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Superconductivity in the Iron Age

Zlatko Tesanovic, Johns Hopkins University
zbt@pha.jhu.edu http://www.pha.jhu.edu/~zbt

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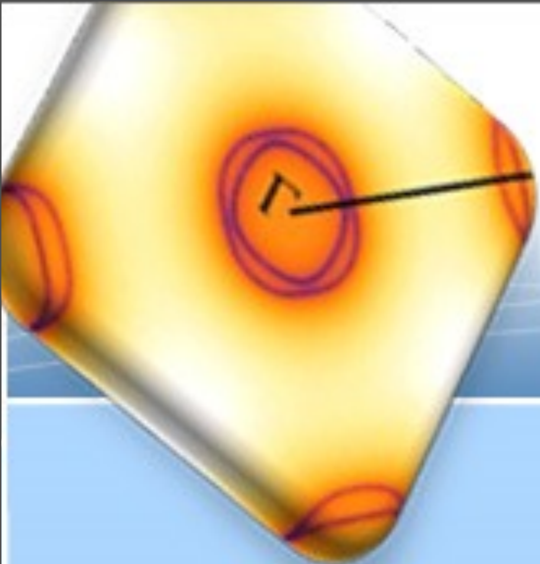

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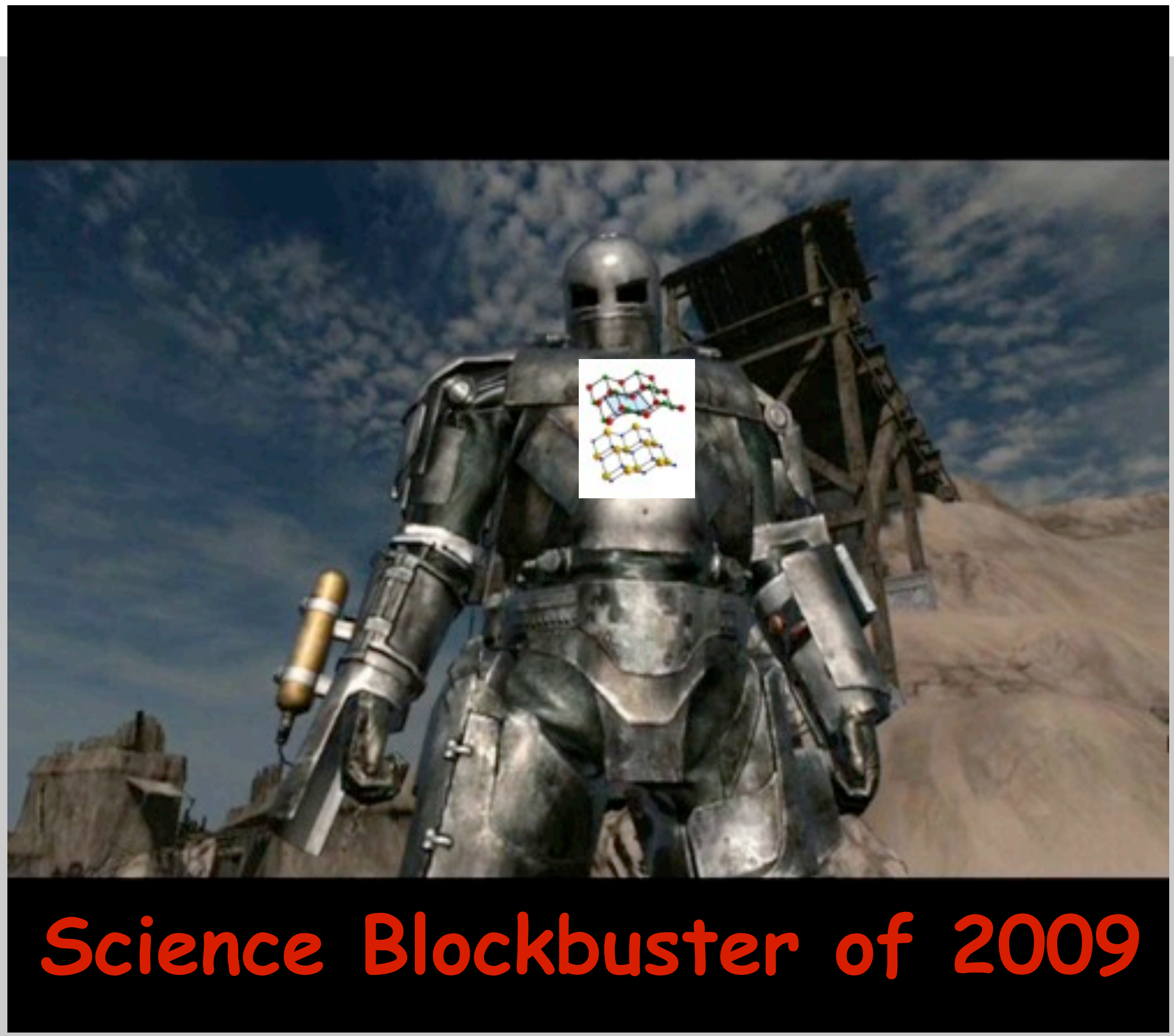

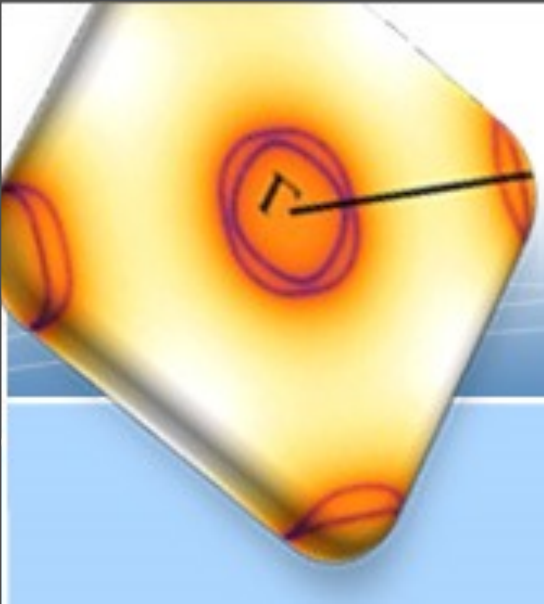

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USA TODAY

Swine flu, space interest scientists most in 2009

By Dan Vergano, USA TODAY

Science marches on, sometimes with headlines and awards, but most often with little fanfare.

A look at the year's most-cited papers in science, ones that scientists themselves referenced in their own work, for example, finds studies that did and didn't make any "Top Ten" lists.

"What scientists themselves are interested in often differs a good bit from the public's interests," says analyst David Pendlebury of Thomson Reuters, the international specialty information firm. "Often the stories that really matter in science are the ones still unfolding."

