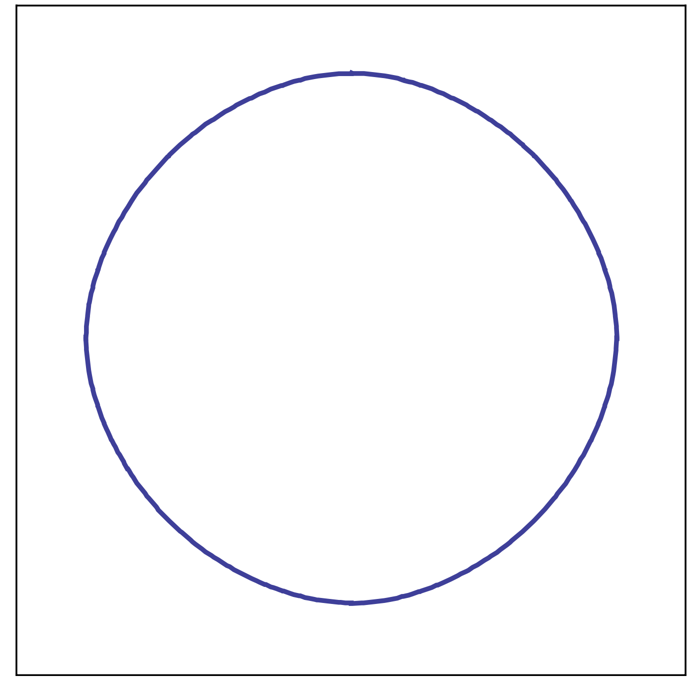
Electron and hole pockets in antiferromagnetic phase with $\langle \vec{\varphi} \rangle \neq 0$

Fermi surface+antiferromagnetism



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

Metal with electron and hole pockets



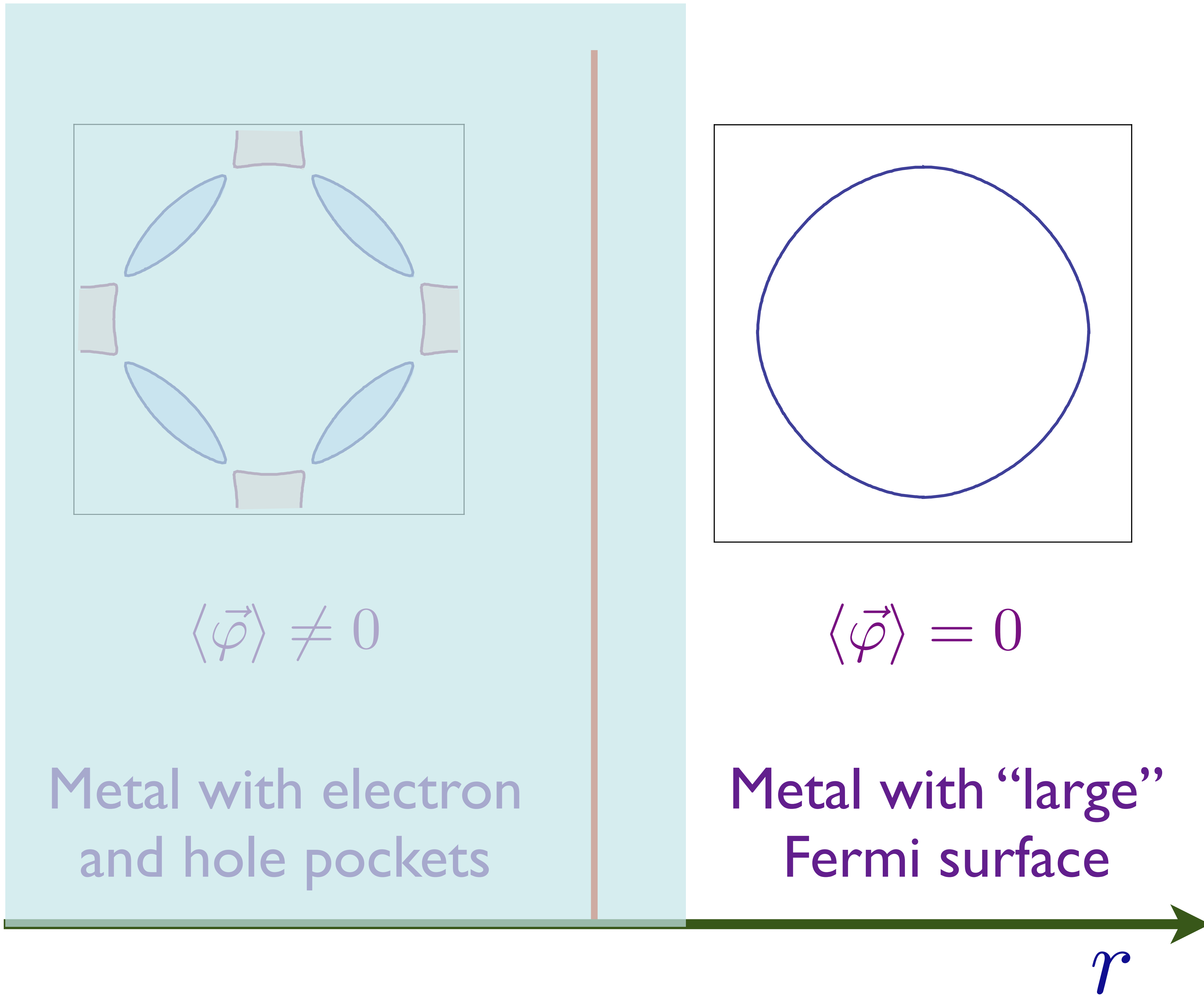
$\langle \vec{\varphi} \rangle = 0$

Metal with "large" Fermi surface

r

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



Rest of the talk

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).

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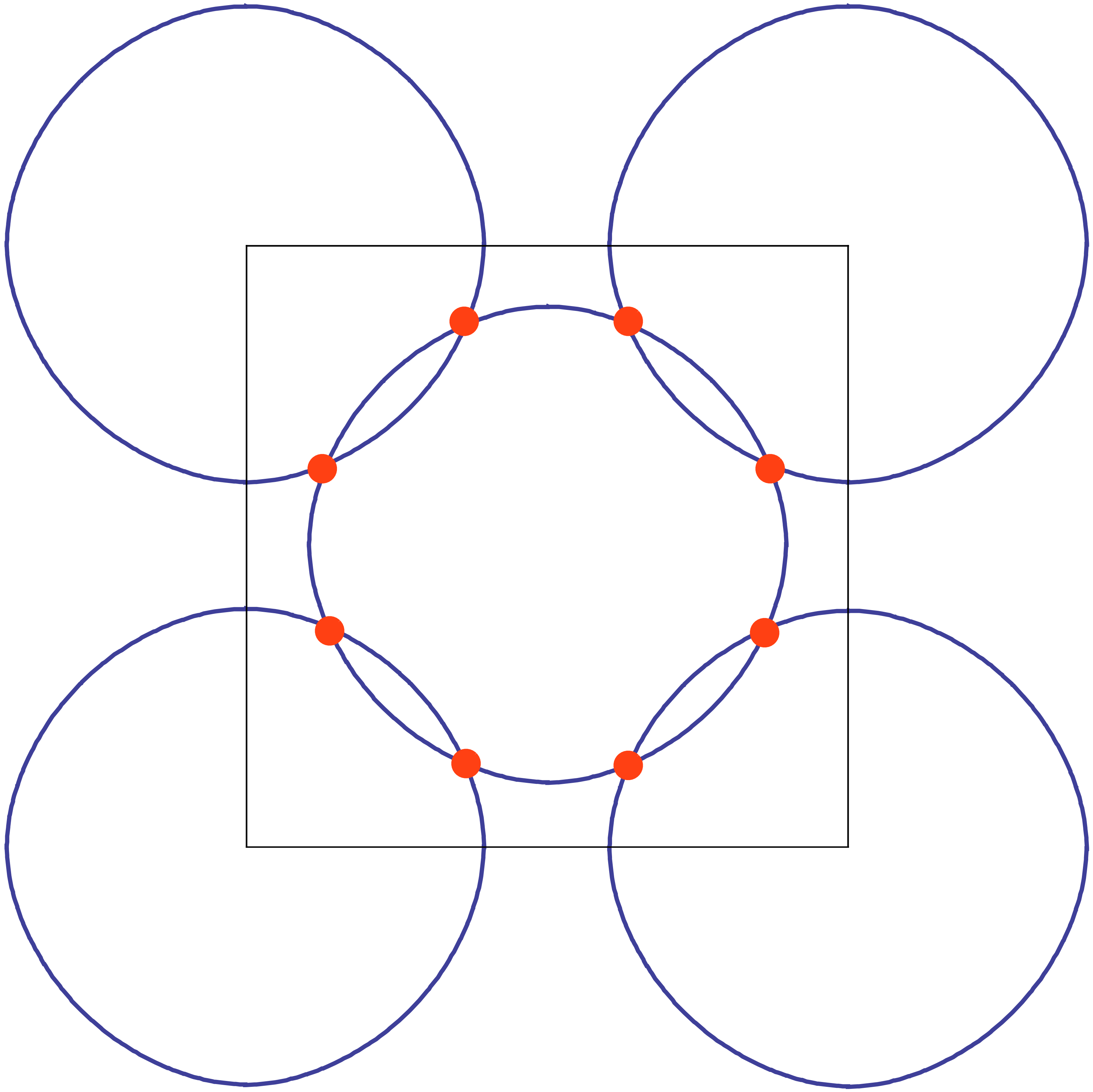
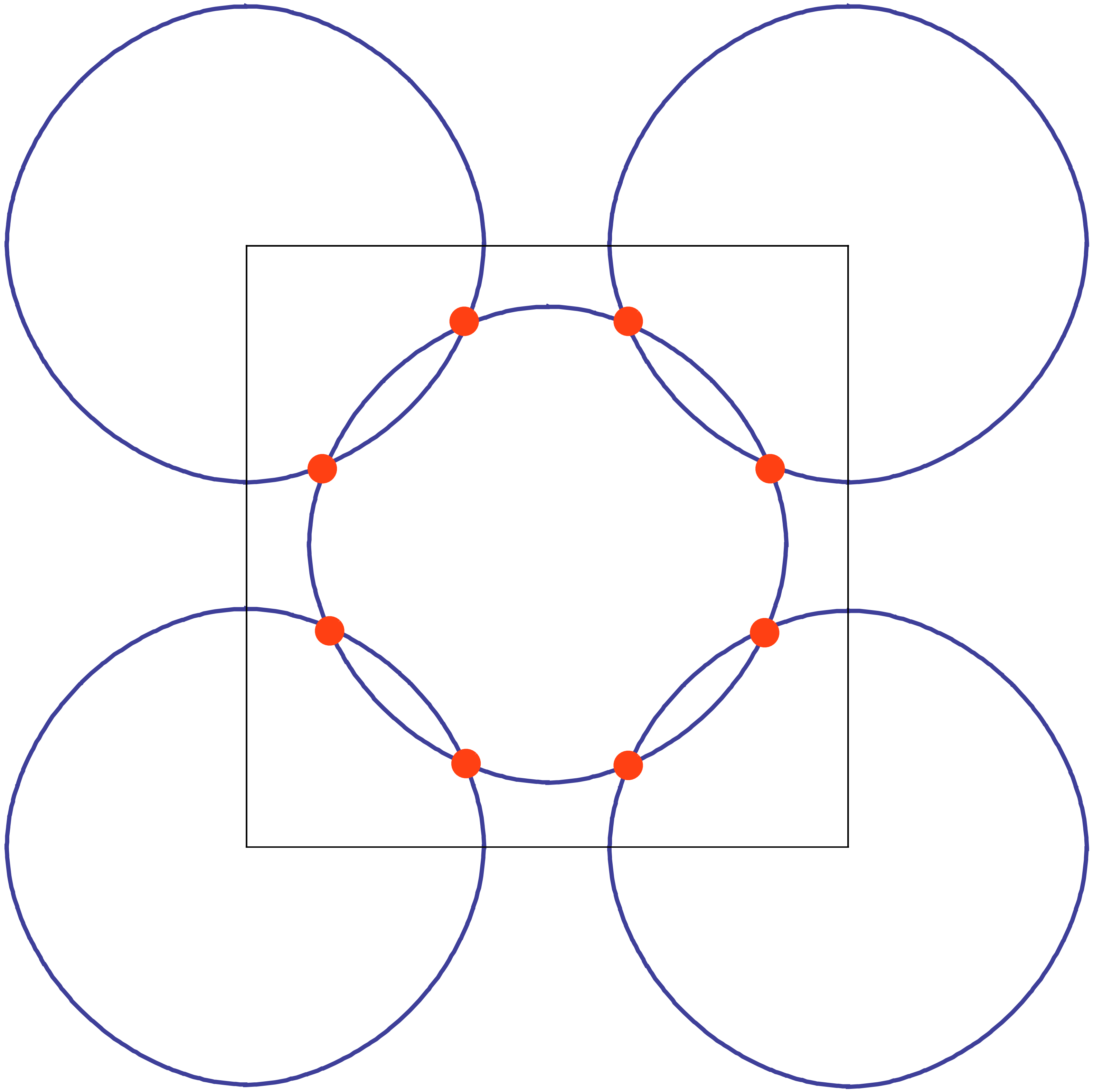
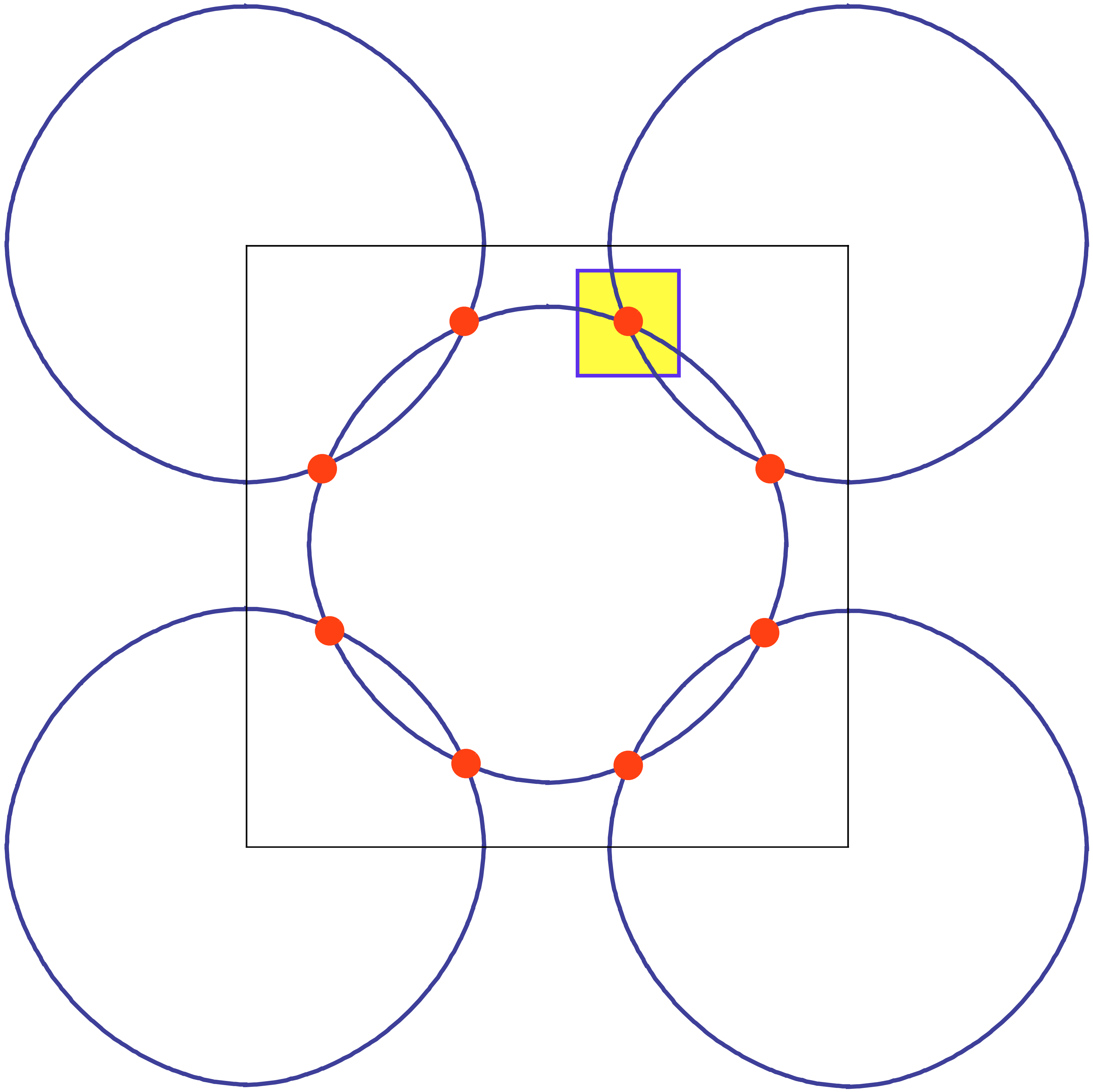


“Hot” spots

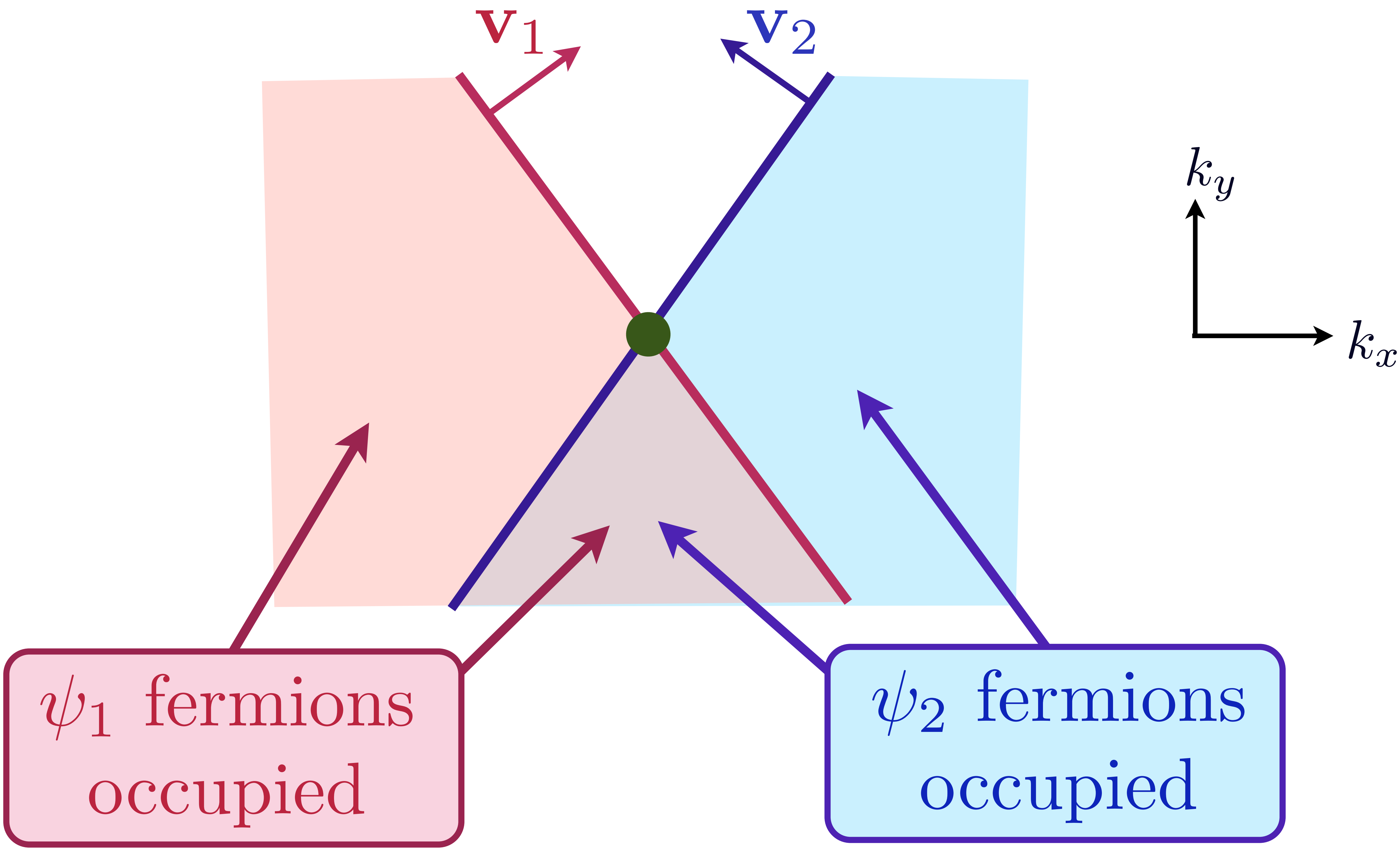


Low energy theory for critical point near hot spots



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



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Pairing by SDW fluctuation exchange

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

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

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.

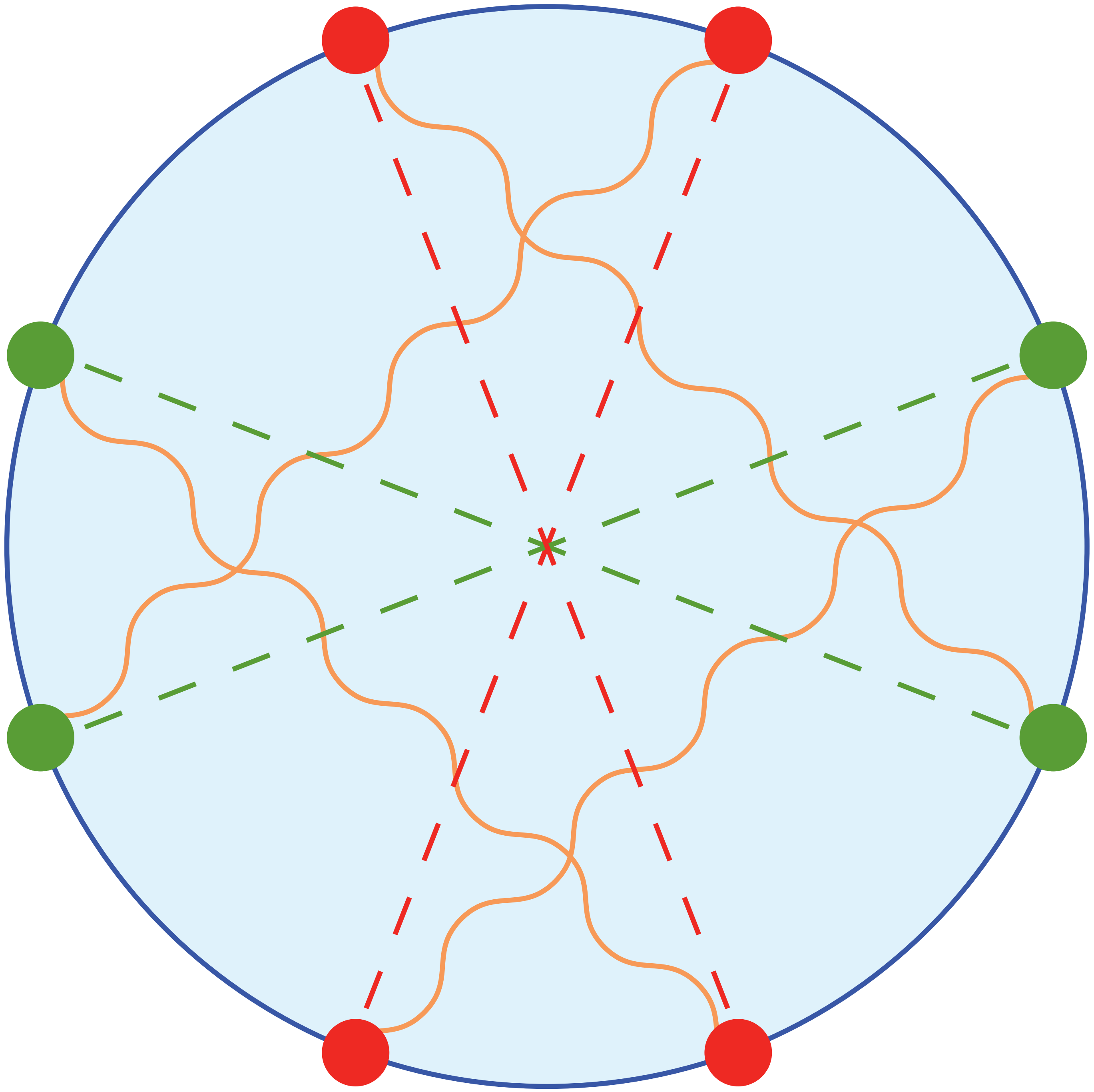
BCS Gap equation

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

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

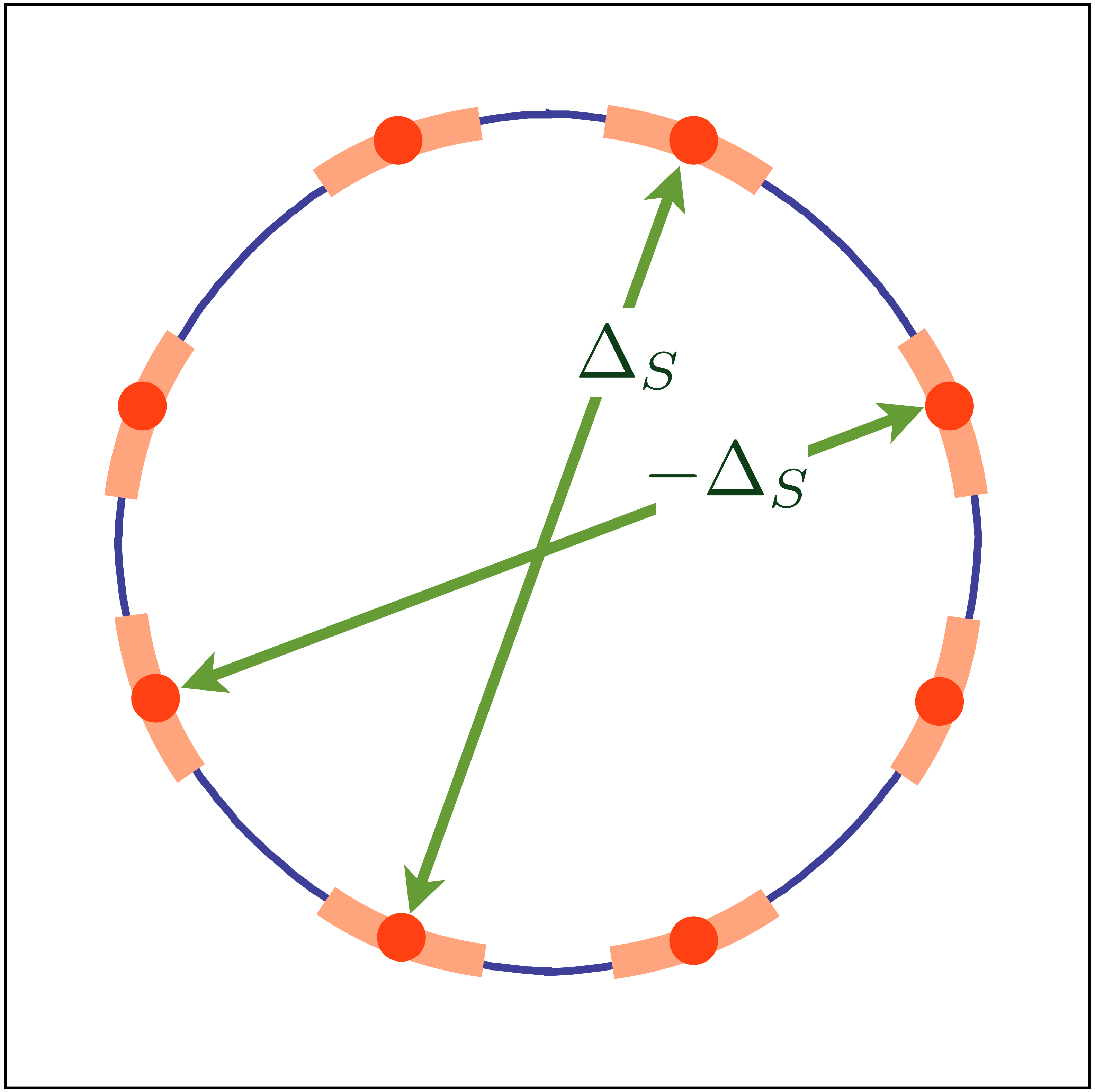
Non-zero solutions of this equation require that $\Delta_{\mathbf{k}}$ and $\Delta_{\mathbf{p}}$ have opposite signs when $\mathbf{p} - \mathbf{k} \approx \mathbf{K}$.

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)

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



Unconventional pairing at *and near* hot spots

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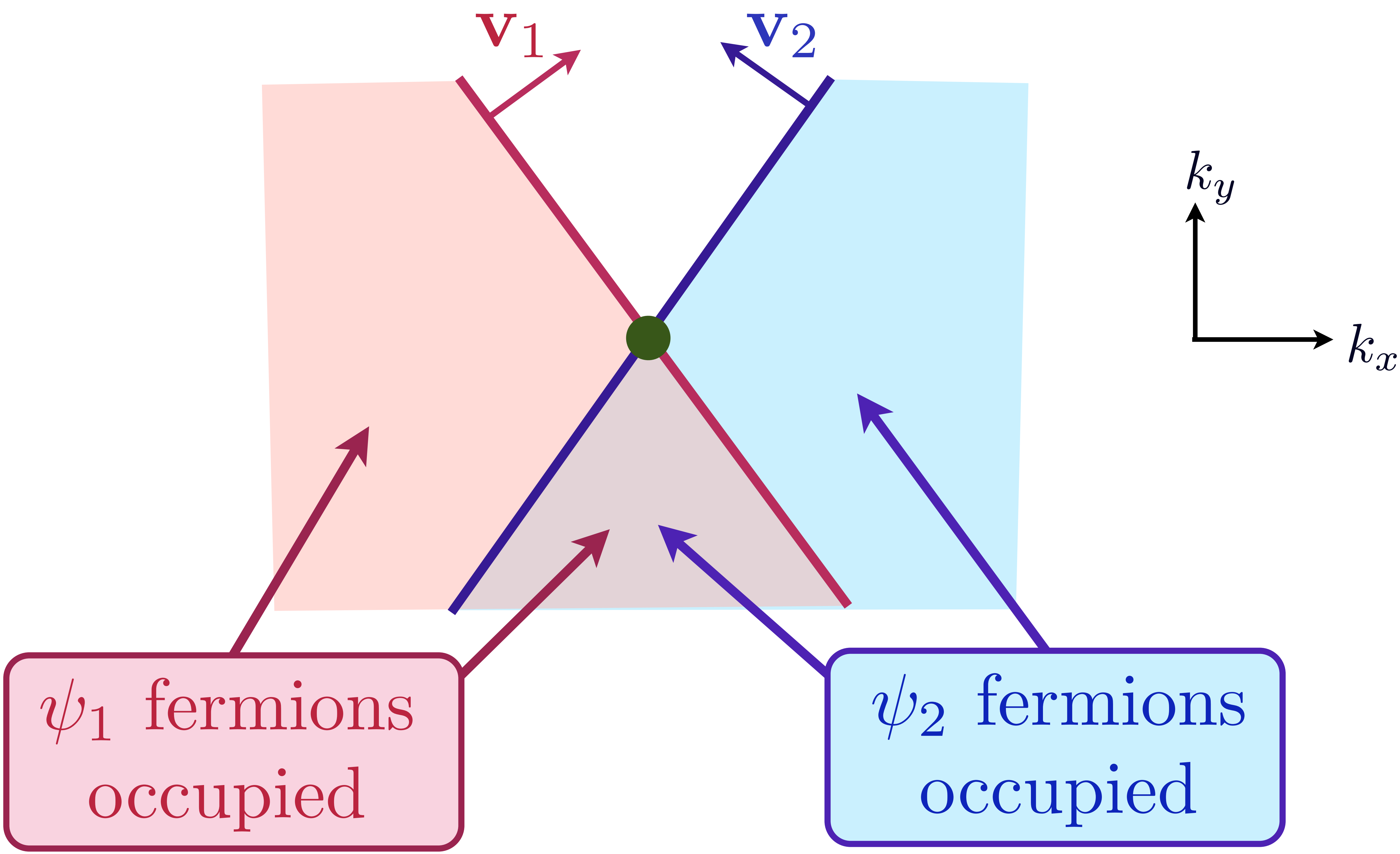
Theory has fermions $\psi_{1,2}$ (with Fermi velocities $\mathbf{v}_{1,2}$) and boson order parameter $\vec{\varphi}$, interacting with coupling λ



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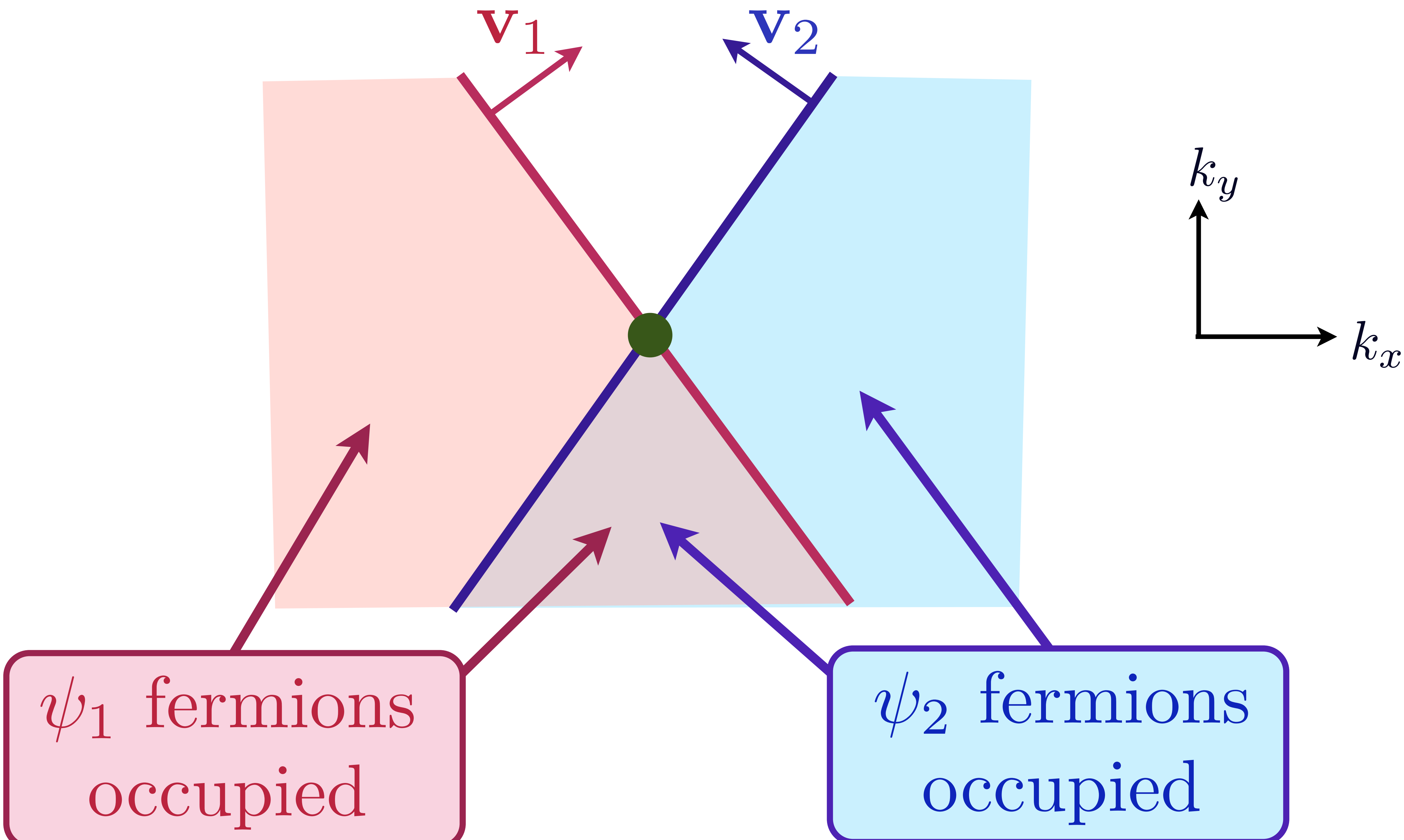