As part of his efforts for the ScienceWatch.com website, Pendlebury compiled 2009's top topics in science, by citation, using an "Essential Science Indicators" database of publications, citations and trends in all disciplines. Here are the top 10:

•NASA's measures of the age, expansion and distribution of galaxies throughout the universe based on observations by its WMAP probe, launched in 2001. Not on a lot of lists, but, "the studies just provide a wealth of data that everyone in physics from cosmology to high-energy physicists will use for years," Pendlebury says.

•Prostate cancer studies suggesting that screening and Vitamin E had few benefits in treating the disease. These made news but were also highly cited by other researchers.

•*New England Journal of Medicine* and *Journal of the American Medical Association* studies showing problems with the blood-thinning drug Clopidogrel for heart patients. Another newsmaker.

•Diabetes treatment consensus statements that were updated this year. "Such articles are typically highly cited," Pendlebury says.

•Swine flu studies. They racked up a lot of citations this year. (You may not be too surprised.)

•Iron-based superconductors, which rivaled swine flu for citations among scholars. For two decades, physicists have chased after superconductors, which transmit juice with zero power loss, to replace less efficient copper wires. Iron superconductors look like the latest hope. "Recent discovery of superconductivity in iron-based layered compounds may have opened a new pathway to room temperature superconductivity," begins a highly cited *EPL* journal paper by Vladimir Cvetkovic of Johns Hopkins University in Baltimore. Did you hear about this? You may hear more in the next few years.

•Cancer treatments that target blood vessel growth, or anti-angiogenesis. They also made the news, but for the wrong reasons. Highly-cited papers linked anti-angiogenesis to tumor growth.

•Graphene, single-atom layers of carbon that have semiconductor properties. They "look like a coming revolution in electronics," Pendlebury says. *Science* magazine included graphene on its "Top Ten" list of breakthroughs for the year.

•Small RNA's, genetic materials that regulate genes in cells. They've emerged in "an astounding landscape" notes a highly-cited *Nature Reviews Molecular Cell Biology* survey led by V. Narry Kim of South Korea's Seoul National University. They have potential to treat diseases and reveal how genes work on a fundamental level inside cells. But not a big news item.

•Obesity gene, biology and diet studies. A *New England Journal of Medicine* report that found cutting calories, whatever their origin, mattered the most surprisingly high number of citations, considering it confirmed long-standing advice.

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#6- Iron-based Superconductors,
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$ 1,000,000,000 question:
How to make a 100 K iron-based superconductor ?

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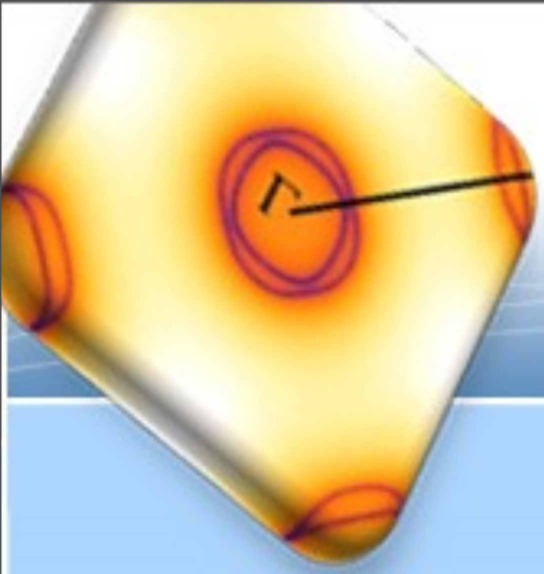

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USA TODAY

$ 100 question: What is the theory of iron-pnictides ?

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PHYSICAL REVIEW B **80**, 024512 (2009)

Valley density-wave and multiband superconductivity in iron-based pnictide superconductors

Vladimir Cvetkovic and Zlatko Tesanovic
Institute for Quantum Matter and Department of Physics & Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218, USA
(Received 5 September 2008; revised manuscript received 22 June 2009; published 20 July 2009)

The key feature of the Fe-based superconductors is their quasi-two-dimensional multiband Fermi surface. By relating the problem to a negative U Hubbard model and its superconducting ground state, we show that the defining instability of such a Fermi surface is the valley density-wave (VDW), a *combined* spin/charge density-wave at the wave vector connecting the electron and hole valleys. As the valley parameters change by doping or pressure, the fictitious superconductor experiences "Zeeman splitting," eventually going into a nonuniform "Fulde-Ferrell-Larkin-Ovchinikov" (FFLO) state, an *itinerant* and often *incommensurate* VDW of the real world, characterized by the metallic conductivity from the ungapped remnants of the Fermi surface. When Zeeman splitting exceeds the "Chandrasekhar-Clogston" limit, the "FFLO" state disappears and the VDW is destabilized. Near this point, the VDW fluctuations and interband pair repulsion are essential ingredients of high-T_c superconductivity in Fe pnictides.

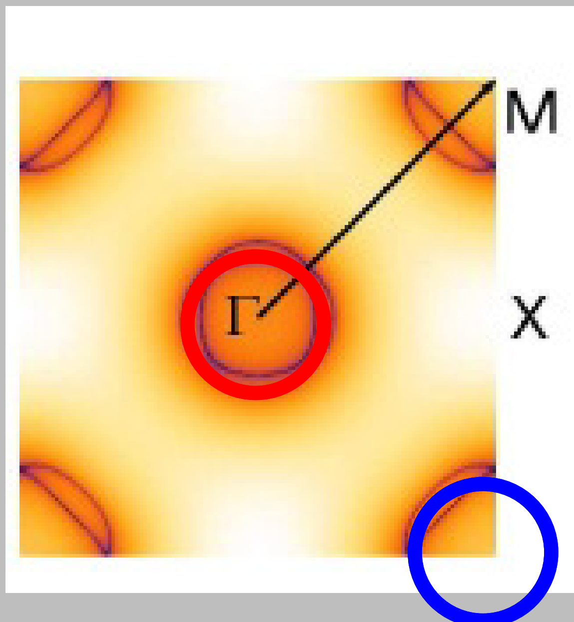
PHYSICAL REVIEW B **83**, 020505(R) (2011)

Theory of the valley-density wave and hidden order in iron pnictides

Jian Kang and Zlatko Tešanović
Institute for Quantum Matter and Department of Physics & Astronomy, The Johns Hopkins University, Baltimore, Maryland 21218, USA
(Received 20 November 2010; revised manuscript received 22 December 2010; published 31 January 2011)

In the limit of perfect nesting, the physics of iron pnictides is governed by the density wave formation at the zone-edge vector **M**. At high energies, various spin- (SDW), charge-, and orbital/pocket- (PDW) density waves, and their linear combinations, all appear equally likely, unified within the unitary order parameter of U(4) × U(4) symmetry. Nesting imperfections and low-energy interactions reduce this symmetry to that of real materials. Nevertheless, the generic ground state preserves a distinct signature of its highly symmetric origins: A SDW along one axis of the iron lattice is predicted to *coexist* with a perpendicular PDW, accompanied by weak charge currents. This "hidden" order induces the structural transition in our theory, naturally insures $T_s \geqslant T_N$, and leads to orbital ferromagnetism and other observable consequences.