Theory has fermions $\psi_{1,2}$ (with Fermi velocities $\mathbf{v}_{1,2}$)
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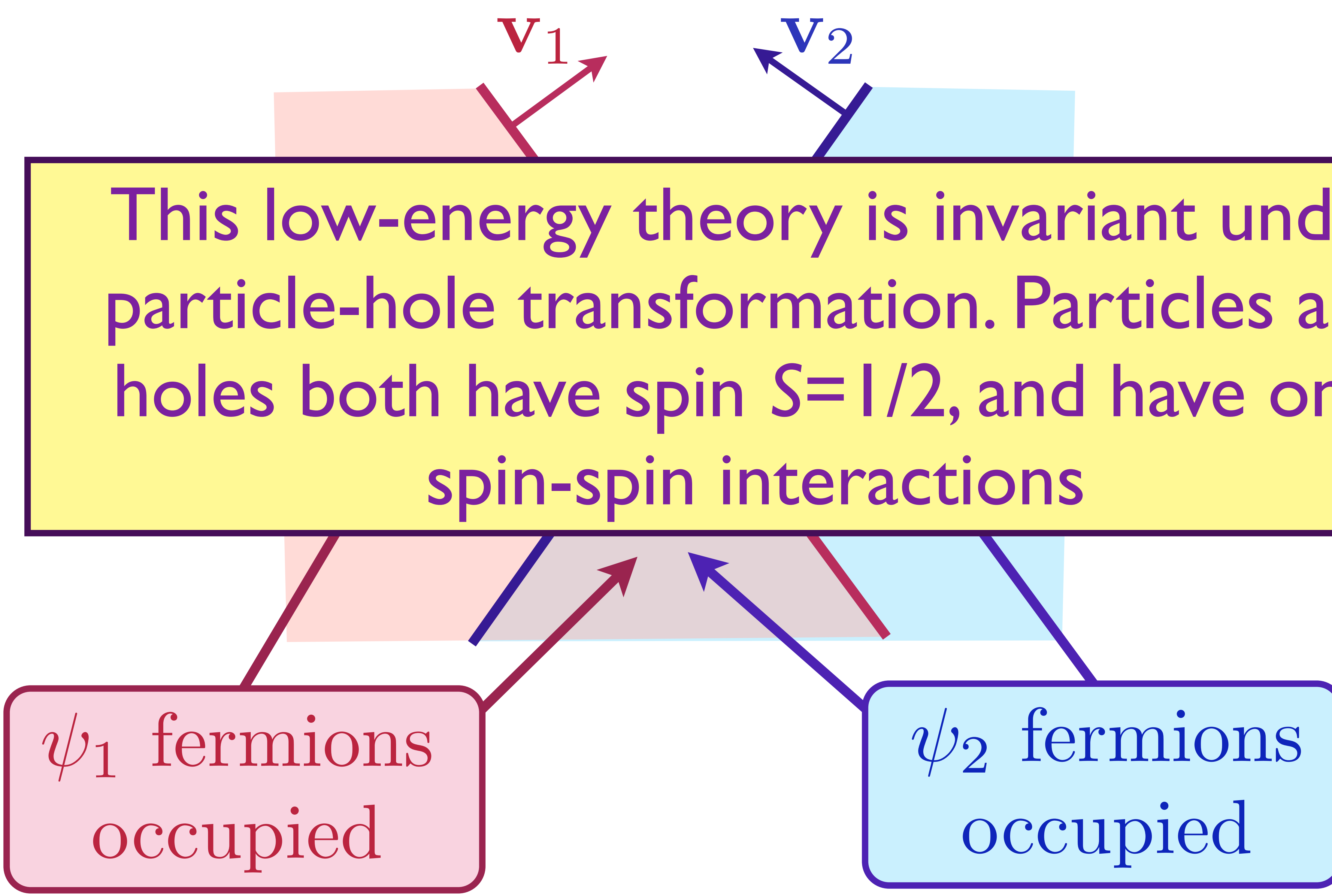
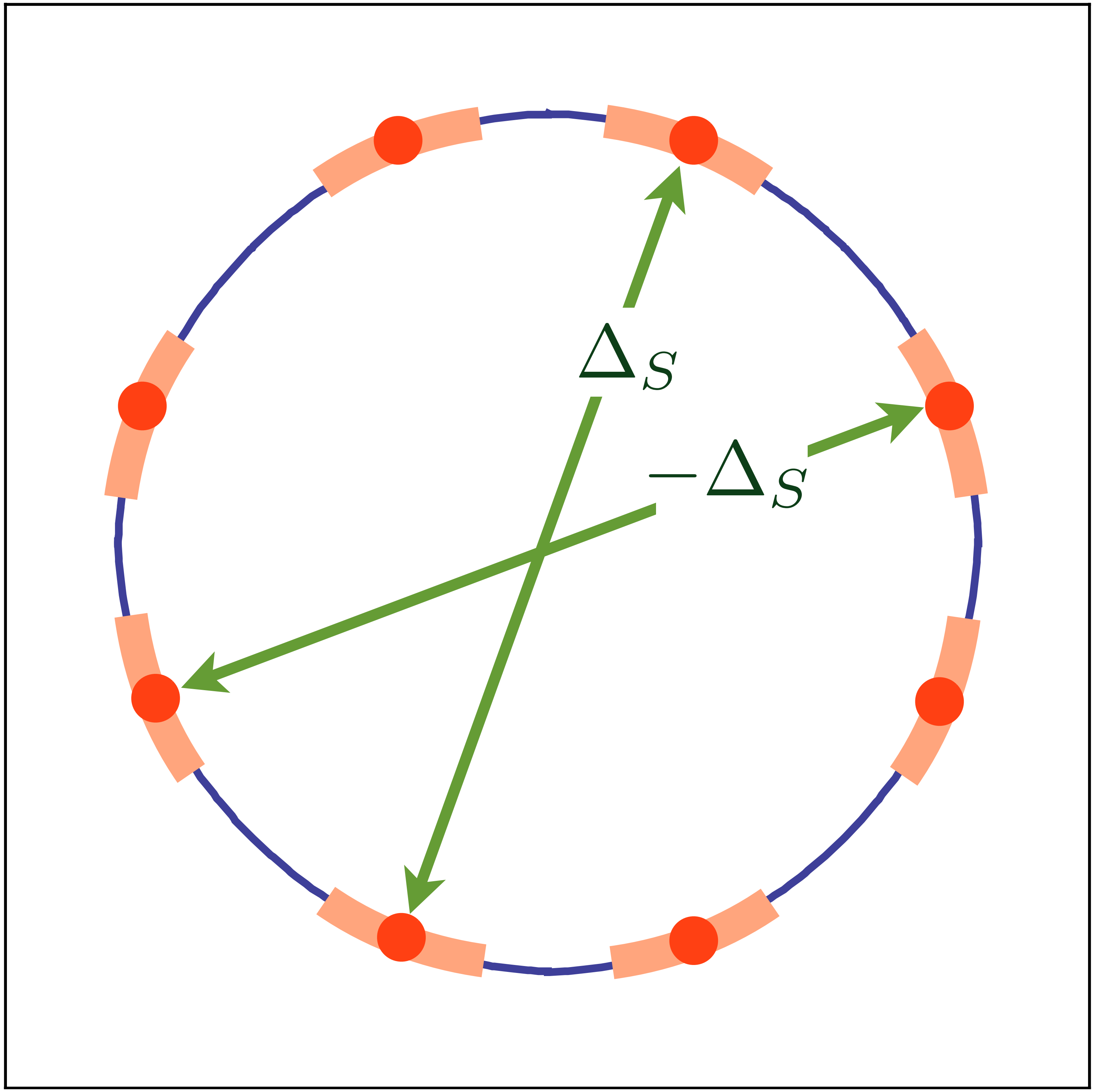


This low-energy theory is invariant under particle-hole transformation. Particles and holes both have spin S=1/2, and have only spin-spin interactions

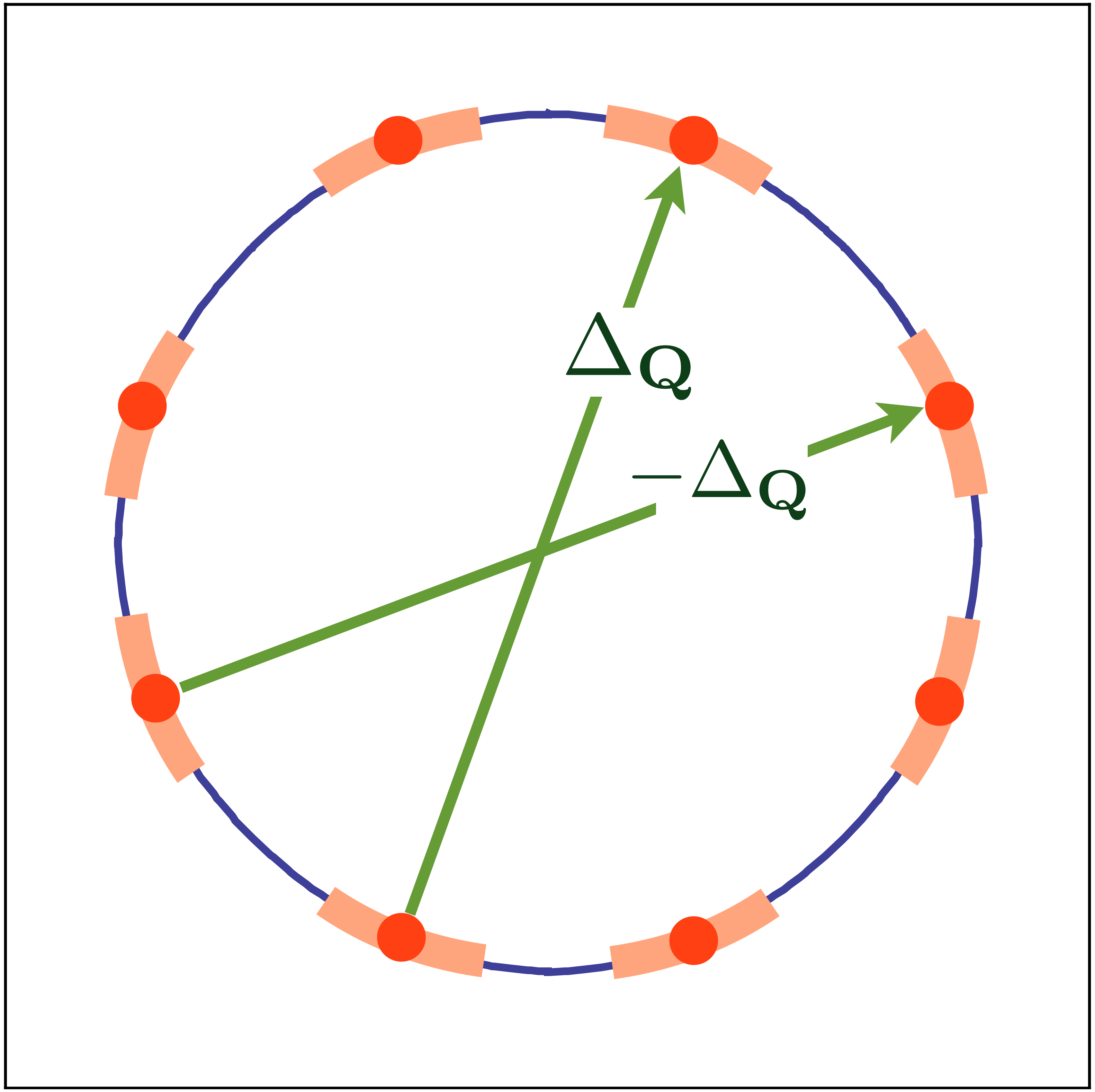
$$\left\langle c^\dagger_{\mathbf{k}\alpha} c^\dagger_{-\mathbf{k}\beta} \right\rangle = \varepsilon_{\alpha\beta} \Delta_S (\cos k_x - \cos k_y)$$



Unconventional pairing at *and near* hot spots

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

After pseudospin rotation



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

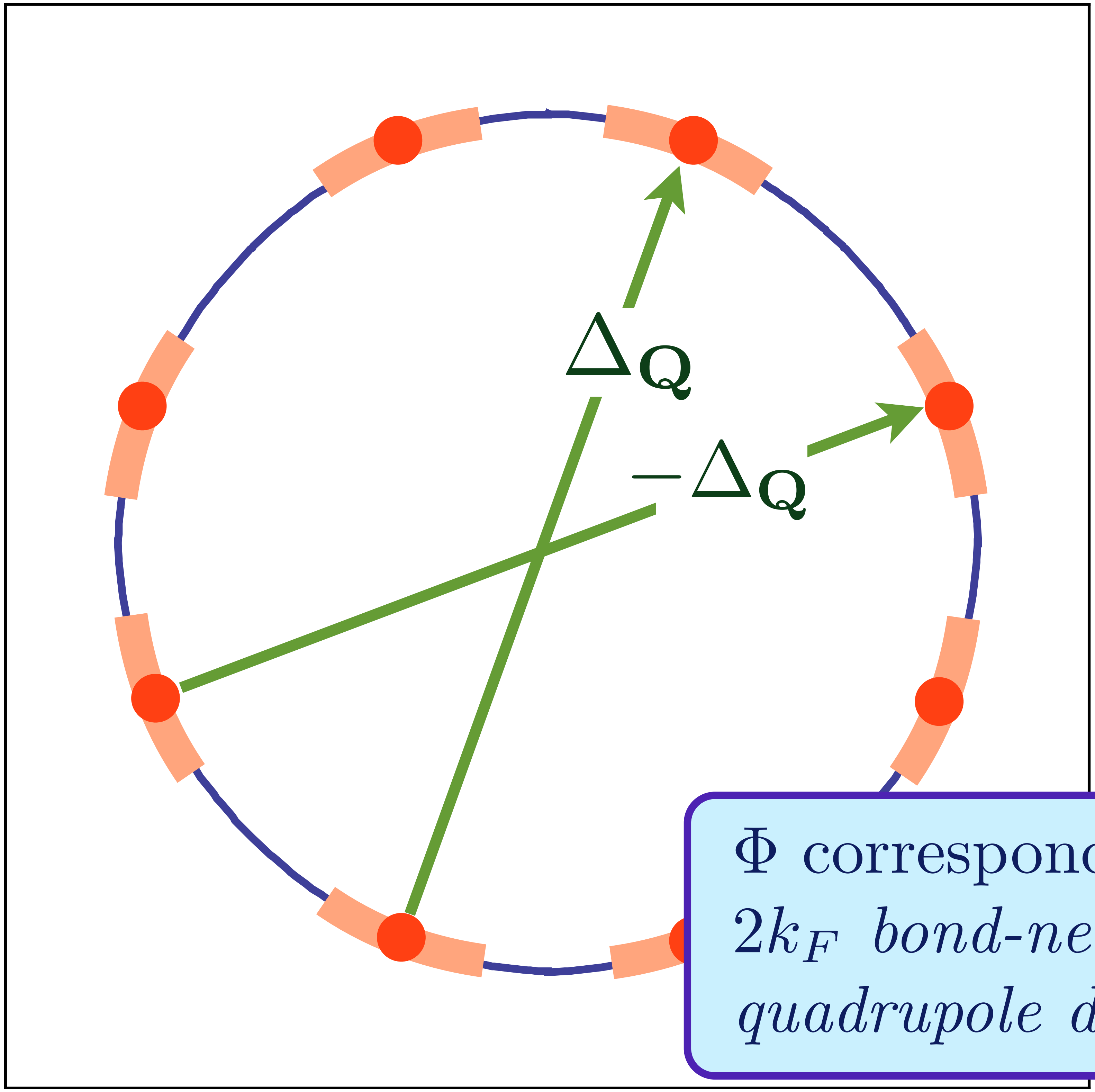
M. A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)

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

Unconventional particle-hole pairing at *and near* hot spots

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

After pseudospin rotation



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

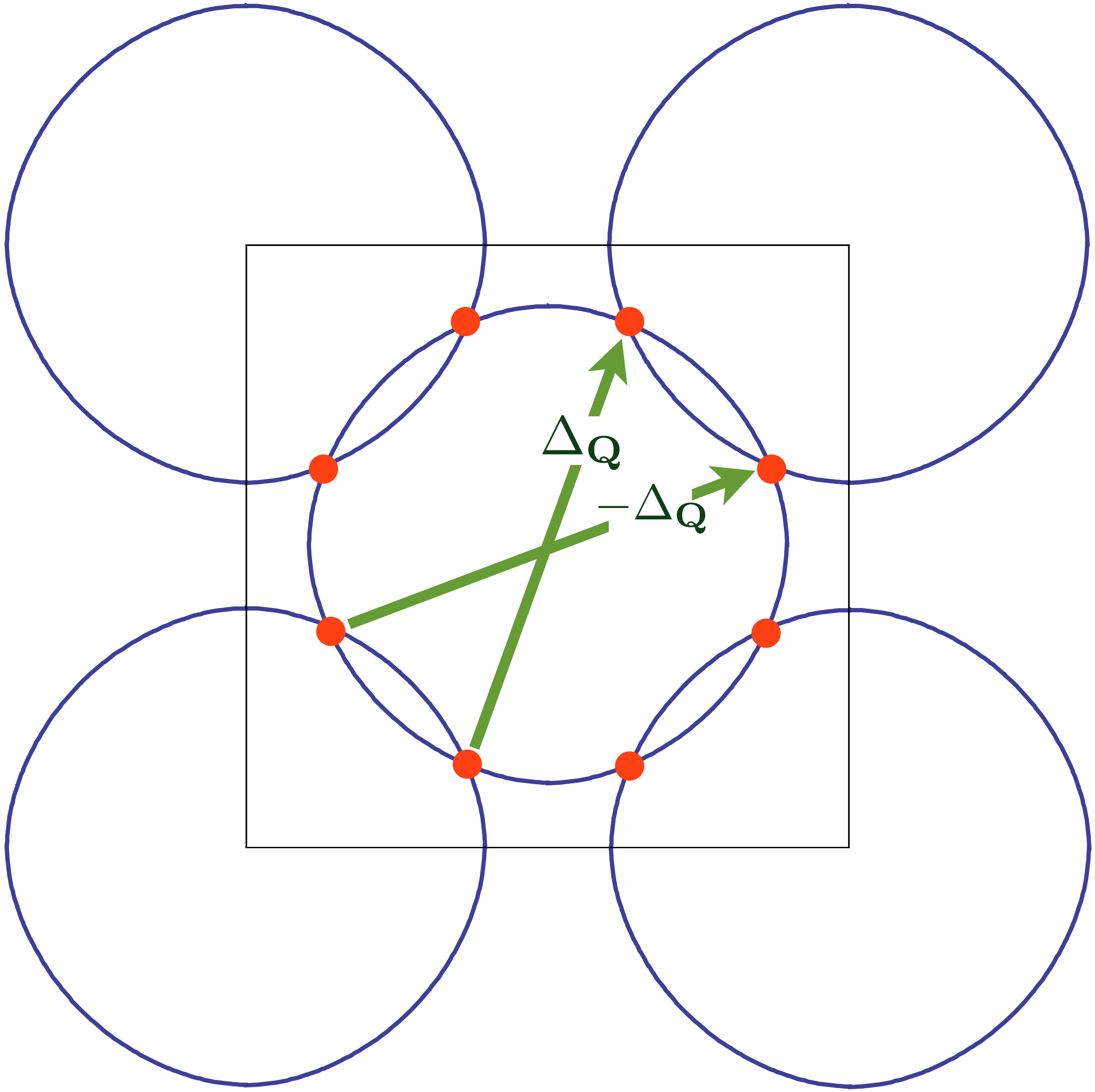
M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)

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

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

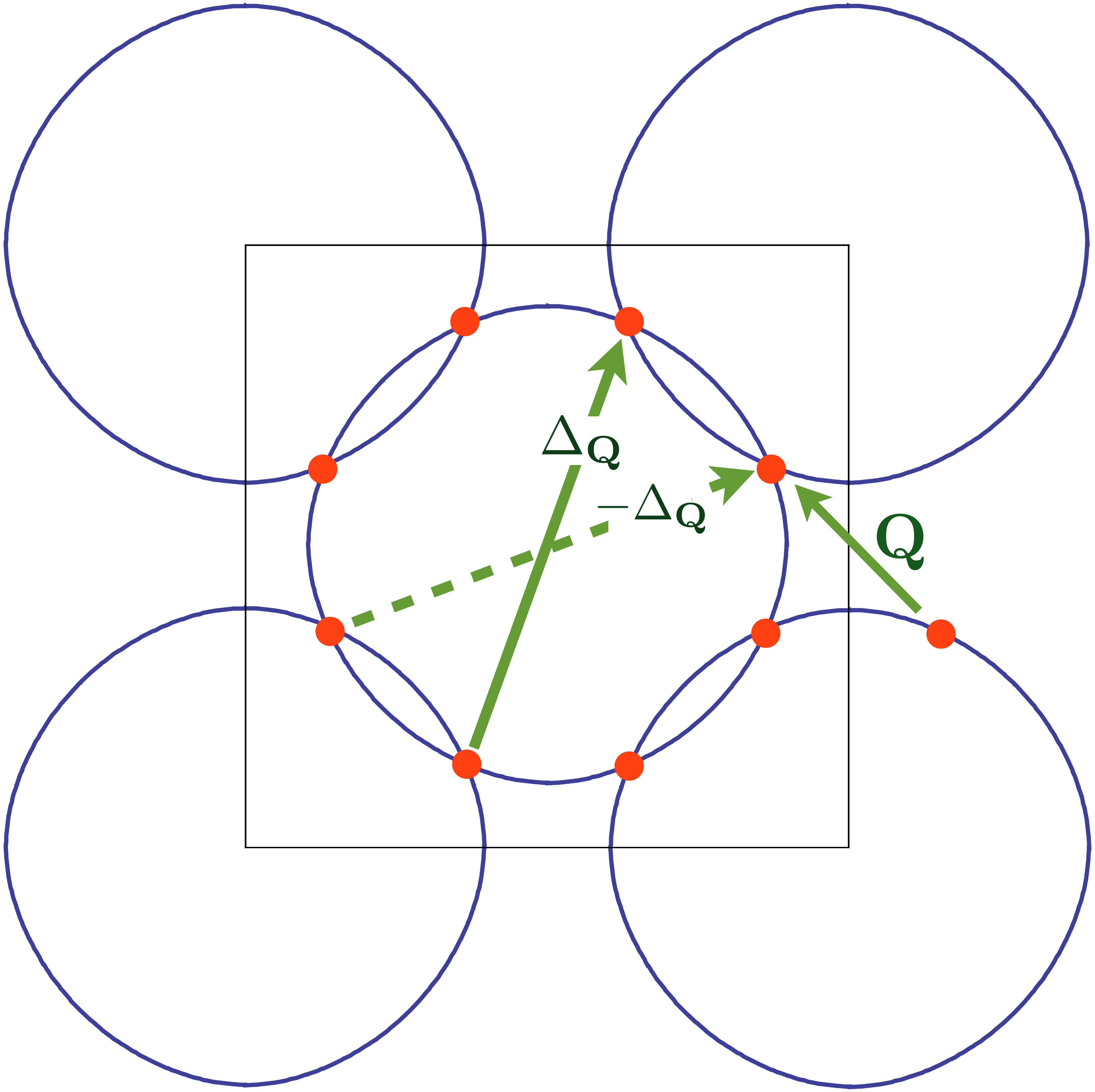
Unconventional particle-hole pairing at *and near* hot spots

Incommensurate bond order



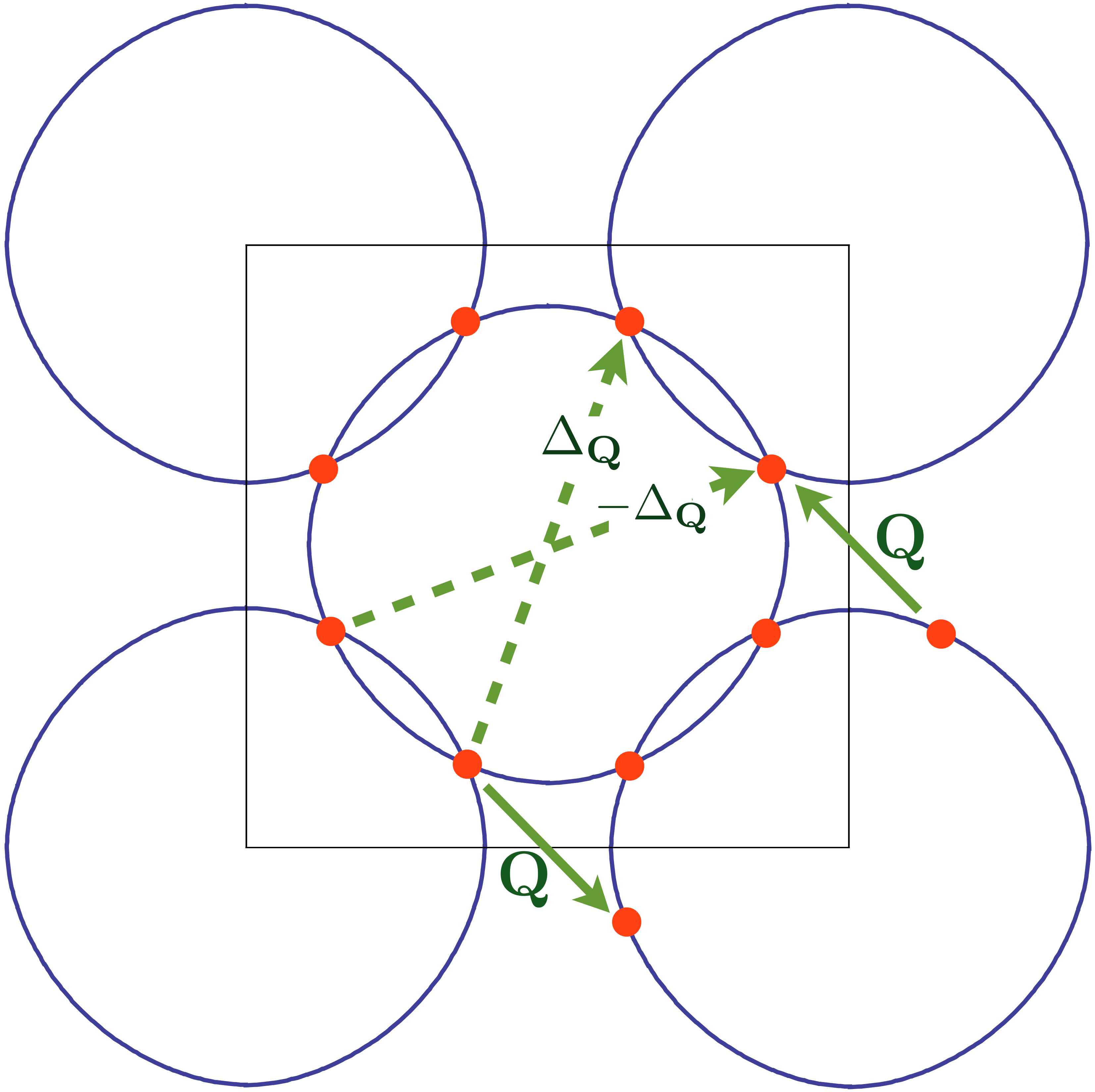
$$\left\langle c^\dagger_{\mathbf{k}-\mathbf{Q}/2,\alpha} c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \right\rangle = \Delta_{\mathbf{Q}} (\cos k_x - \cos k_y)$$

Incommensurate bond order



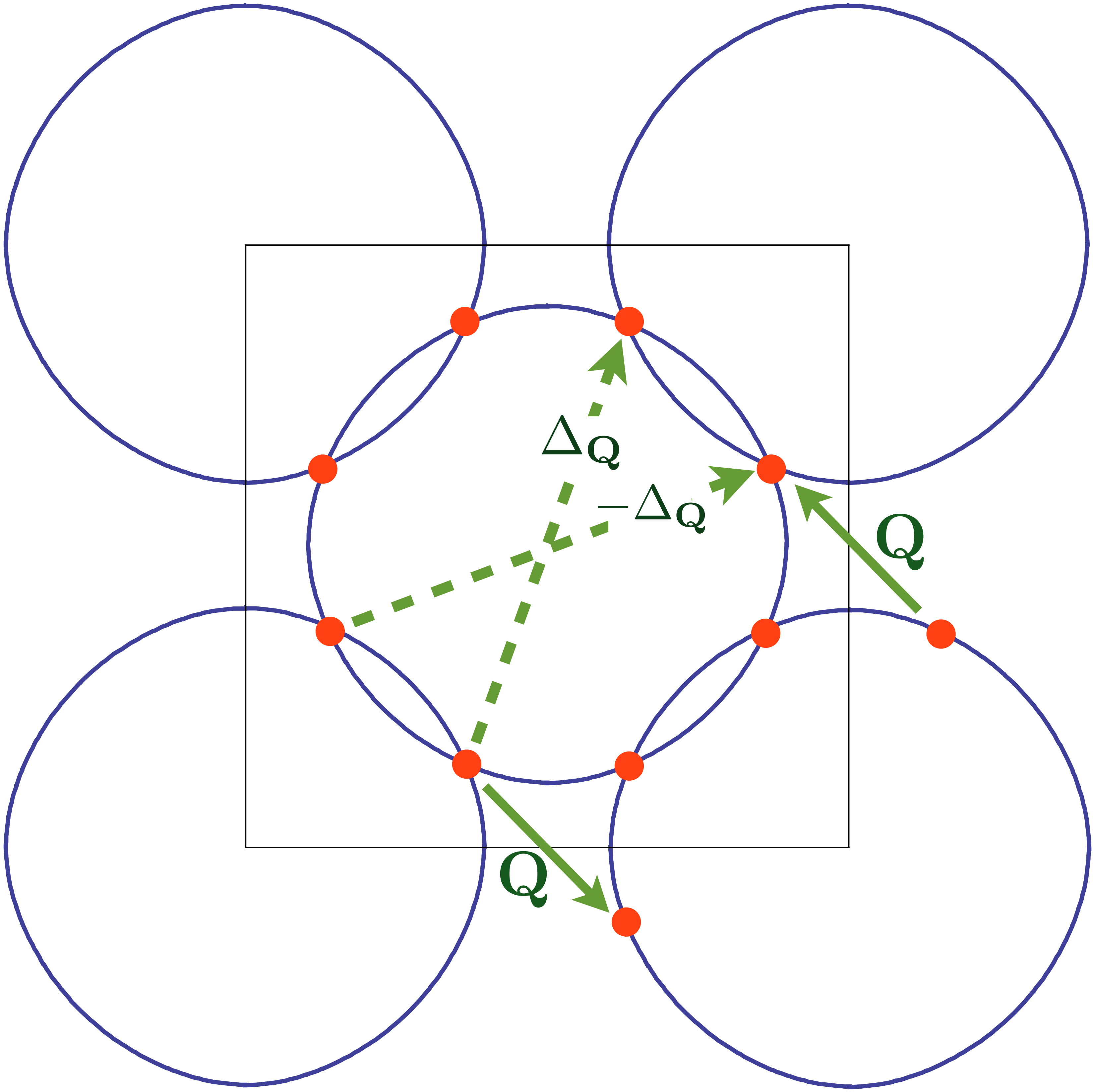
$$\left\langle c^\dagger_{\mathbf{k}-\mathbf{Q}/2,\alpha} c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \right\rangle = \Delta_{\mathbf{Q}} (\cos k_x - \cos k_y)$$

Incommensurate bond order



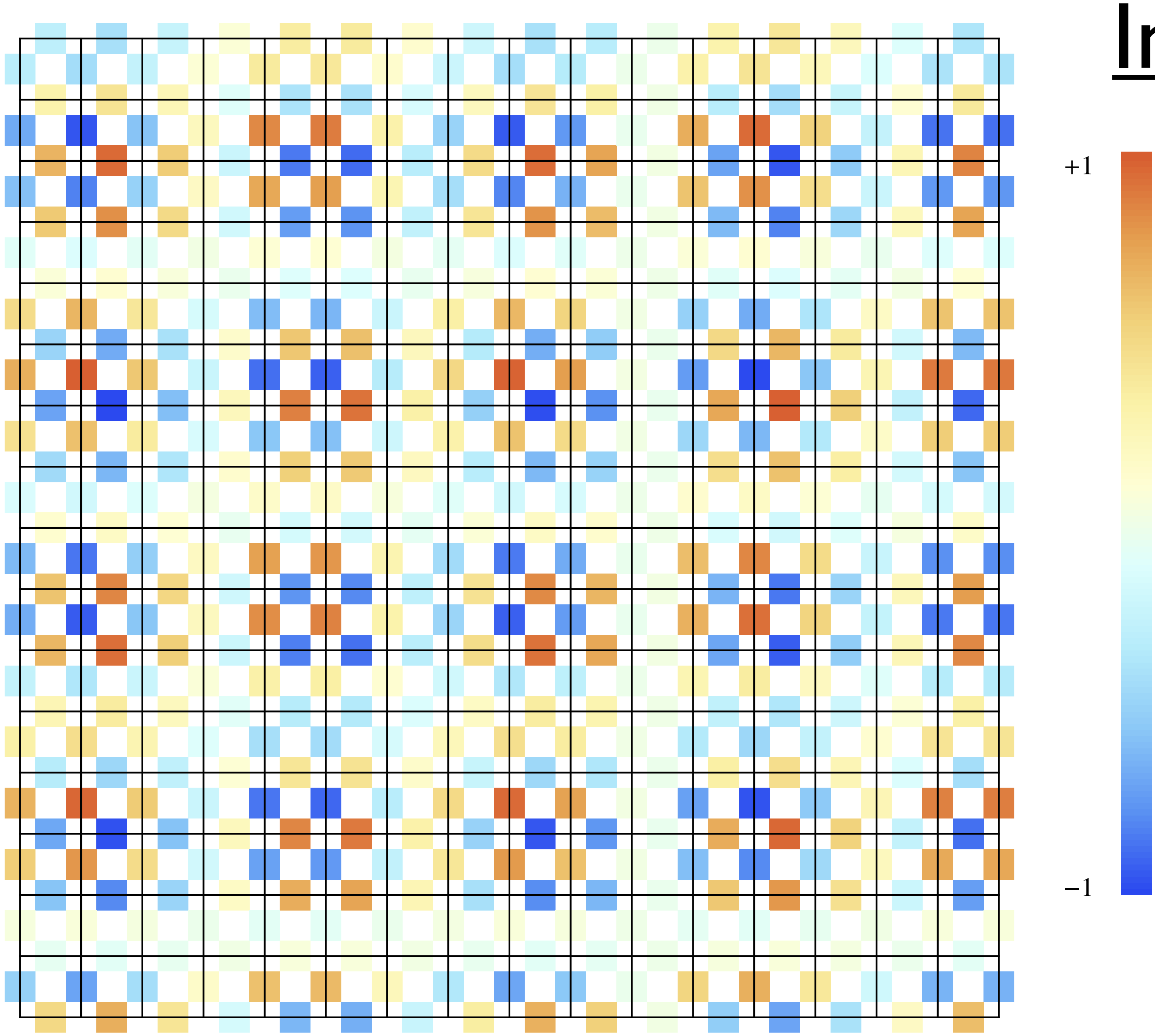
$$\left\langle c^{\dagger}_{\mathbf{k}-\mathbf{Q}/2,\alpha} c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \right\rangle = \Delta_{\mathbf{Q}} (\cos k_x - \cos k_y)$$

Incommensurate bond order



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

Incommensurate 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)

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

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Hartree-Fock computation on lattice model

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

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

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

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$$H_{MF} = \sum_{\boldsymbol{k}} \Bigg[\varepsilon(\boldsymbol{k})\, c^\dagger_{\boldsymbol{k},\alpha} c_{\boldsymbol{k},\alpha} + \Delta_S(\boldsymbol{k})\, \epsilon_{\alpha\beta}\, c_{\boldsymbol{k},\alpha} c_{-\boldsymbol{k}\beta} + \text{H.c.}$$

$$+ \sum_{\boldsymbol{Q}} \Delta_{\boldsymbol{Q}}(\boldsymbol{k})\, c^\dagger_{\boldsymbol{k}+\boldsymbol{Q}/2,\alpha} c_{\boldsymbol{k}-\boldsymbol{Q}/2,\alpha} \Bigg],$$

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

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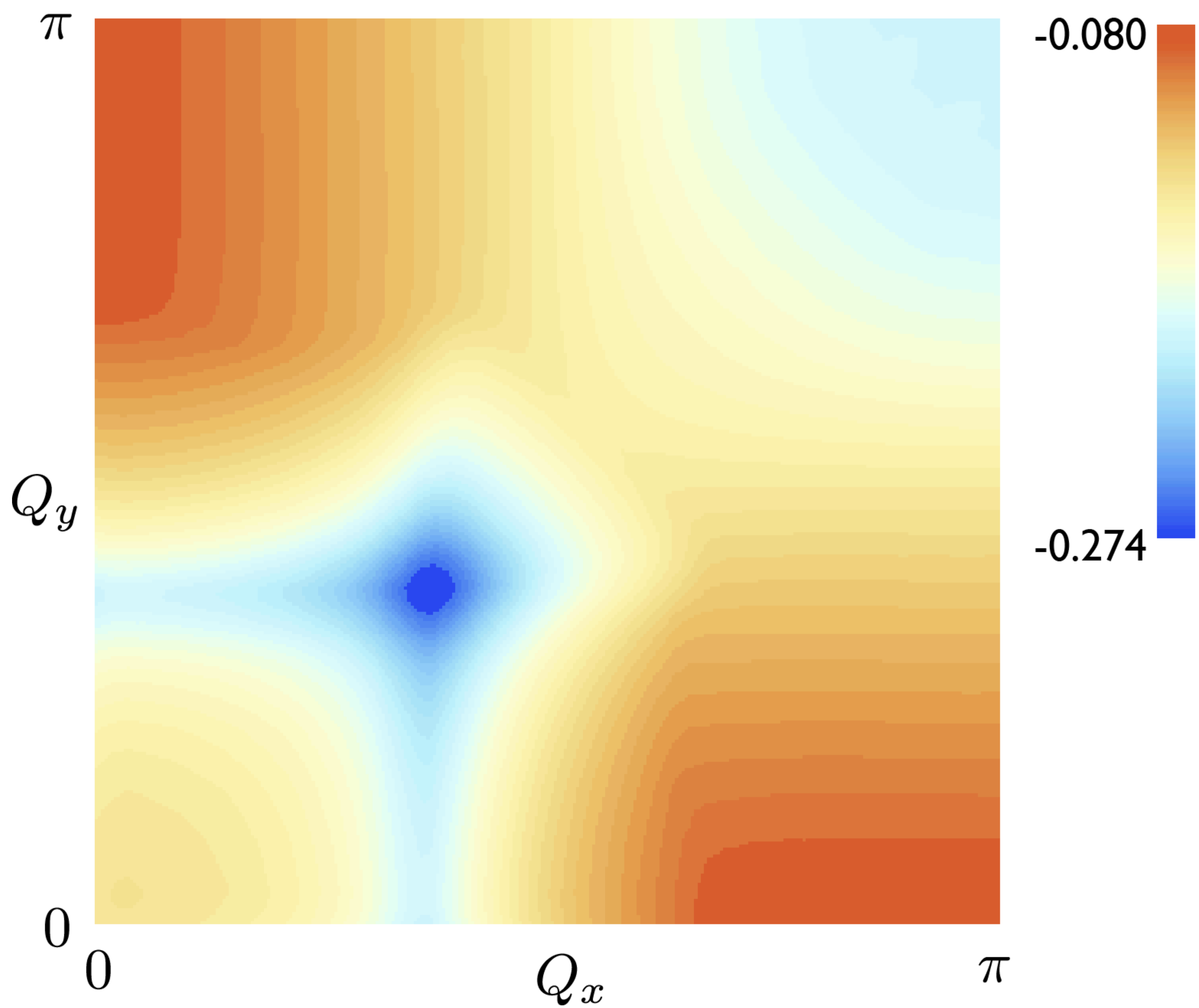
$$+ \sum_{\boldsymbol{Q}} \Delta_{\boldsymbol{Q}}(\boldsymbol{k}) \, c^{\dagger}_{\boldsymbol{k}+\boldsymbol{Q}/2,\alpha} c_{\boldsymbol{k}-\boldsymbol{Q}/2,\alpha} \Big],$$

Expand F to second order in $\Delta_S(\mathbf{k})$ and $\Delta_{\mathbf{Q}}(\mathbf{k})$, and obtain lowest eigenvalues λ_S and $\lambda_{\mathbf{Q}}$ and corresponding eigenvectors $\Delta_S(\mathbf{k})$ and $\Delta_{\mathbf{Q}}(\mathbf{k})$.