What is a (THE) Model for Iron-Pnictides ? → U(4)×U(4) Theory of Valley-Density Wave (VDW)



The first question: Itinerant or Localized? ⇒
Itinerant starting point for high T_c Fe-pnictides

All e and h bands are identical ⇒
H_0 has SU(8) internal symmetry

$$H_0 = \sum_{\mathbf{k},\sigma} \xi^{(0)}_{\mathbf{k}} [\sum_\alpha h^{(\alpha)\dagger}_{\mathbf{k}} h^{(\alpha)}_{\mathbf{k}} + \sum_\beta e^{(\beta)\dagger}_{\mathbf{k}} e^{(\beta)}_{\mathbf{k}}]$$

This is highly idealized. In the real world:

- Pockets are not of same size (particularly h_2)
- Their shape differs ("elliptical" e versus "circular" h)

Eremin, Knolle

Key assumption I:

Differences among (e,h) pockets $\ll$ effective bandwidth $D \sim E_F$

Furthermore, in real world, Γs have strong orbital content:

- Vertices U, W, G_1, and G_2 differ for $e(h)$ pockets
- They have significant angular variation $\delta\Gamma$ around FS

Hirschfeld, Kuroki, Bernevig, Thomale, Chubukov, Eremin,

Key assumption II:

$U, W \sim D \gg G_1, G_2$
$\delta(U,W) \ll (U,W)$

for moderate correlations
$U_d \sim t$, $J_{\mathrm{Hund}} \ll U_d$

U(4)×U(4) Theory of Valley-Density Wave (VDW)

V. Cvetkovic and ZT, PRB **80**, 024512 (2009);
J. Kang and ZT, arXiv:1011.2499

All e and h bands are identical $\Rightarrow$
H_0 has SU(8) internal symmetry

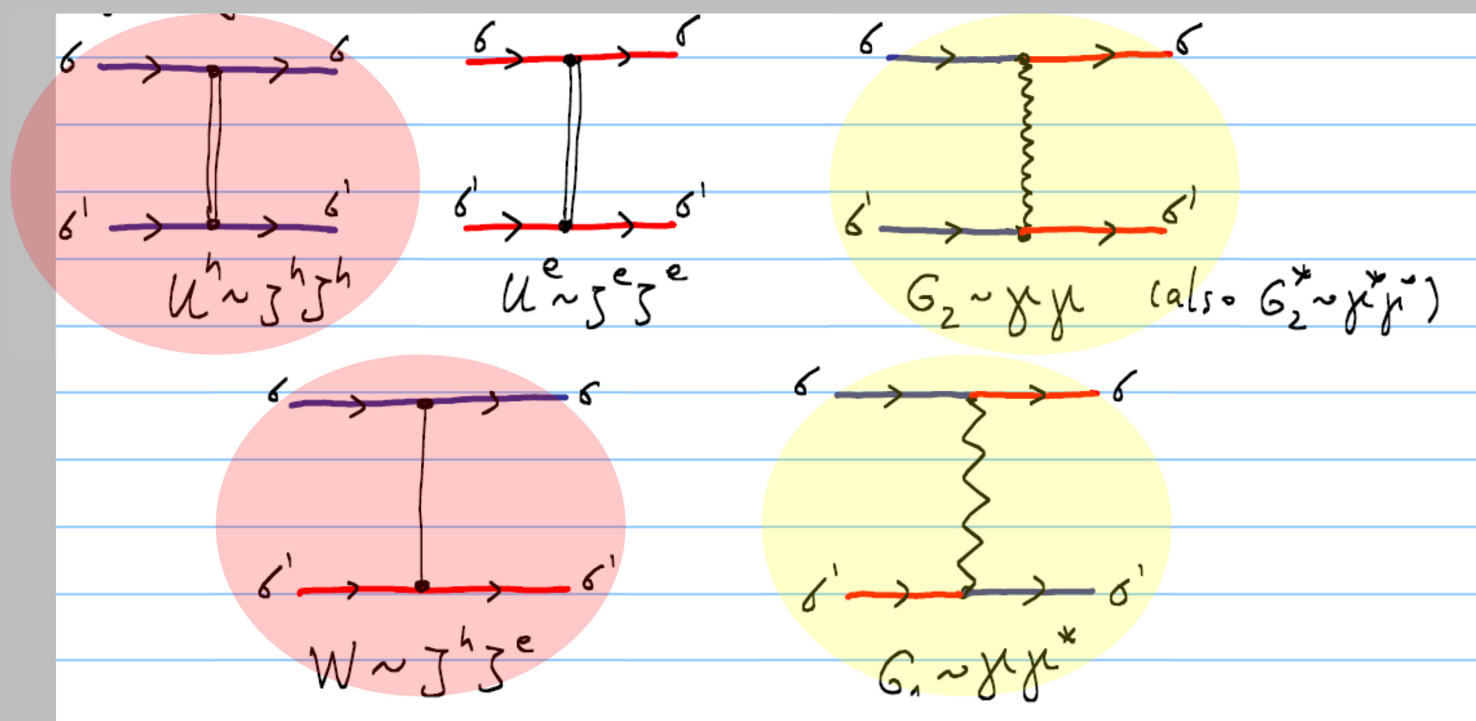
$$H_0 = \sum_{\mathbf{k},\sigma} \xi^{(0)}_{\mathbf{k}} [\sum_\alpha h^{(\alpha)\dagger}_{\mathbf{k}} h^{(\alpha)}_{\mathbf{k}} + \sum_\beta e^{(\beta)\dagger}_{\mathbf{k}} e^{(\beta)}_{\mathbf{k}}]$$

Effective interaction at the Fermi surface:

$$\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \Gamma_{\alpha,\beta,\gamma,\delta}(\mathbf{k},\mathbf{k}';\mathbf{q}) f^\dagger_{\mathbf{k}+\mathbf{q},\alpha} f^\dagger_{\mathbf{k}'-\mathbf{q},\beta} f_{\mathbf{k}',\delta} f_{\mathbf{k},\gamma} \quad \rightarrow \quad U, W, G_1, G_2$$