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

Hartree-Fock computation on lattice model



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

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

Hartree-Fock computation on lattice model

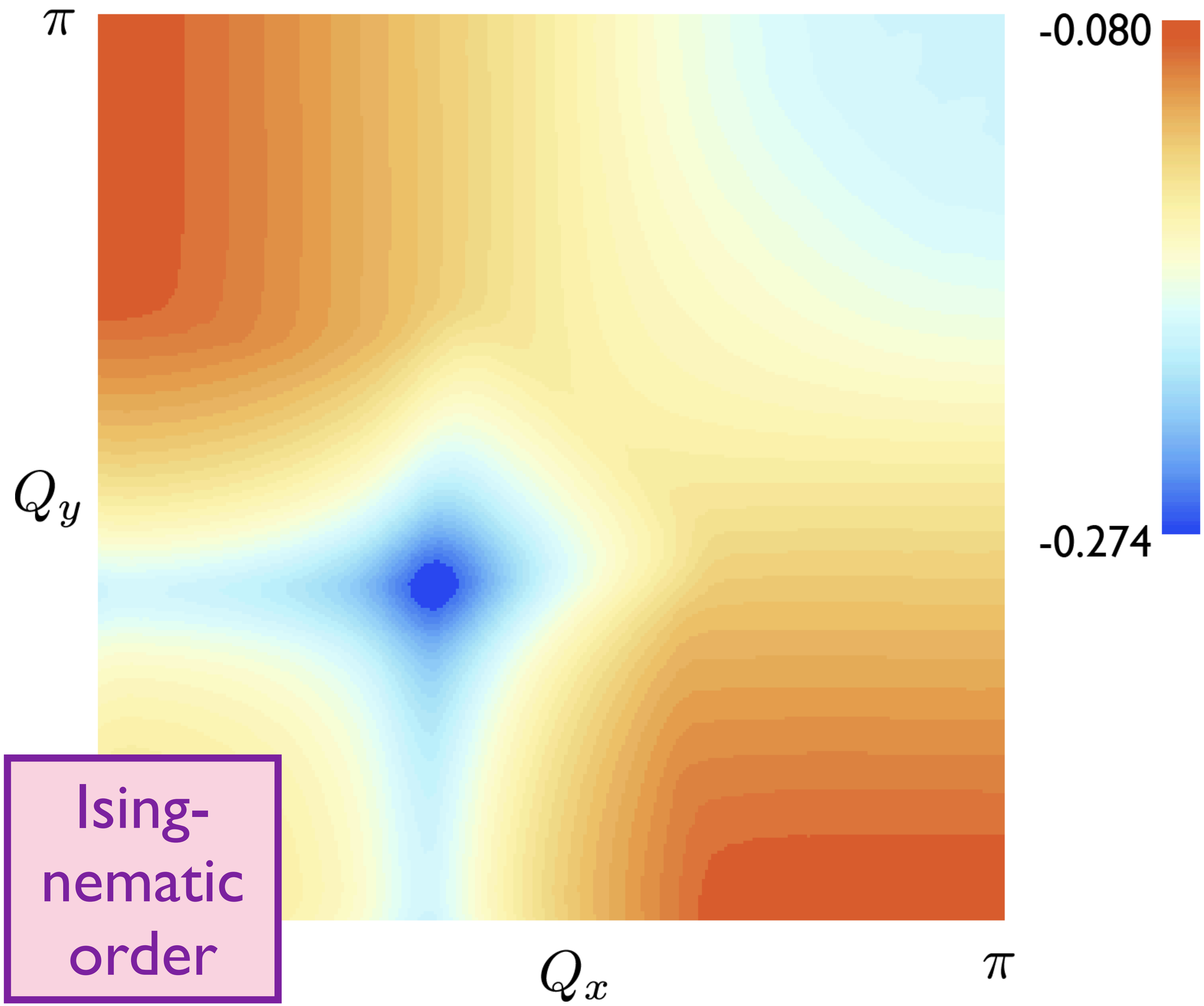
$$\Delta_{\boldsymbol{Q}}(\boldsymbol{k}) = \sum_{\gamma} c_{\boldsymbol{Q},\gamma}\, \psi_\gamma(\boldsymbol{k})$$

γ	$\psi_\gamma(\boldsymbol{k})$	$\boldsymbol{Q}=$ (1.15,1.15)	$\boldsymbol{Q}=$ (1.15, 0)	$\boldsymbol{Q}=$ (0,0)	$\boldsymbol{Q}=$ (π,π)	$\Delta_S(\boldsymbol{k})$
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

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

Hartree-Fock computation on lattice model



Ising-nematic order

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

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

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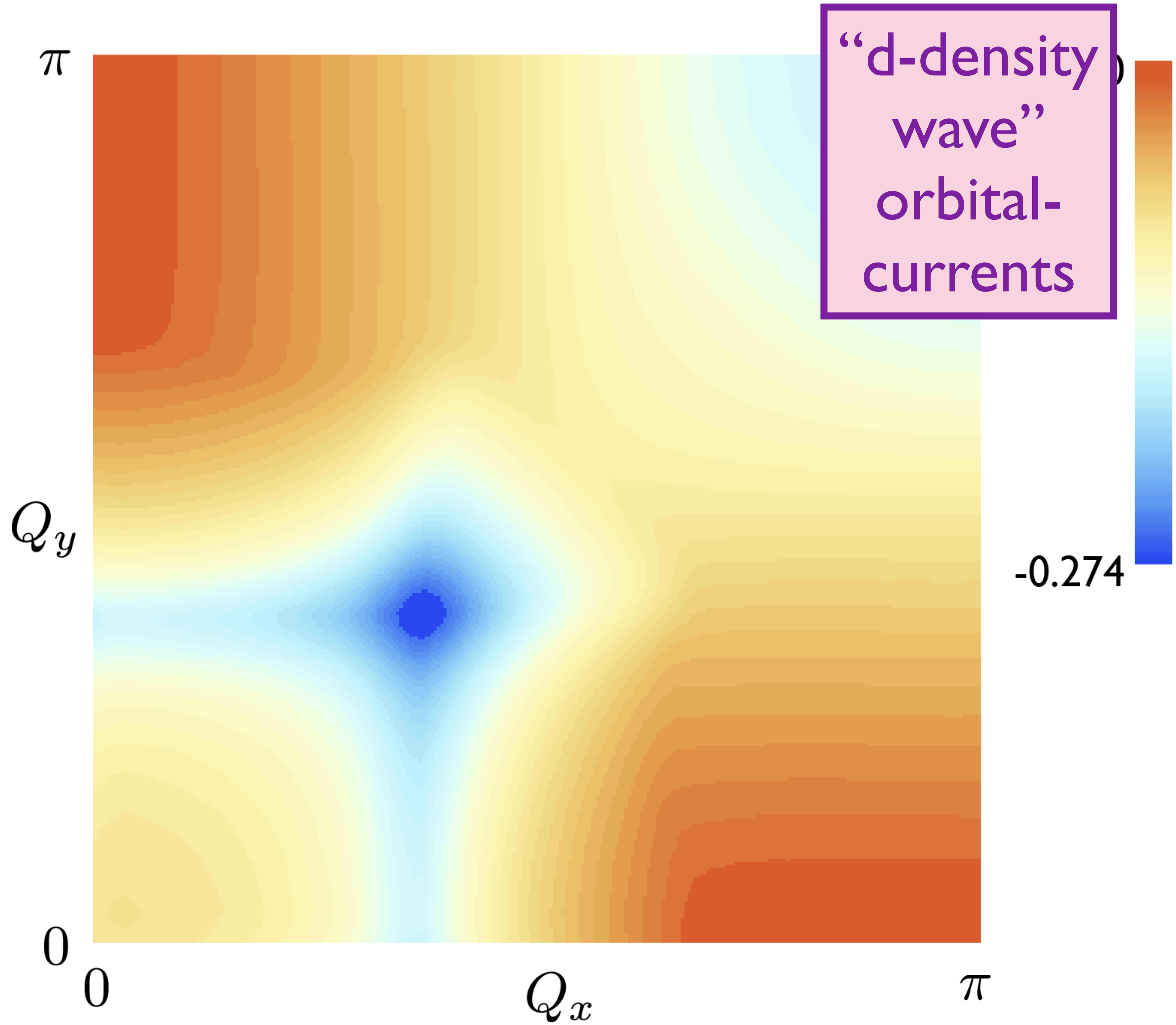

Charge-ordering eigenvalue $\lambda_{\mathbf{Q}}$.

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

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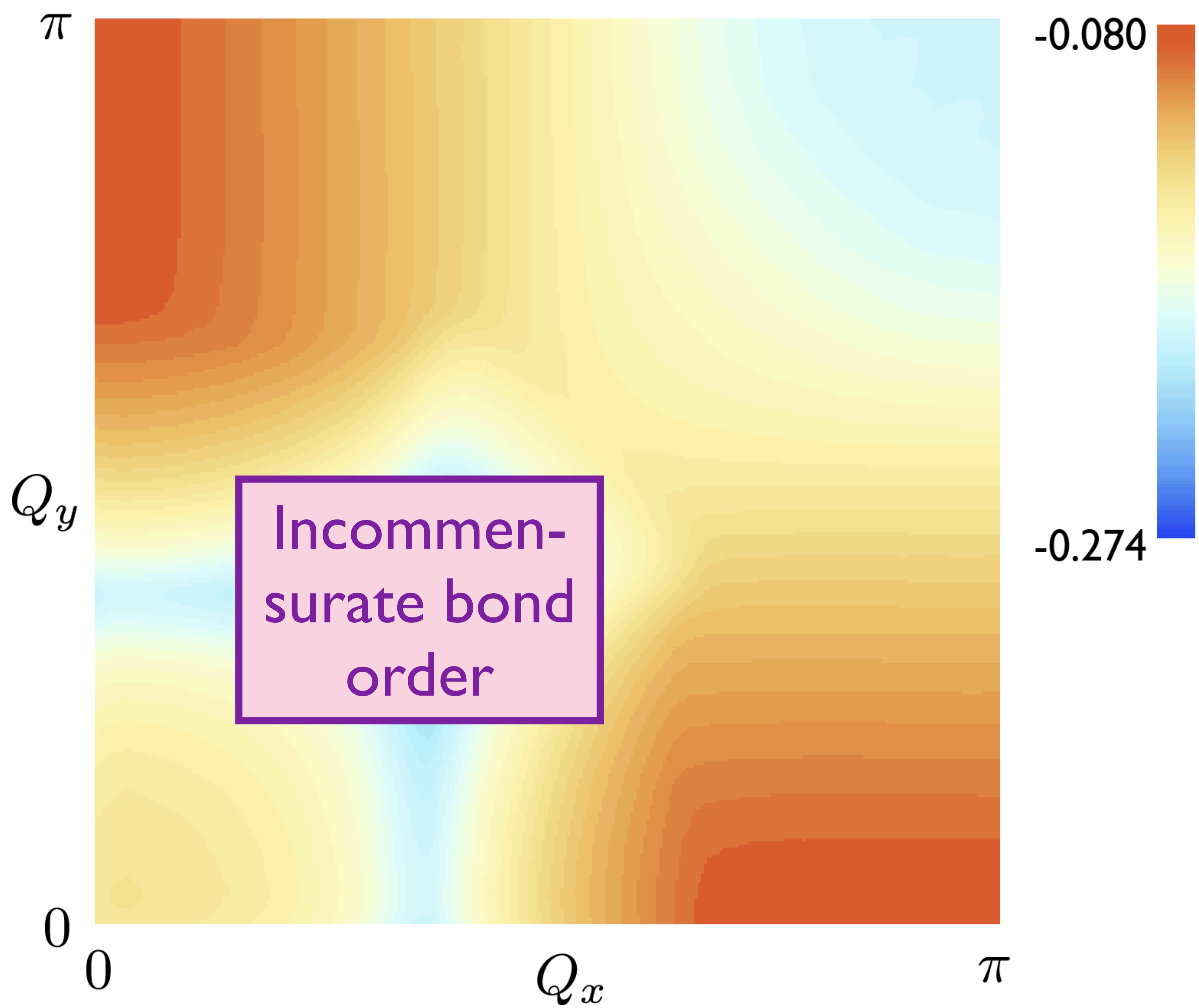
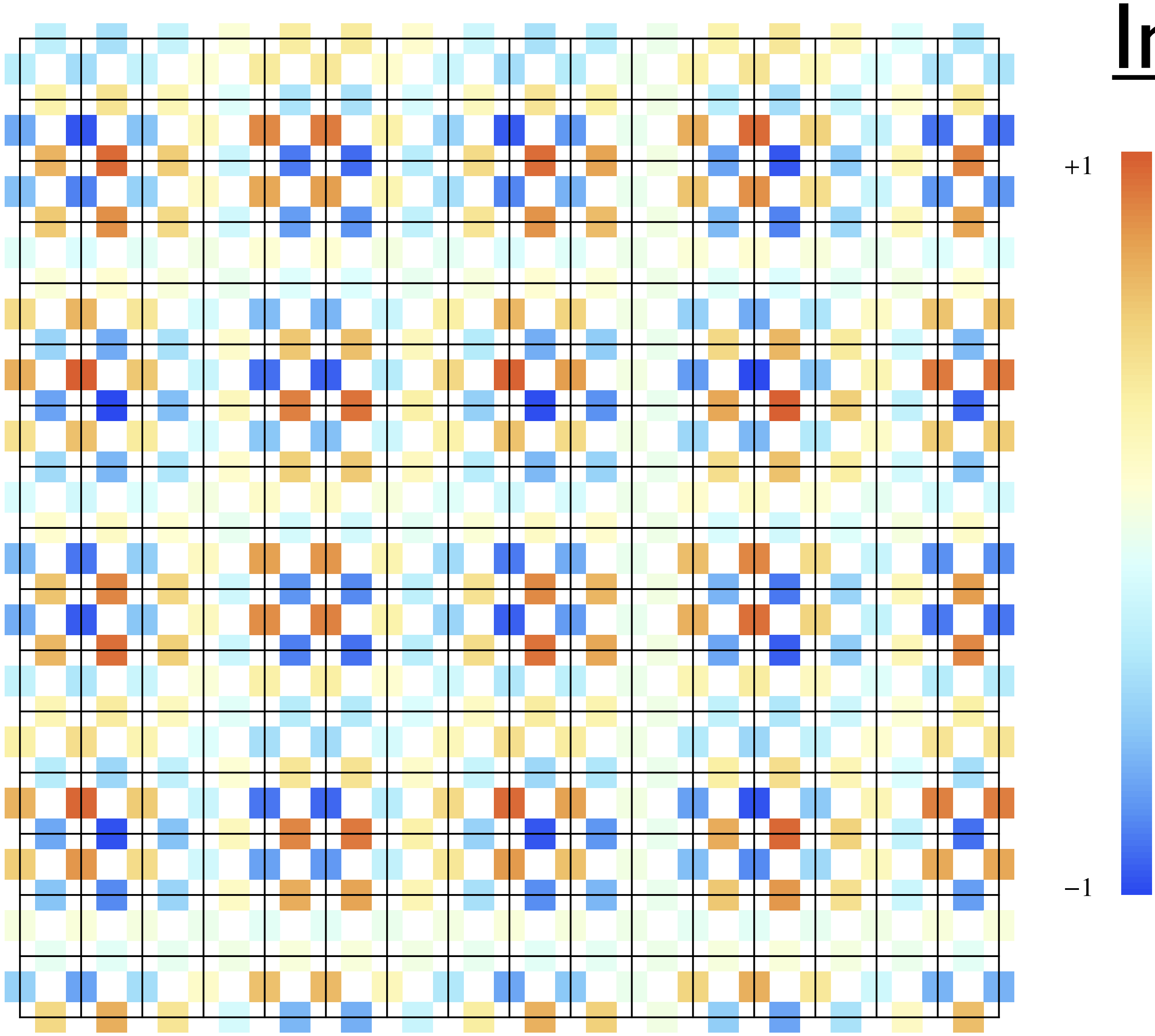


Charge-ordering eigenvalue $\lambda_{\mathbf{Q}}$.

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

Incommensurate bond order



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

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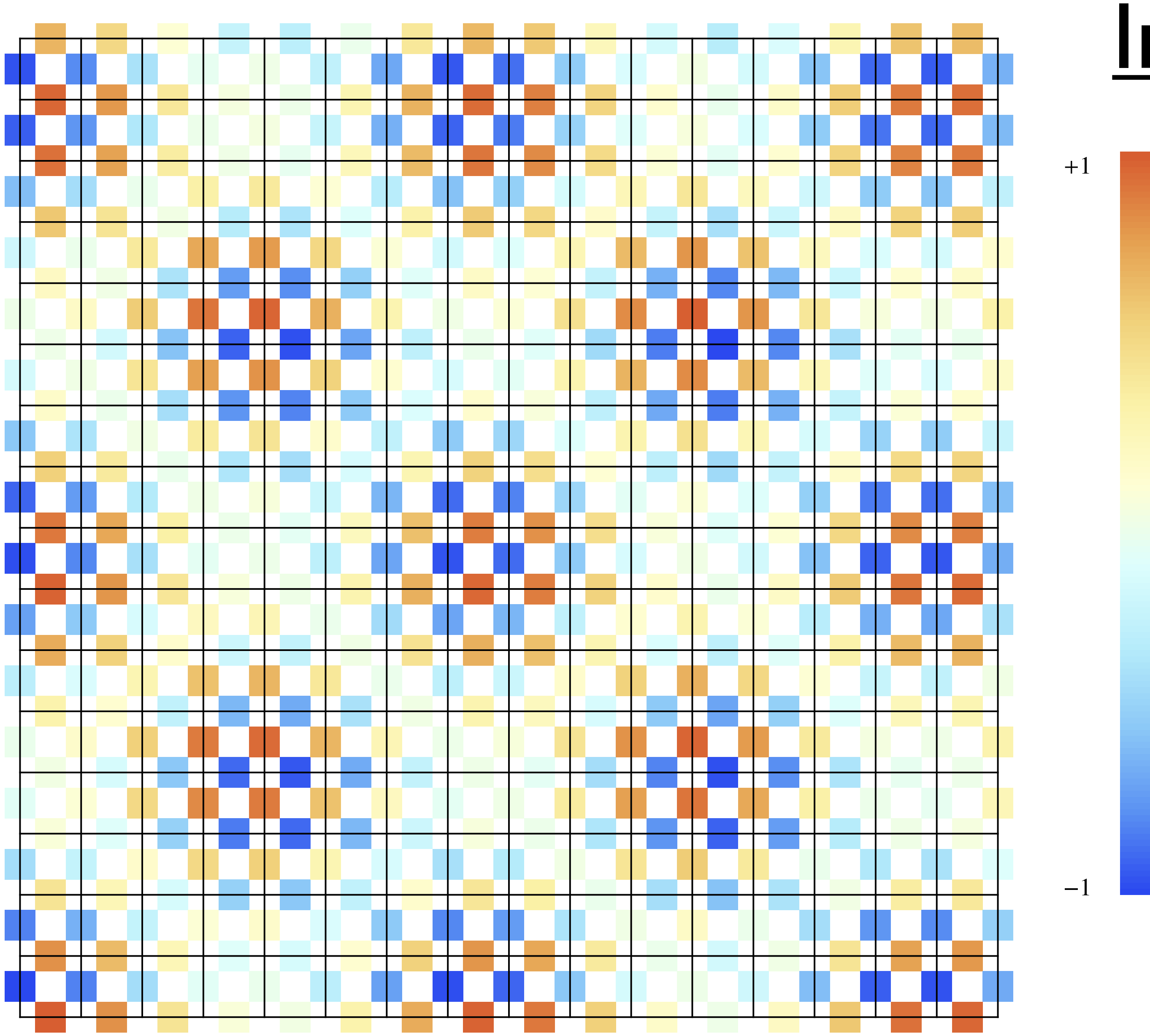

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where $\mathbf{Q}$ extends over $\mathbf{Q} = (\pm Q_0, 0), (0, \pm Q_0)$ with $Q_0 = 2\pi/(7.3)$ and

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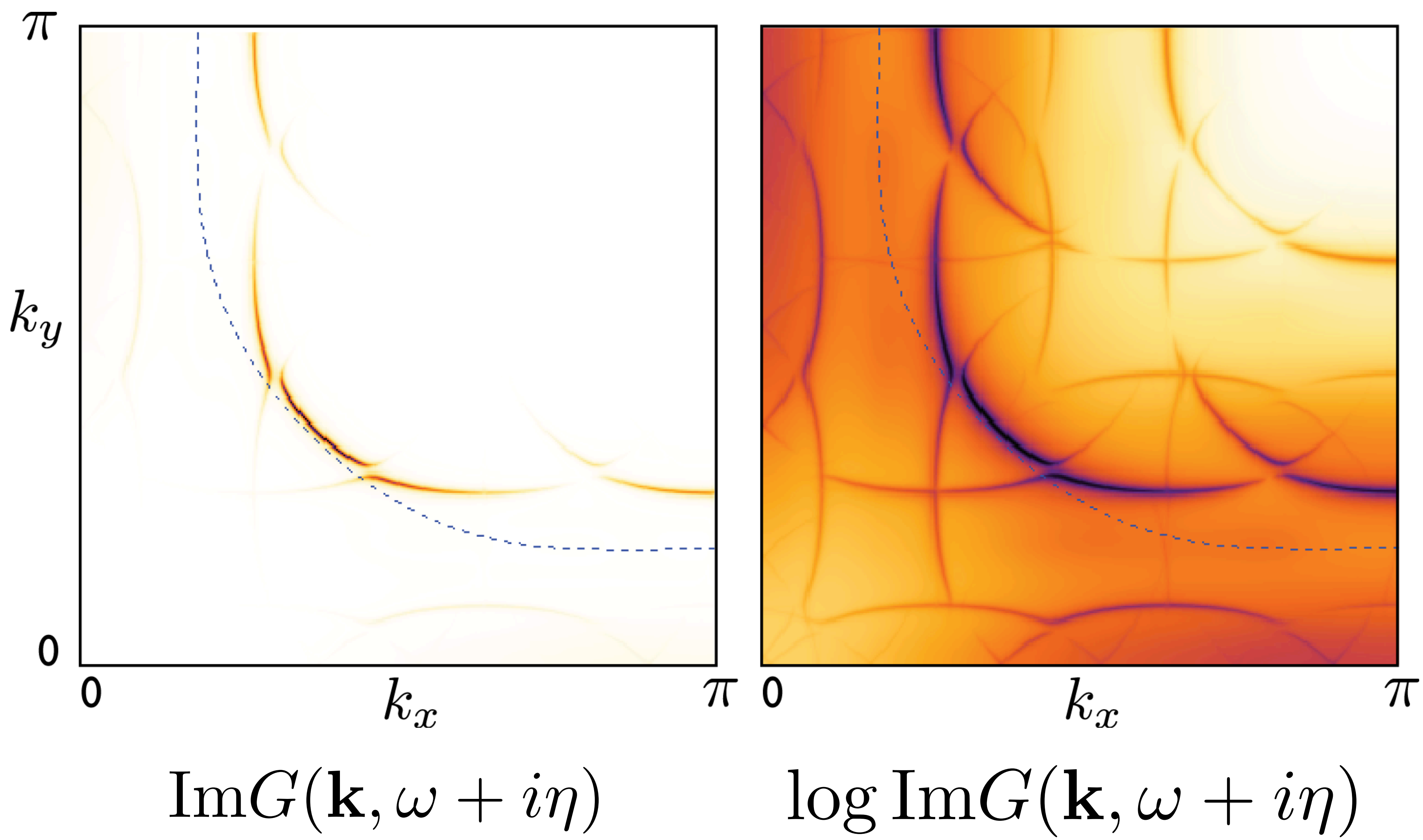
Hartree-Fock computation on lattice model



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

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

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

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

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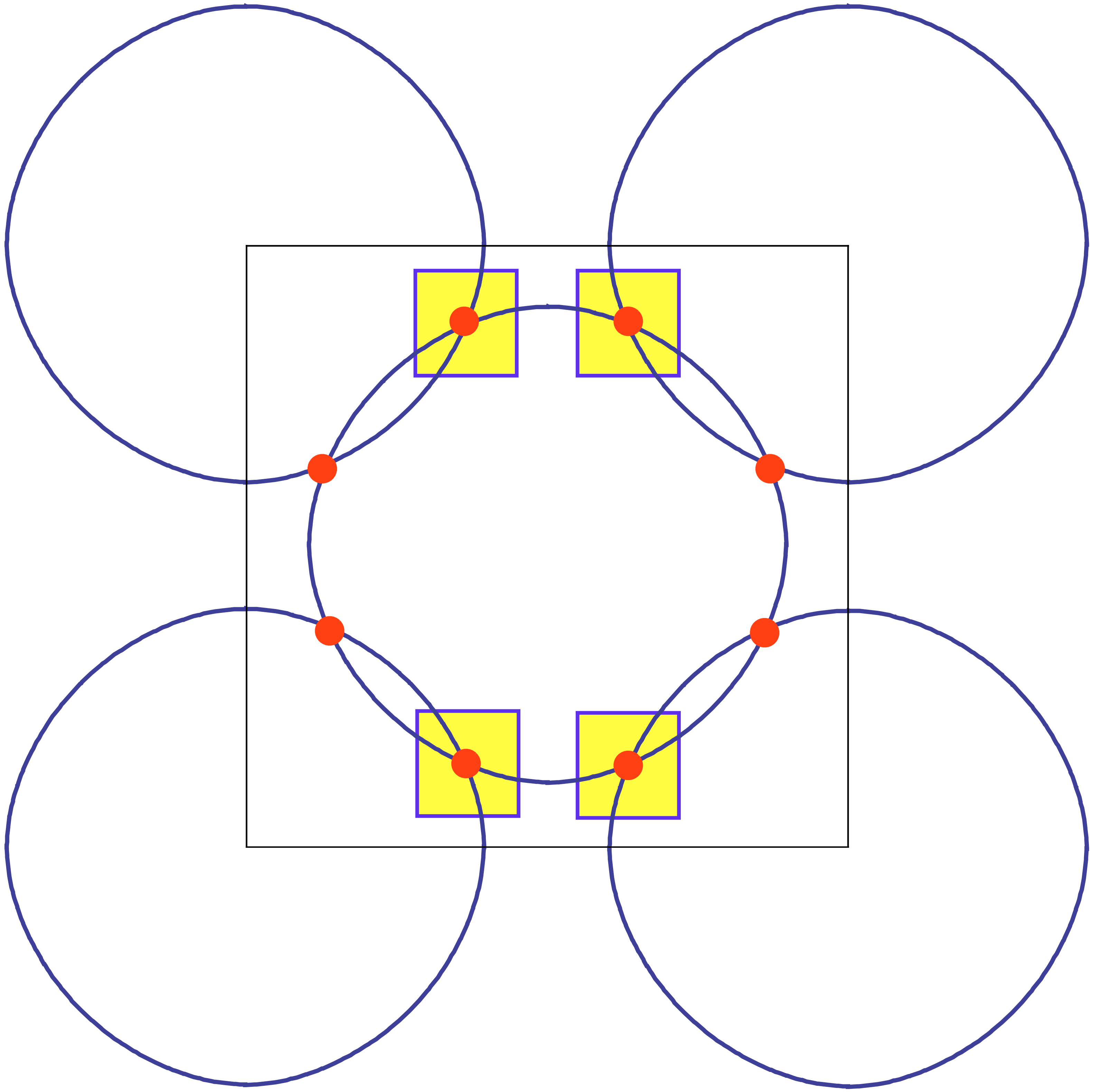
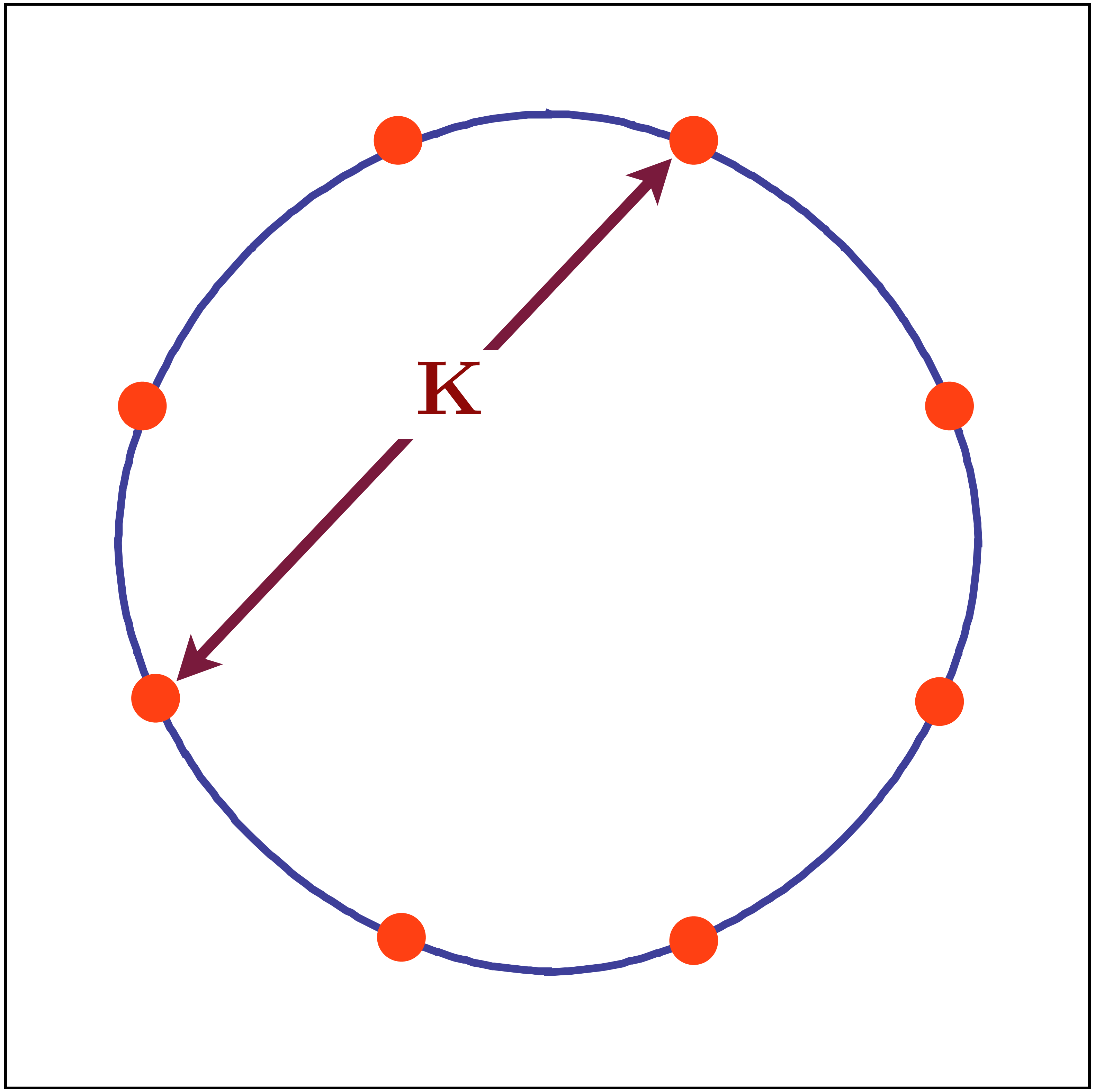


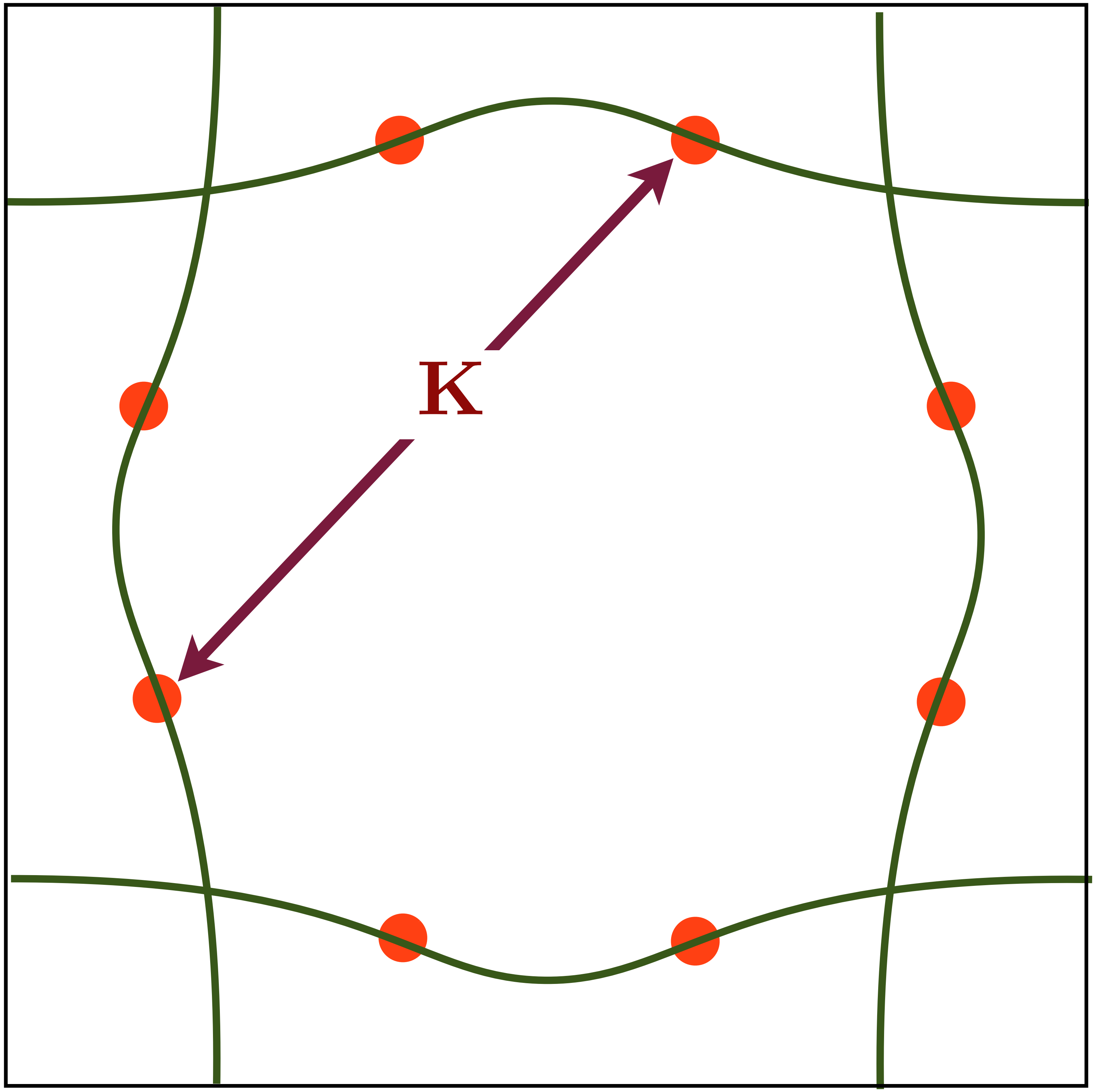
Low energy theory for critical point near hot spots

QMC for the onset of antiferromagnetism



Hot spots in a single band model

QMC for the onset of antiferromagnetism

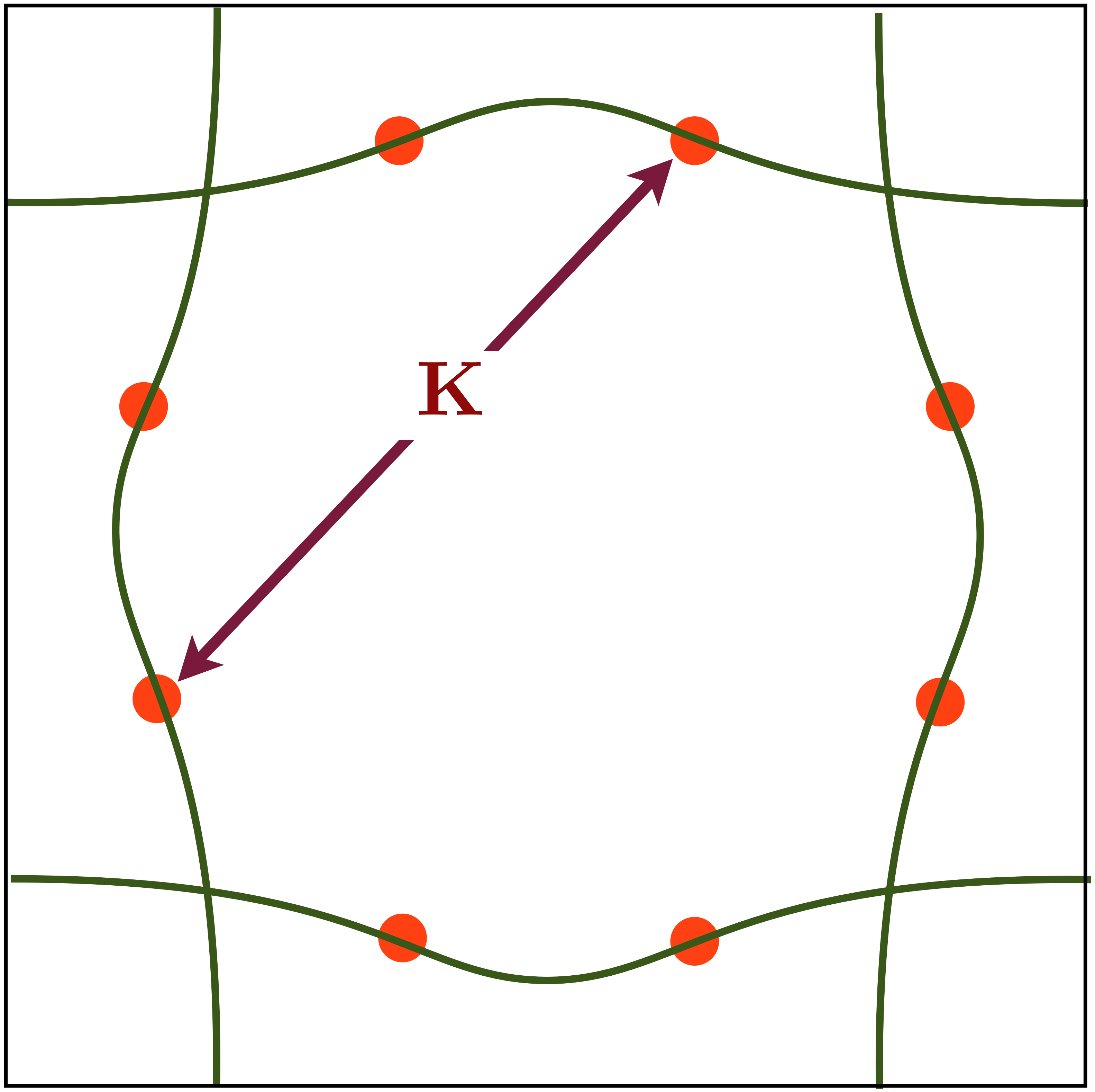


Hot spots in a two band model

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

QMC for the onset of antiferromagnetism

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



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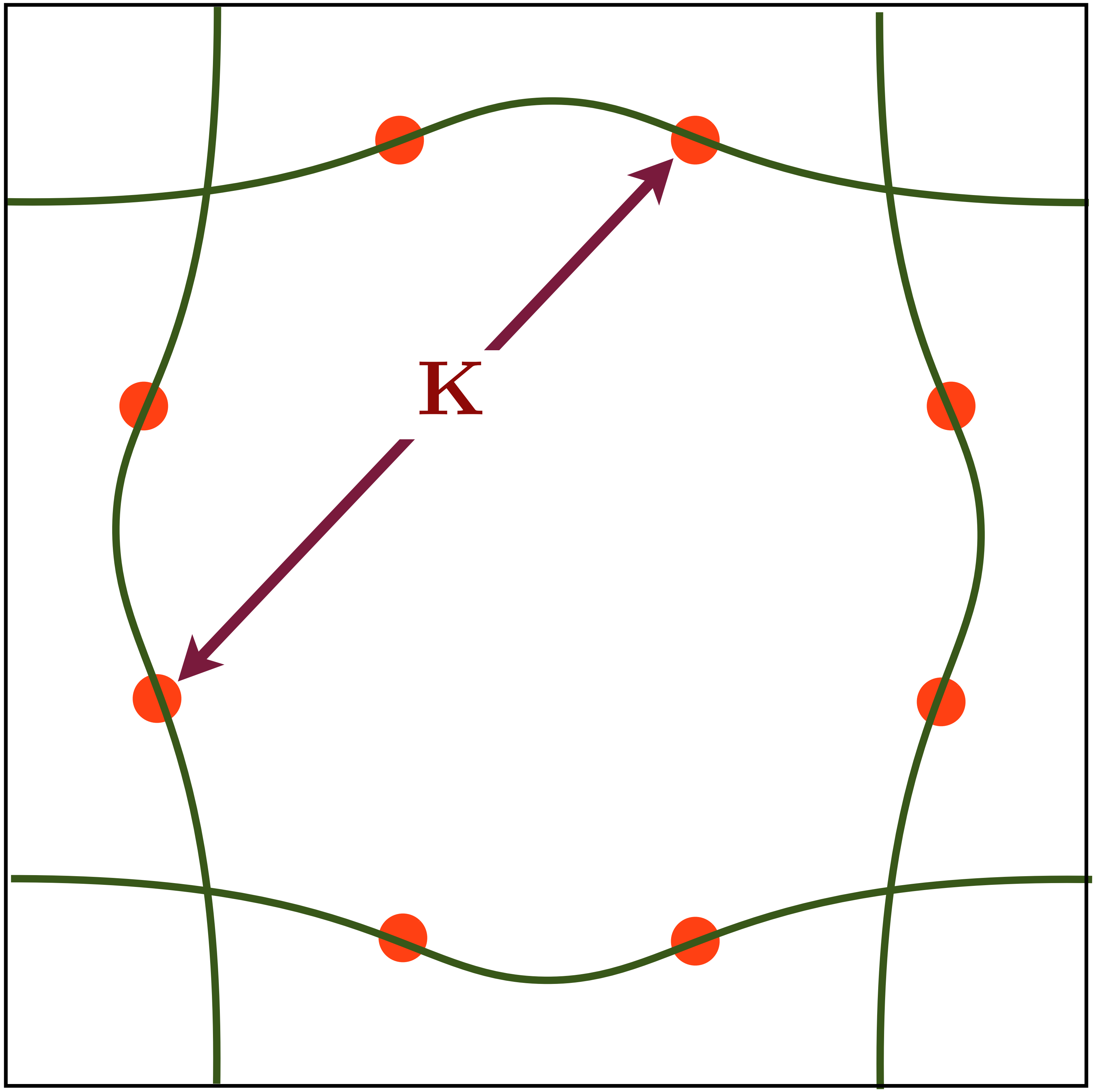