Flavor-conserving vertices U and W

$U, W \sim D$



Flavor-changing vertices G_2 and G_1

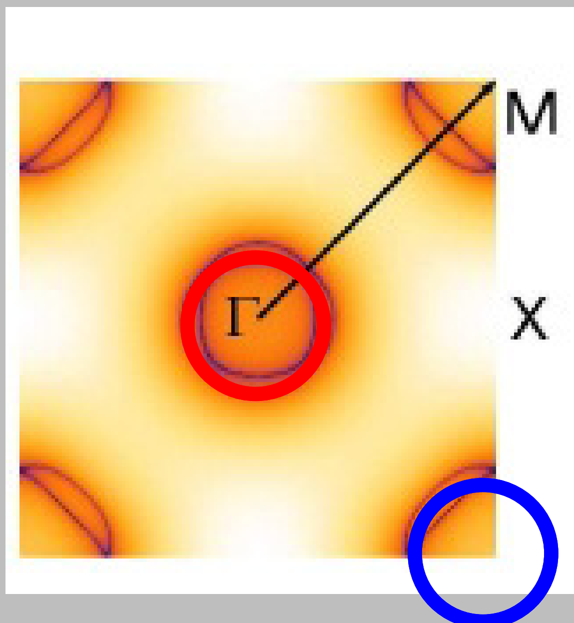
~~$G_2, G_1 \ll D$~~

$$H_{\rm int} \rightarrow U^{(h)} \sum_{\alpha\alpha'\sigma\sigma'} h^{(\alpha)\dagger}_{\sigma} h^{(\alpha')\dagger}_{\sigma'} h^{(\alpha')}_{\sigma'} h^{(\alpha)}_{\sigma} + U^{(e)} \sum_{\beta\beta'\sigma\sigma'} e^{(\beta)\dagger}_{\sigma} e^{(\beta')\dagger}_{\sigma'} e^{(\beta')}_{\sigma'} e^{(\beta)}_{\sigma} + 2W \sum_{\alpha\beta\sigma\sigma'} e^{(\beta)\dagger}_{\sigma'} h^{(\alpha)\dagger}_{\sigma} h^{(\alpha)}_{\sigma} e^{(\beta)}_{\sigma'} + (\cdots)$$

→ U(4)×U(4) symmetry → unified spin and pocket/orbital flavors

Hierarchy of RG Energy Scales U, W >> G_1, G_2 → U(4)×U(4) Theory of Valley-Density Wave (VDW)

V. Cvetkovic and ZT, PRB **80**, 024512 (2009); J. Kang and ZT, arXiv:1011.2499



$$H_0 = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}^{(0)} [\sum_\alpha h_{\mathbf{k}}^{(\alpha)\dagger} h_{\mathbf{k}}^{(\alpha)} + \sum_\beta e_{\mathbf{k}}^{(\beta)\dagger} e_{\mathbf{k}}^{(\beta)}]$$

All e and h bands are identical ⇒ H_0 has SU(8) internal symmetry

Orbital flavor-conserving vertices (U, W) reduce this to U(4)×U(4):

	T_S (K)	T_N (K)	m_{ord} (μ_B)
LaFeAsO	155	137	0.36
CeFeAsO	155	140	0.83
PrFeAsO	153	127	0.48
NdFeAsO	150	141	0.9
CaFeAsF	134	114	0.49
SrFeAsF	175	120	
$CaFe_2As_2$	173	173	0.8
$SrFe_2As_2$	220	220	0.94-1.0
$BaFe_2As_2$	140	140	0.9

$$H_{\rm int} \to U^{(h)} \sum_{\alpha\alpha'\sigma\sigma'} h_\sigma^{(\alpha)\dagger} h_{\sigma'}^{(\alpha')\dagger} h_{\sigma'}^{(\alpha')} h_\sigma^{(\alpha)} + U^{(e)} \sum_{\beta\beta'\sigma\sigma'} e_\sigma^{(\beta)\dagger} e_{\sigma'}^{(\beta')\dagger} e_{\sigma'}^{(\beta')} e_\sigma^{(\beta)} +$$
$$2W \sum_{\alpha\beta\sigma\sigma'} e_{\sigma'}^{(\beta)\dagger} h_\sigma^{(\alpha)\dagger} h_\sigma^{(\alpha)} e_{\sigma'}^{(\beta)} + (\cdots)$$

$U(4)\times U(4)$ symmetry is reasonable since U and W do not vary much in different (e, h) channels

	(h1)	(h2)	(e1)	(e2)	(h1,e1)	(h1,e2)	(h2,e1)	(h2,e2)	(h1,e1)	(h1,e1)
s	0.44	0.31	0.35	0.35	0.21	0.25	0.27	0.29	0.14	0.14
p	0.04	0.21	0.17	0.20	0.22	0.21	0.22	0.22	0.01	0.01
d	0.22	0.12	0.09	0.10	0.11	0.13	0.09	0.11	0.03	0.02

Finally, flavor-mixing vertices $G_{1,2}(\ll U, W)$ have the highest symmetry that physics will allow:

$$(\ldots) \to 2G_1 \sum_{\alpha\beta\sigma\sigma'} (\sigma\sigma') e_\sigma^{(\beta)\dagger} h_{-\sigma}^{(\alpha)\dagger} h_{-\sigma'}^{(\alpha)} e_{\sigma'}^{(\beta)} +$$
$$G_2 \sum_{\alpha\alpha'\beta\beta'\sigma\sigma'} (\sigma\sigma') h_{-\sigma}^{(\alpha)} e_\sigma^{(\beta)} h_{-\sigma'}^{(\alpha')} e_{\sigma'}^{(\beta')} \epsilon^{\alpha\alpha'} \epsilon^{\beta\beta'} + h.c.$$

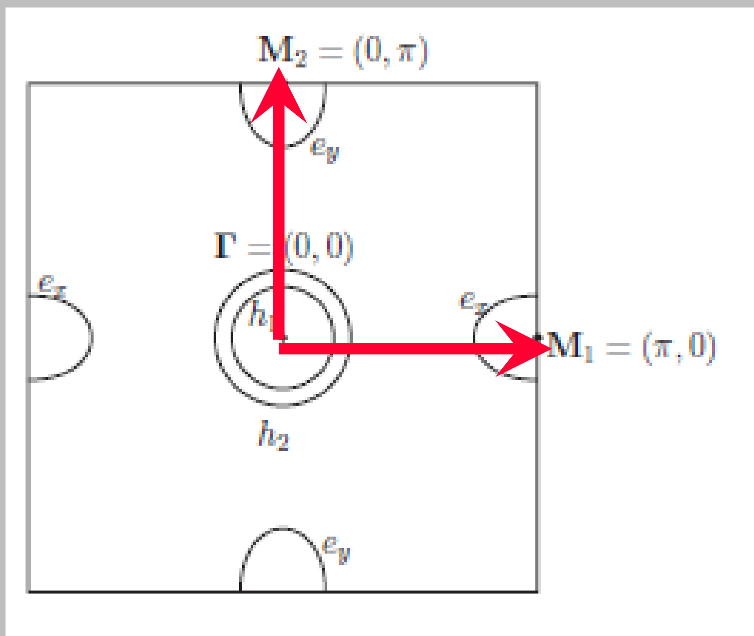
VDW in Fe-pnictides is a (nearly) U(4)×U(4) symmetric combination: SDW/CDW/ODW