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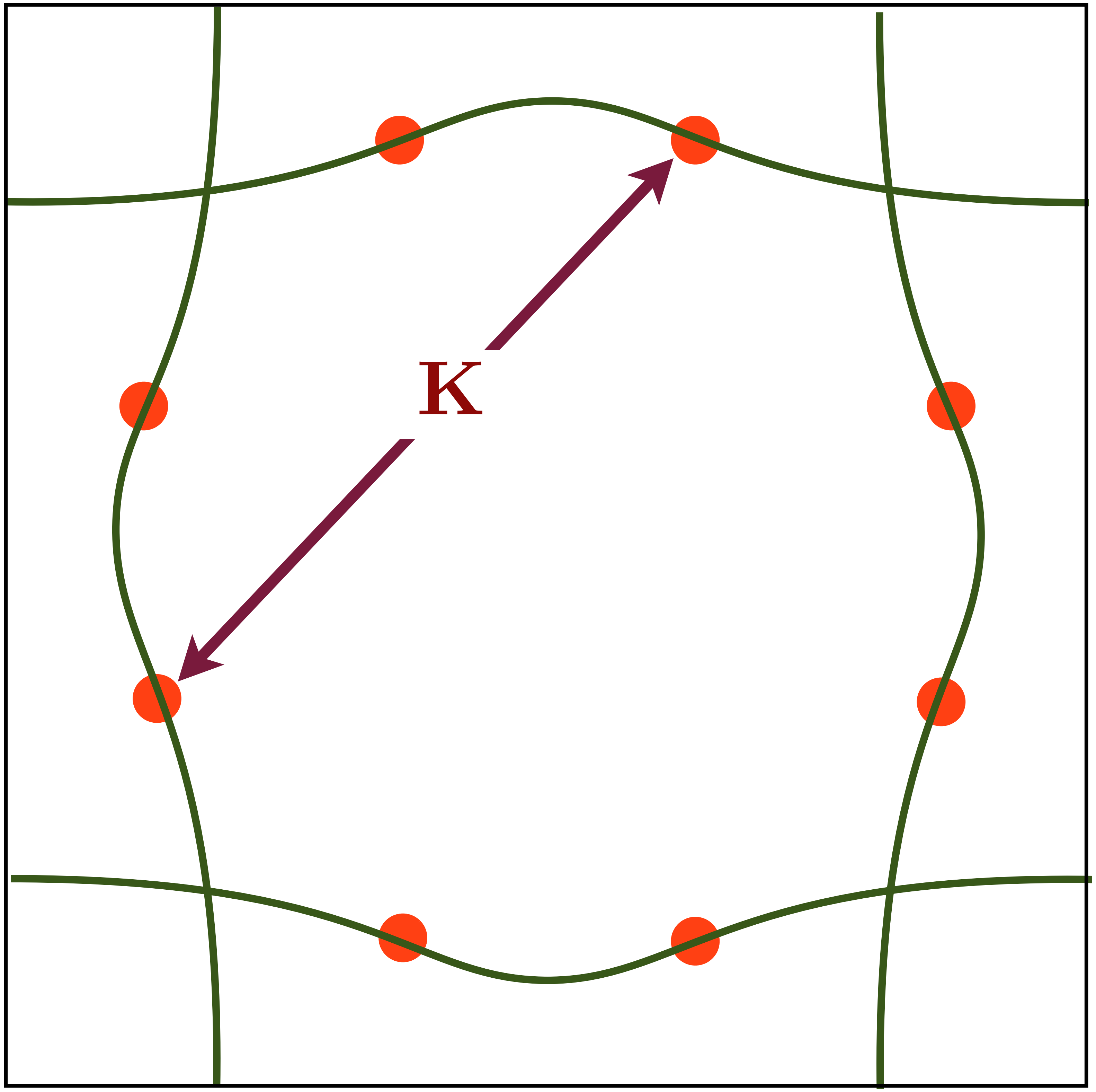
QMC for the onset of antiferromagnetism

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



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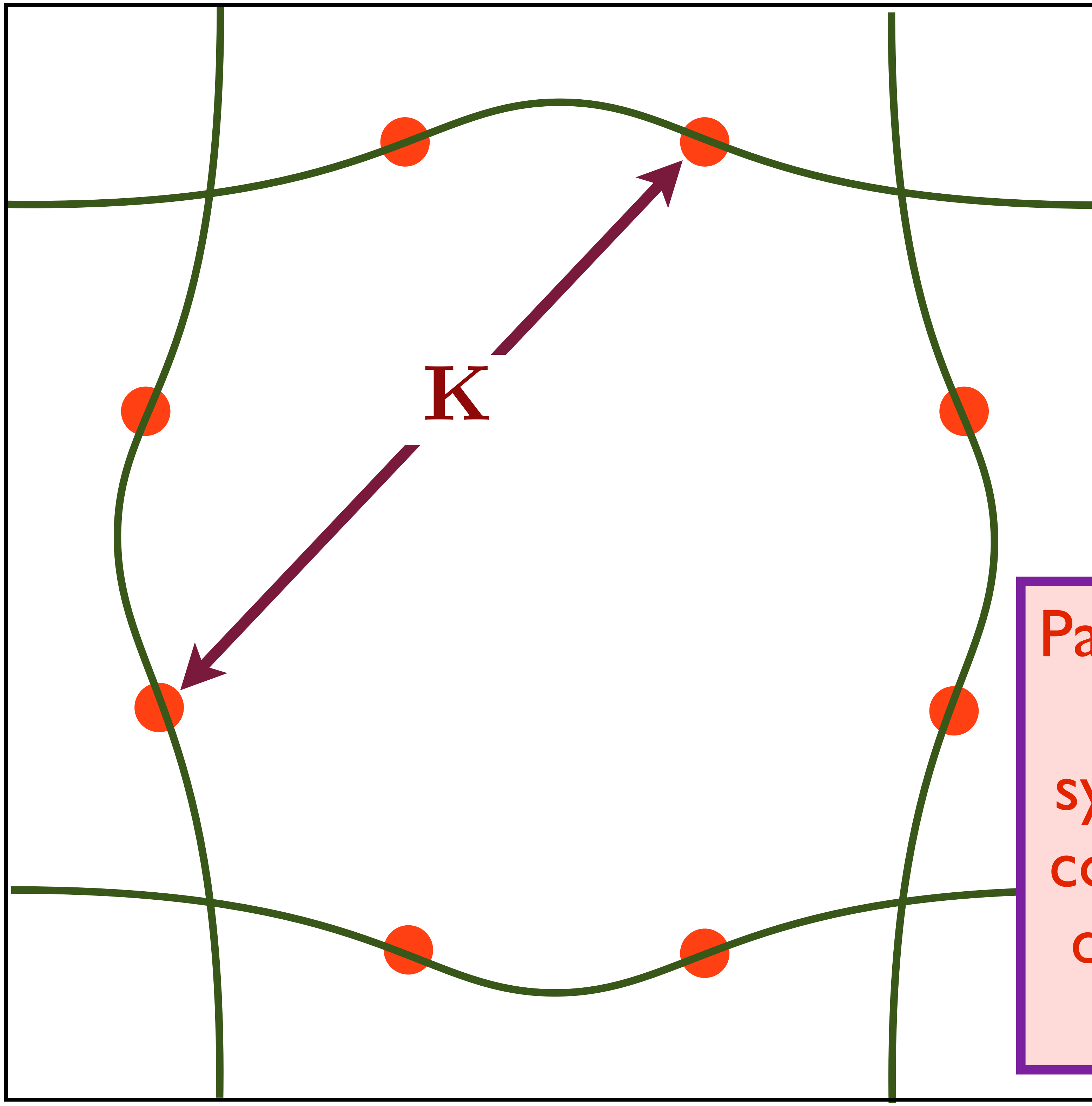

Hot spots in a two band model

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

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

QMC for the onset of antiferromagnetism

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

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No sign problem !

QMC for the onset of antiferromagnetism

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

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

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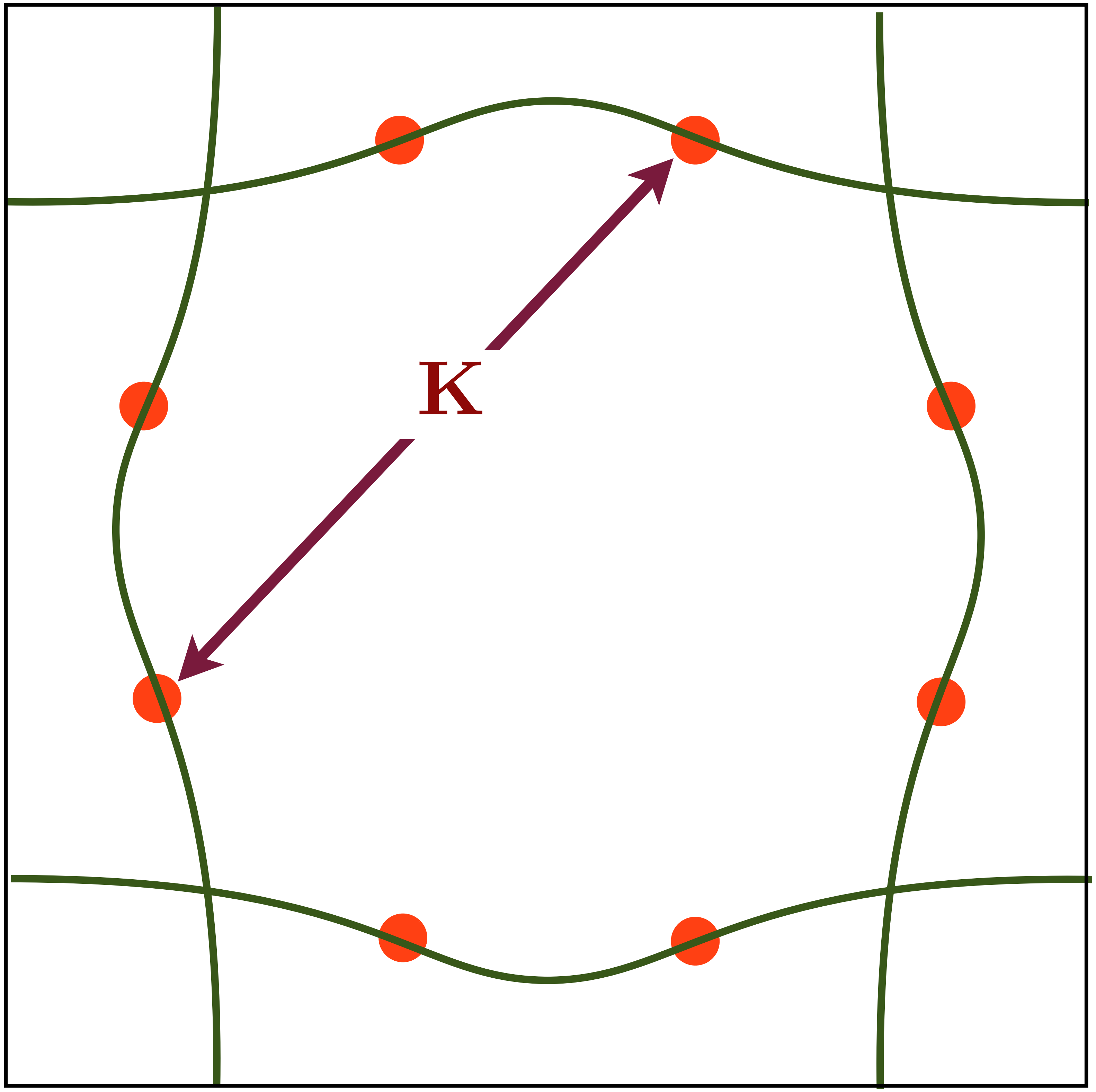
E. Berg, M. Metlitski, and S. Sachdev, *Science* **338**, 1606 (2012).

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



Hot spots in a two band model

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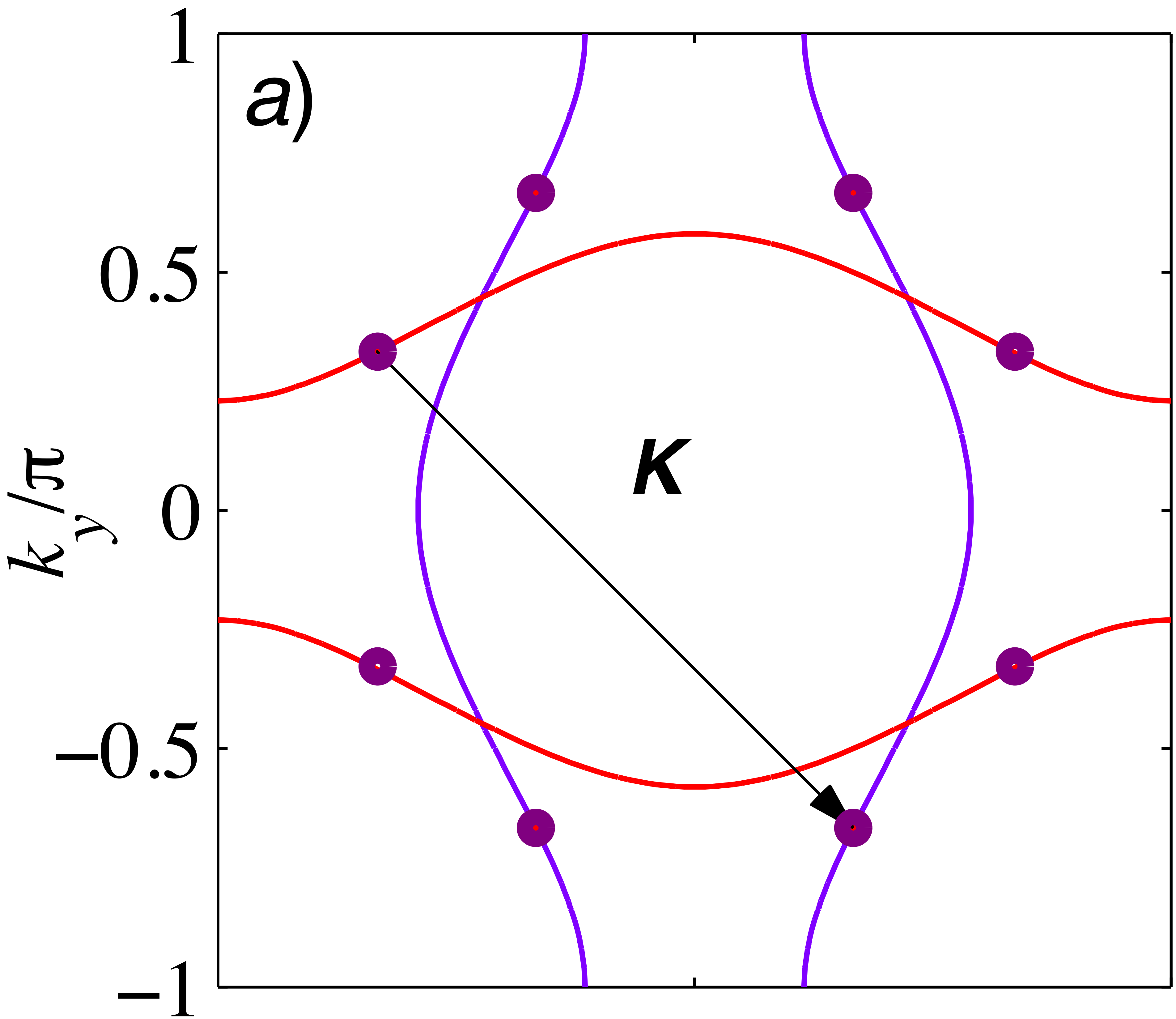
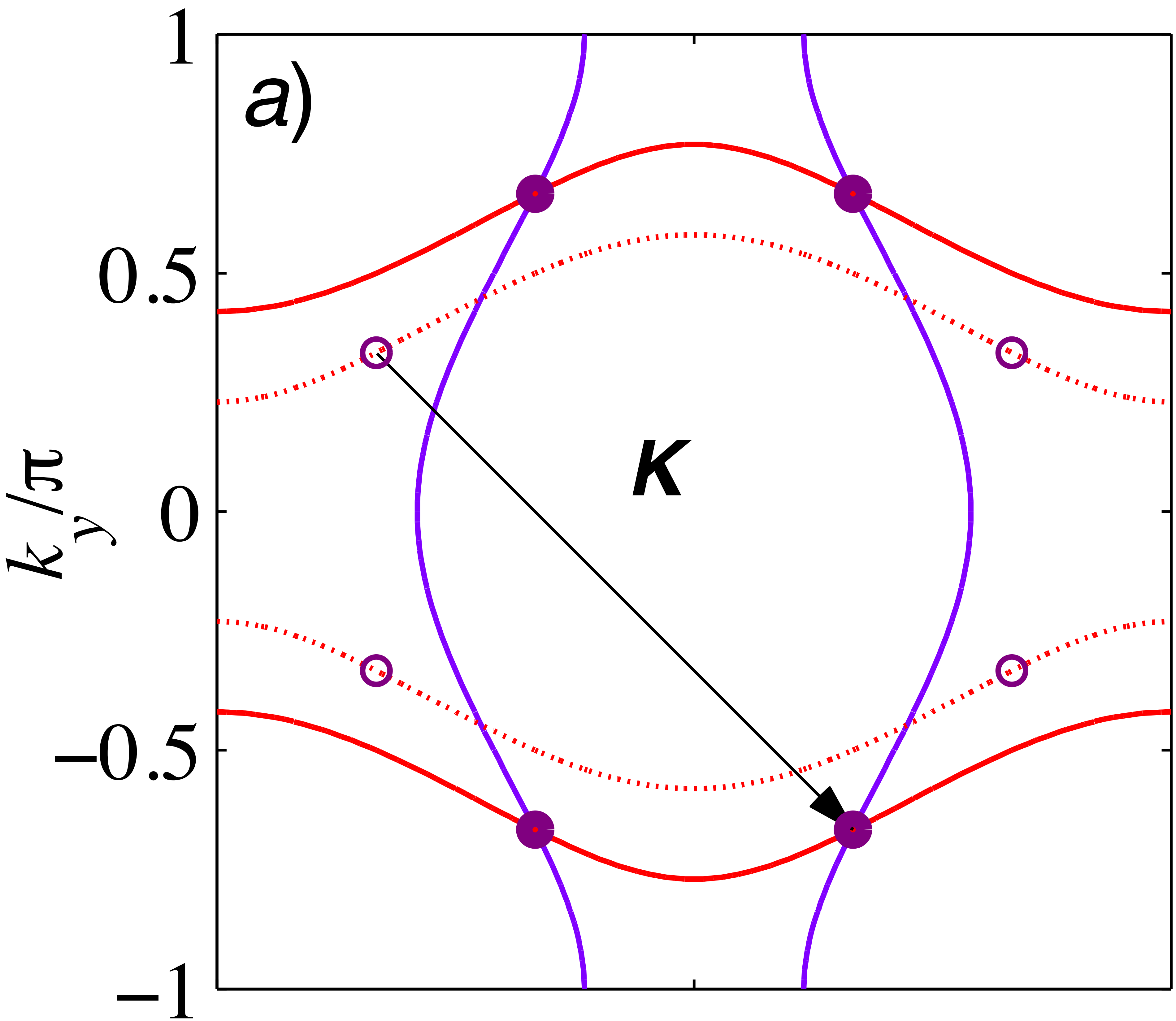
QMC for the onset of antiferromagnetism