“Near” U(4)×U(4) Symmetry and Experiments

J. Kang and ZT, arXiv:1011.2499

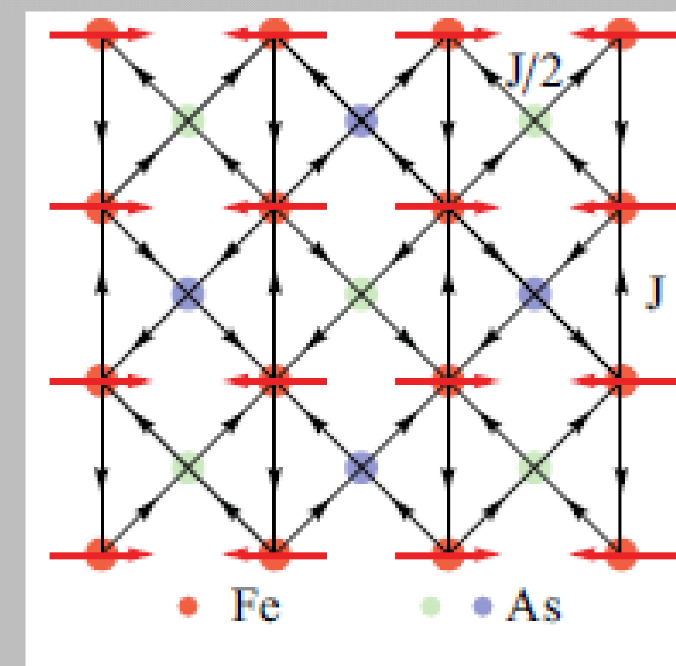
"Direction" of U(4)×U(4) symmetry breaking fixed by flavor-mixing vertices $G_{1,2} (\ll U, W)$:

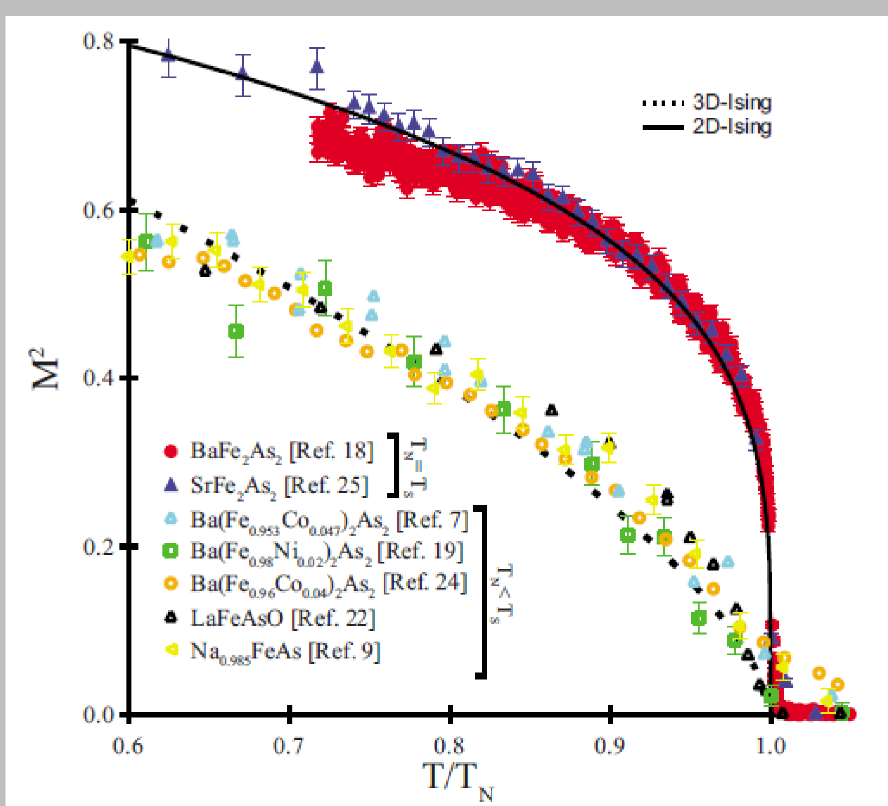
$$2G_1 \sum_{\alpha\beta\sigma\sigma'} (\sigma\sigma') e_\sigma^{(\beta)\dagger} h_{-\sigma}^{(\alpha)\dagger} h_{-\sigma'}^{(\alpha)} e_{\sigma'}^{(\beta)} + G_2 \sum_{\alpha\alpha'\beta\beta'\sigma\sigma'} (\sigma\sigma') h_{-\sigma}^{(\alpha)} e_\sigma^{(\beta)} h_{-\sigma'}^{(\alpha')} e_{\sigma'}^{(\beta')} \epsilon^{\alpha\alpha'} \epsilon^{\beta\beta'} + h.c.$$



Two main predictions:
i) SDW along x accompanied by imaginary PWD along y → orbital/charge currents

ii) Structural transition driven by PDW → $T_s \geq T_N$.





PHYSICAL REVIEW B **81**, 014501 (2010)

Universal magnetic and structural behaviors in the iron arsenides

Stephen D. Wilson,[1] C. R. Rotundu,[1] Z. Yamani,[2] P. N. Valdivia,[3] B. Freelon,[4] E. Bourret-Courchesne,[1] and R. J. Birgeneau[1,3,4]

Orbital “AF” → Can this modulated current pattern be observed by neutrons? μSR?

Friedel-Like Oscillations from Interstitial Iron in Superconducting $Fe_{1+y}Te_{0.62}Se_{0.38}$

V. Thampy,[1] J. Kang,[1] J. A. Rodriguez-Rivera,[2,3] W. Bao,[4] A. T. Savici,[5] J. Hu,[6] T. J. Liu,[6] B. Qian,[6] D. Fobes,[6] Z. Q. Mao,[6] C. B. Fu,[7,8,9] W. C. Chen,[3,9] Q. Ye,[5] R. W. Erwin,[2] T. R. Gentile,[9] Z. Tesanovic,[1] and C. Broholm[1,2]

[1]*Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland 21218, USA*

[2]*NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA*

[3]*Department of Materials Science and Engineering, University of Maryland, College Park, Maryland 20740, USA*

[4]*Department of Physics, Renmin University of China, Beijing 100872, China*

[5]*NSSD, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

[6]*Department of Physics, Tulane University, New Orleans, Louisiana 70118, USA*

[7]*Department of Physics, Indiana University, Bloomington, Indiana 47408, USA*

[8]*Department of Physics, Shanghai Jiaotong University, Shanghai, 200240, China*

[9]*National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA*

(Received 23 September 2011; published 7 March 2012)

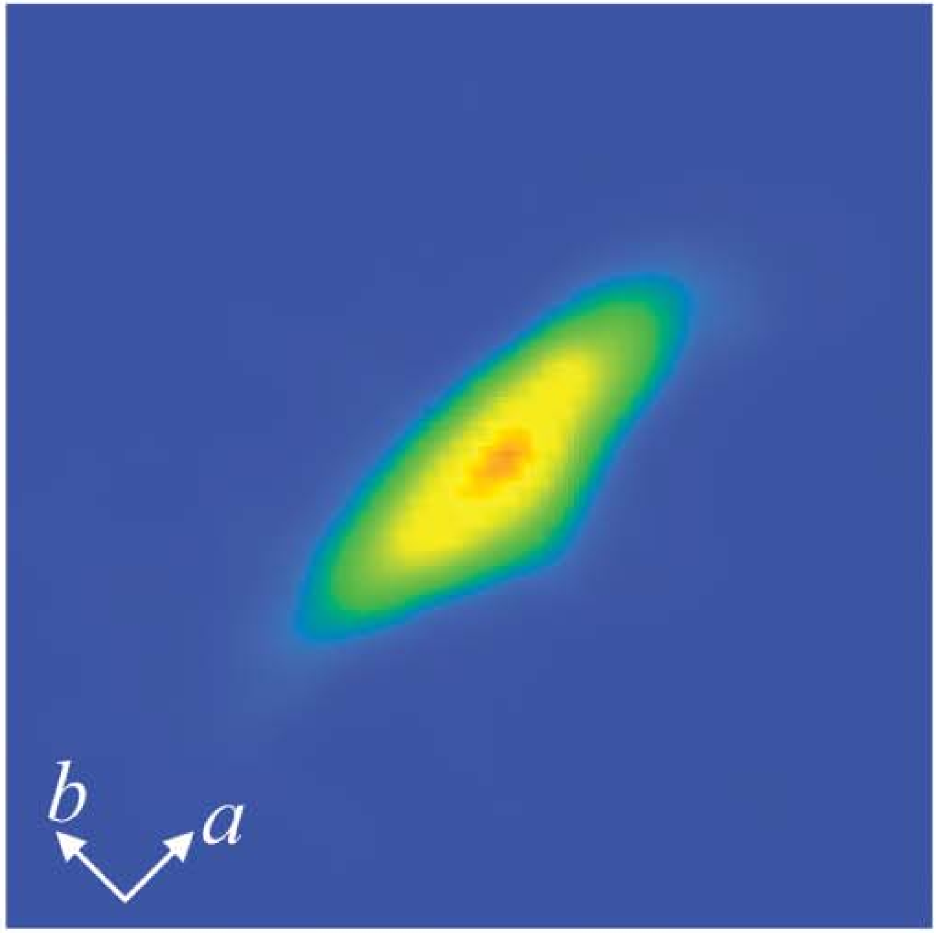
Using polarized and unpolarized neutron scattering, we show that interstitial Fe in superconducting $Fe_{1+y}Te_{1-x}Se_x$ induces a magnetic Friedel-like oscillation that diffracts at $\mathbf{Q}_\perp = (\frac{1}{2}0)$ and involves >50 neighboring Fe sites. The interstitial $>2\mu_B$ moment is surrounded by compensating ferromagnetic four-spin clusters that may seed double stripe ordering in $Fe_{1+y}Te$. A semimetallic five-band model with $(\frac{1}{2}\,\frac{1}{2})$ Fermi surface nesting and fourfold symmetric superexchange between interstitial Fe and two in-plane nearest neighbors largely accounts for the observed diffraction.

Direct Observation of Nodes and Twofold Symmetry in FeSe Superconductor

Can-Li Song,[1,2] Yi-Lin Wang,[2] Peng Cheng,[1] Ye-Ping Jiang,[1,2] Wei Li,[1] Tong Zhang,[1,2] Zhi Li,[2] Ke He,[2] Lili Wang,[2] Jin-Feng Jia,[1] Hsiang-Hsuan Hung,[3] Congjun Wu,[3] Xucun Ma,[2]* Xi Chen,[1]* Qi-Kun Xue[1,2]

We investigated the electron-pairing mechanism in an iron-based superconductor, iron selenide (FeSe), using scanning tunneling microscopy and spectroscopy. Tunneling conductance spectra of stoichiometric FeSe crystalline films in their superconducting state revealed evidence for a gap function with nodal lines. Electron pairing with twofold symmetry was demonstrated by direct imaging of quasiparticle excitations in the vicinity of magnetic vortex cores, Fe adatoms, and Se vacancies. The twofold pairing symmetry was further supported by the observation of striped electronic nanostructures in the slightly Se-doped samples. The anisotropy can be explained in terms of the orbital-dependent reconstruction of electronic structure in FeSe.

17 JUNE 2011 VOL 332 SCIENCE



Progress on the physics of the underdoped cuprates

Zlatko Tesanovic
Memorial Symposium

Johns Hopkins University
March 22, 2013

Subir Sachdev

PHYSICS

HARVARD

Max Metlitski

Erez Berg

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Outline

1. Update on cuprate experiments

2. Antiferromagnetism in metals:
d-wave superconductivity

3. Low energy theory, emergent pseudospin symmetry, and bond order

4. Unrestricted Hartree-Fock-BCS

5. Quantum Monte Carlo without the sign problem

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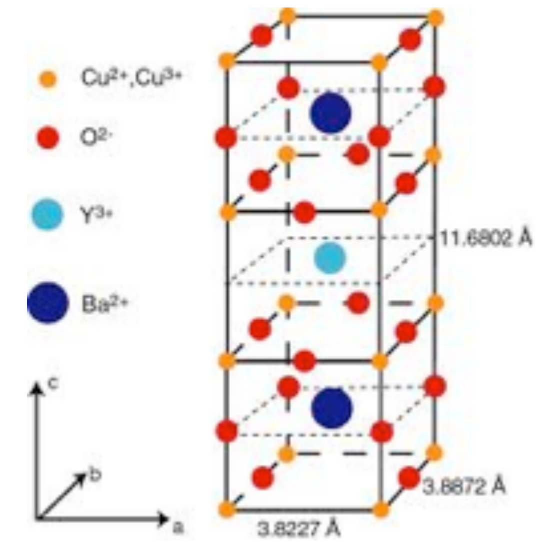