Center Brillouin zone at (π,π,)

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

QMC for the onset of antiferromagnetism



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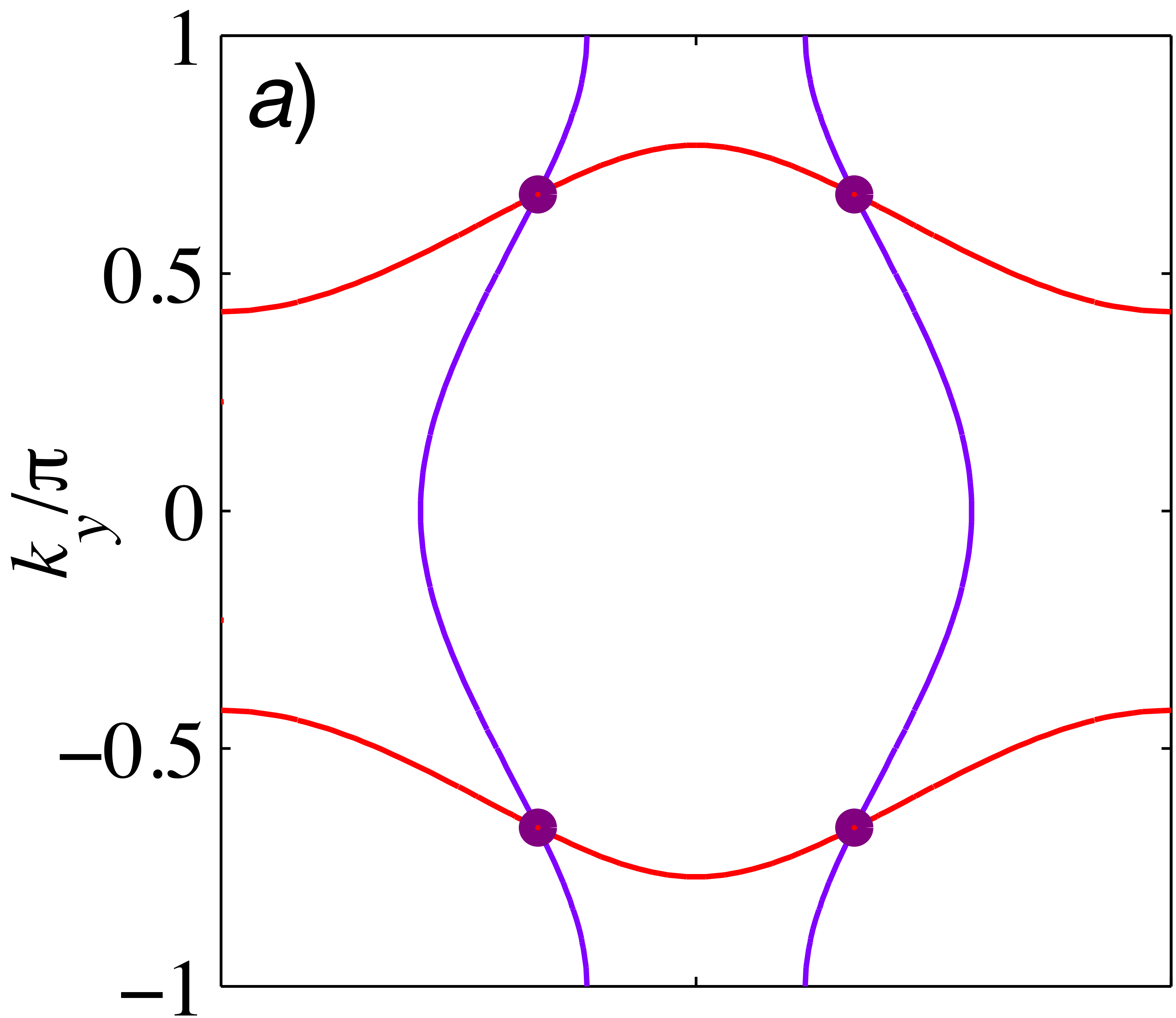
Move one of the Fermi surface by (π,π,)

QMC for the onset of antiferromagnetism



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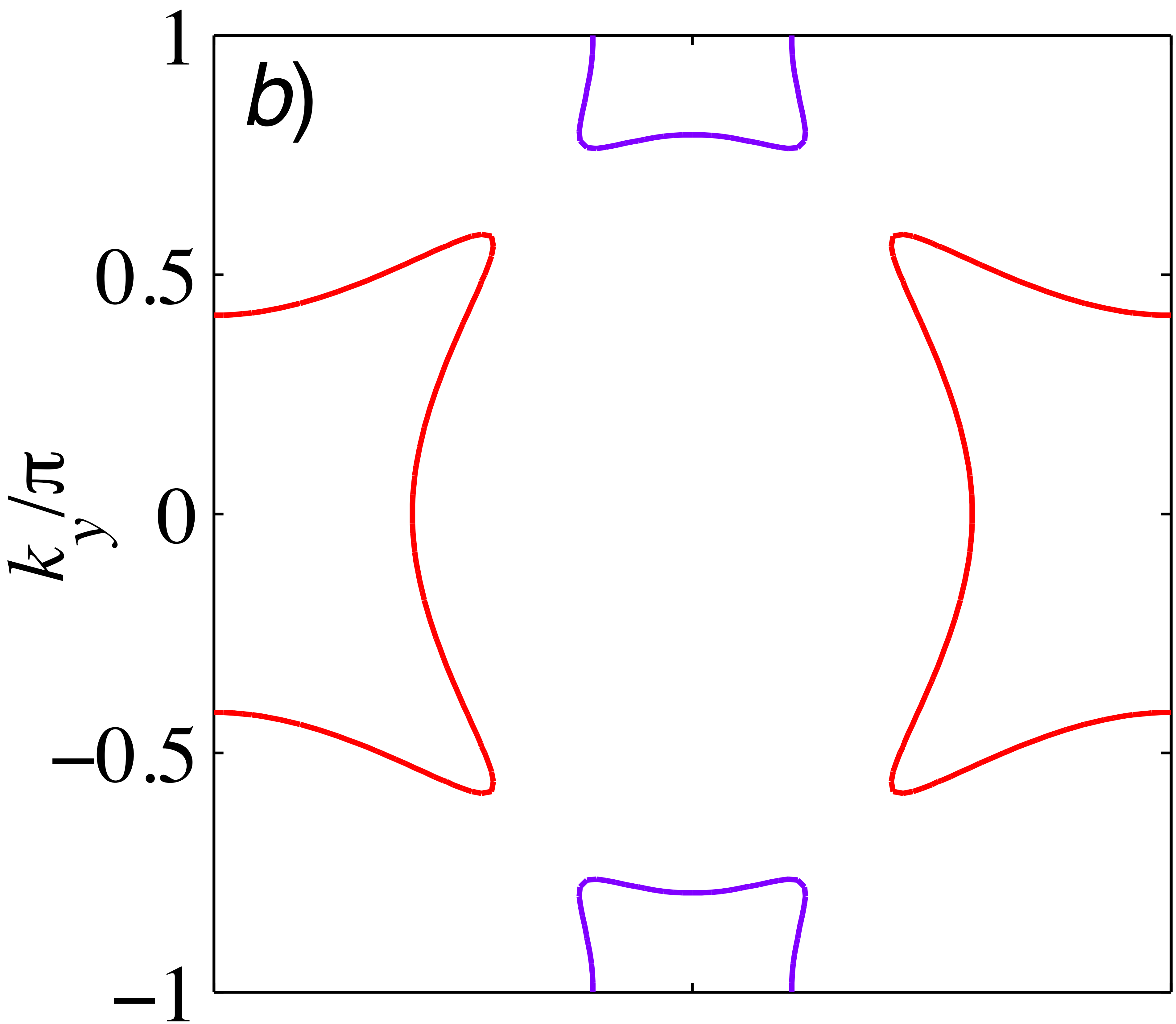
Now hot spots are at Fermi surface intersections

QMC for the onset of antiferromagnetism



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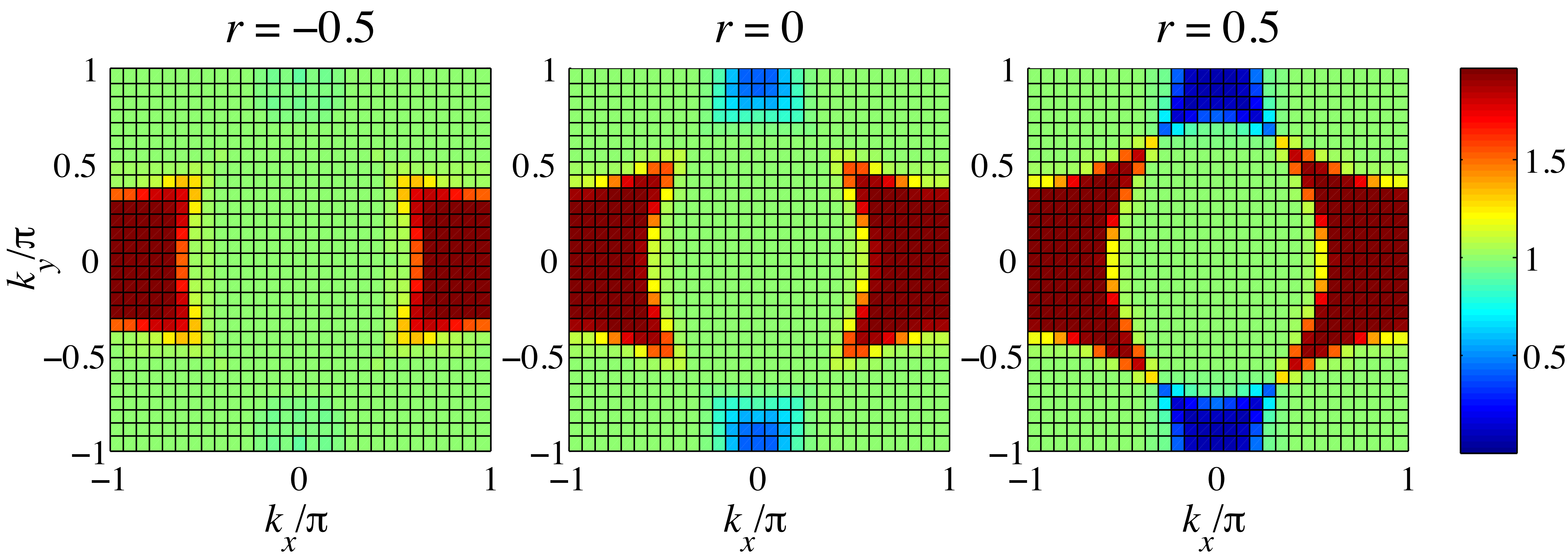
Expected Fermi surfaces in the AFM ordered phase

QMC for the onset of antiferromagnetism



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

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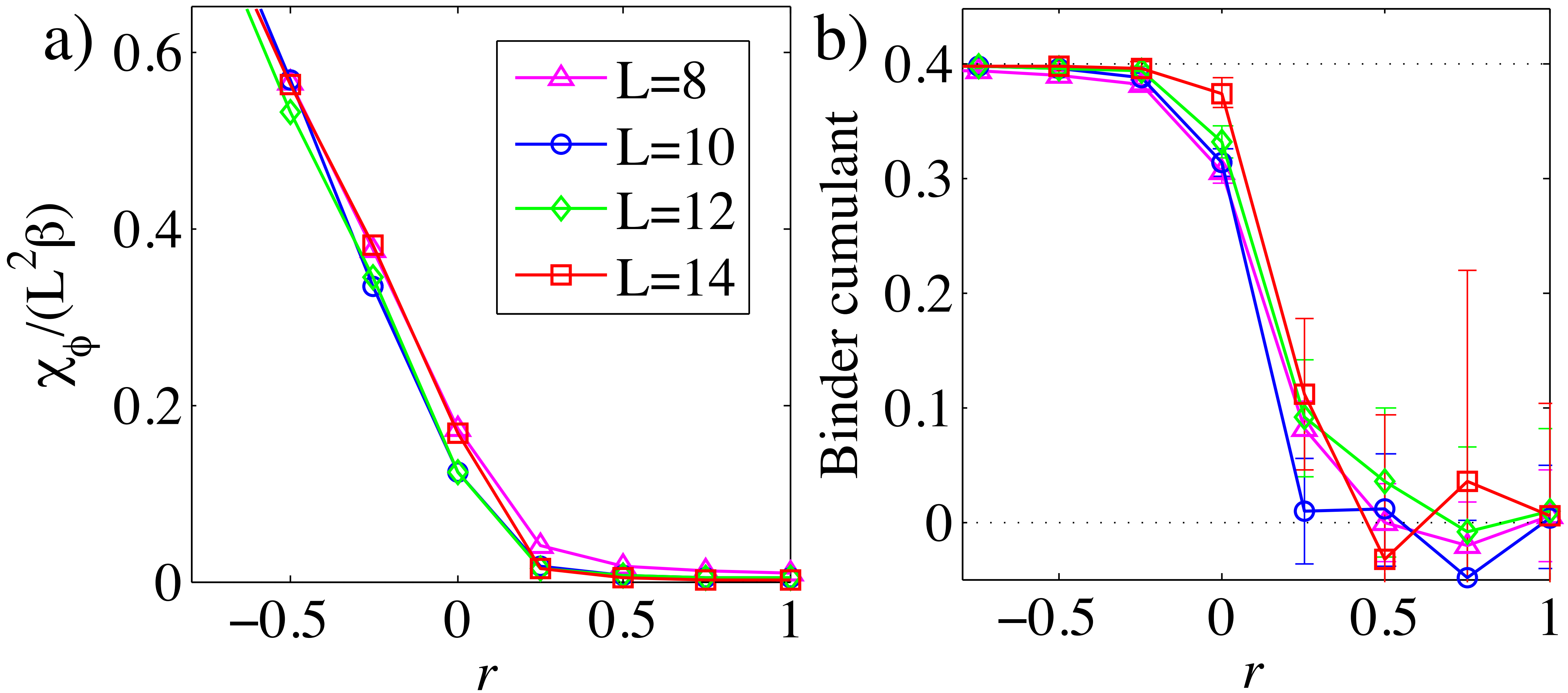
QMC for the onset of antiferromagnetism



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

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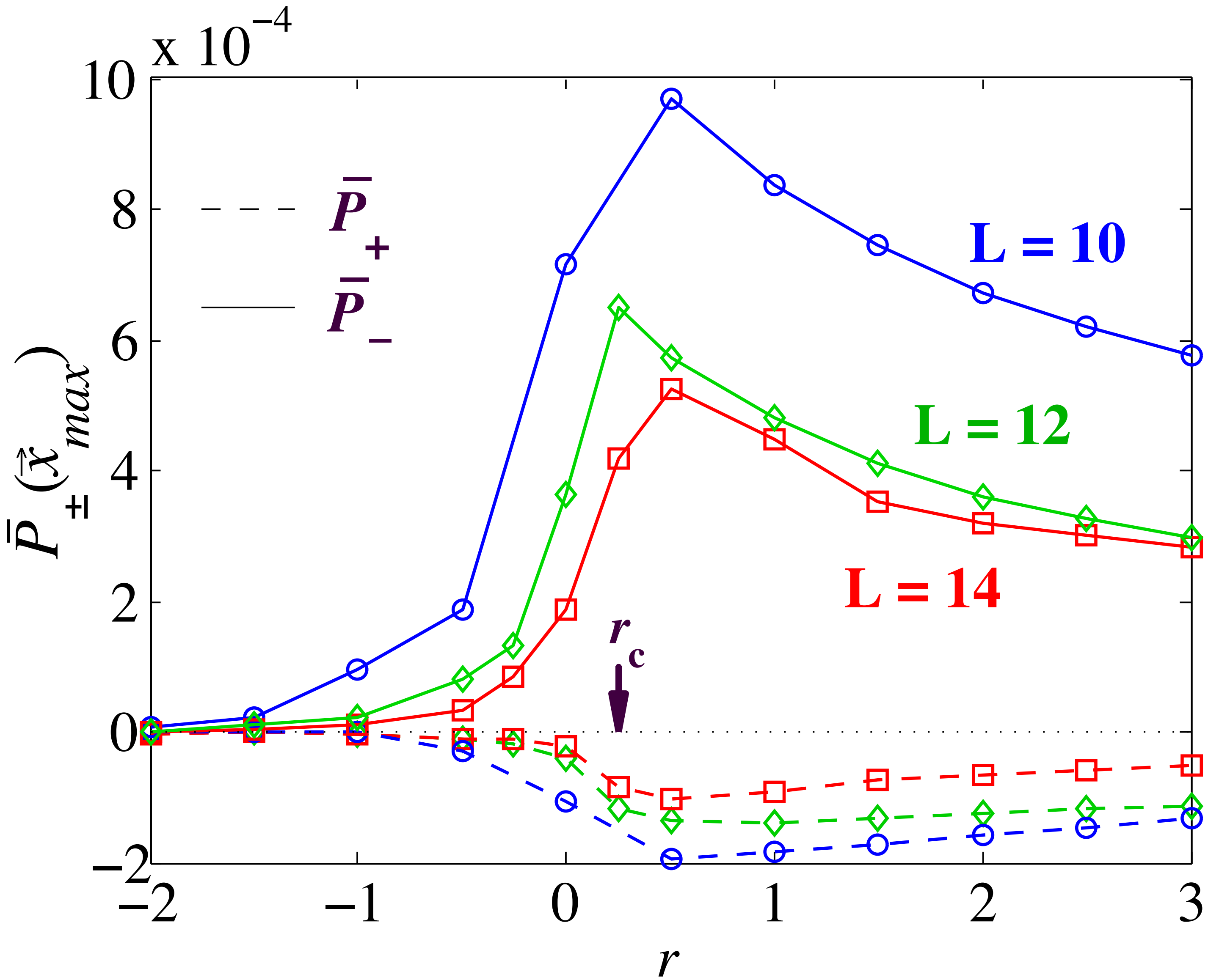

s/d pairing amplitudes P_+/P_-
as a function of the tuning parameter r

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

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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- Good prospects for studying competing charge orders, and non-Fermi liquid physics at non-zero temperature.