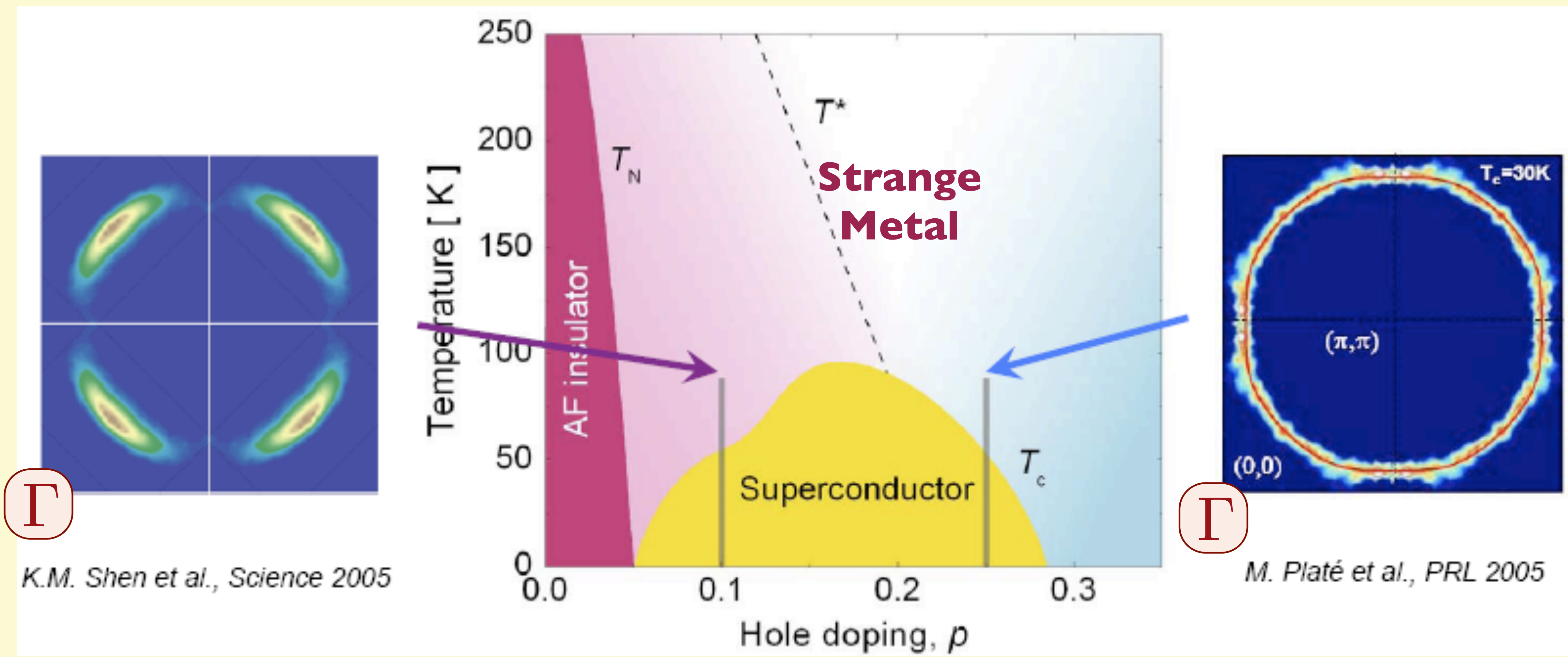

Smaller hole Fermi-pockets

Large hole Fermi surface

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)

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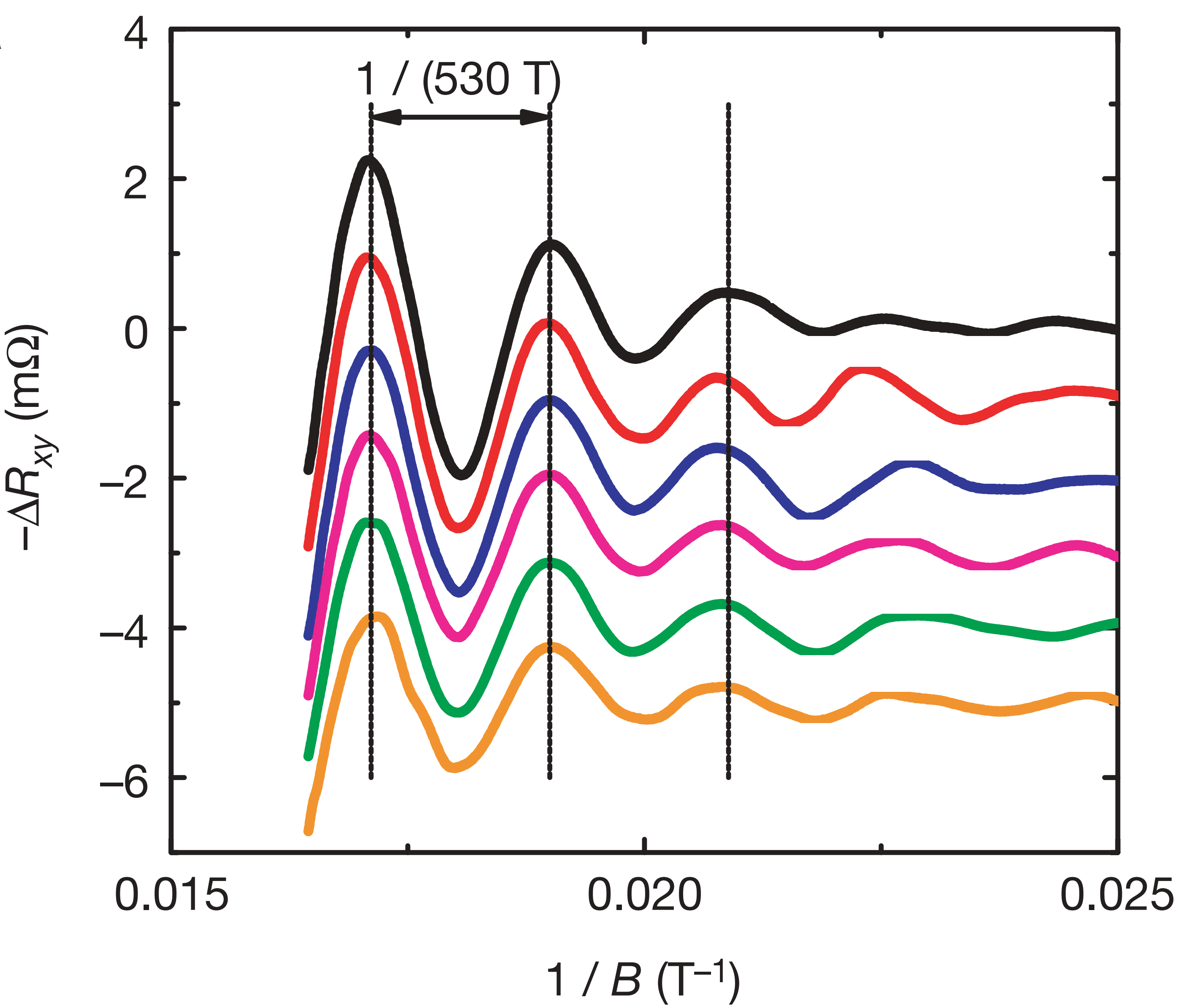
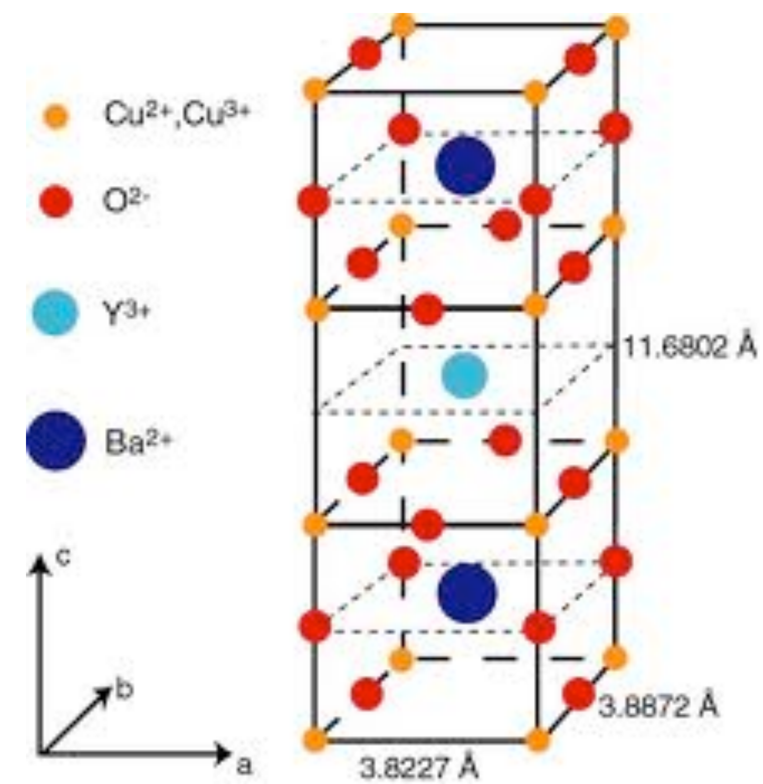
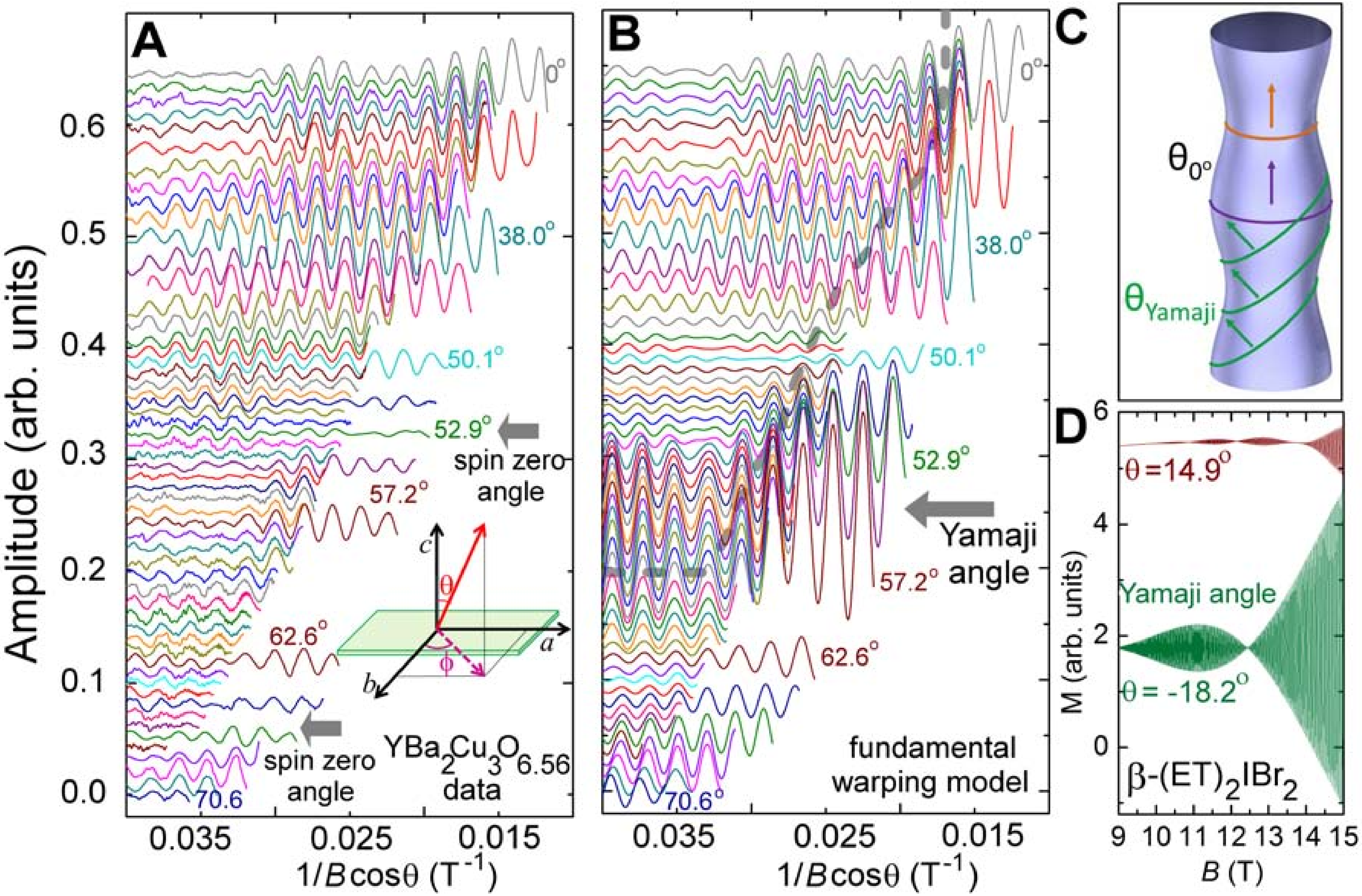






Twofold twisted Fermi surface from staggered order in an underdoped high T_c superconductor

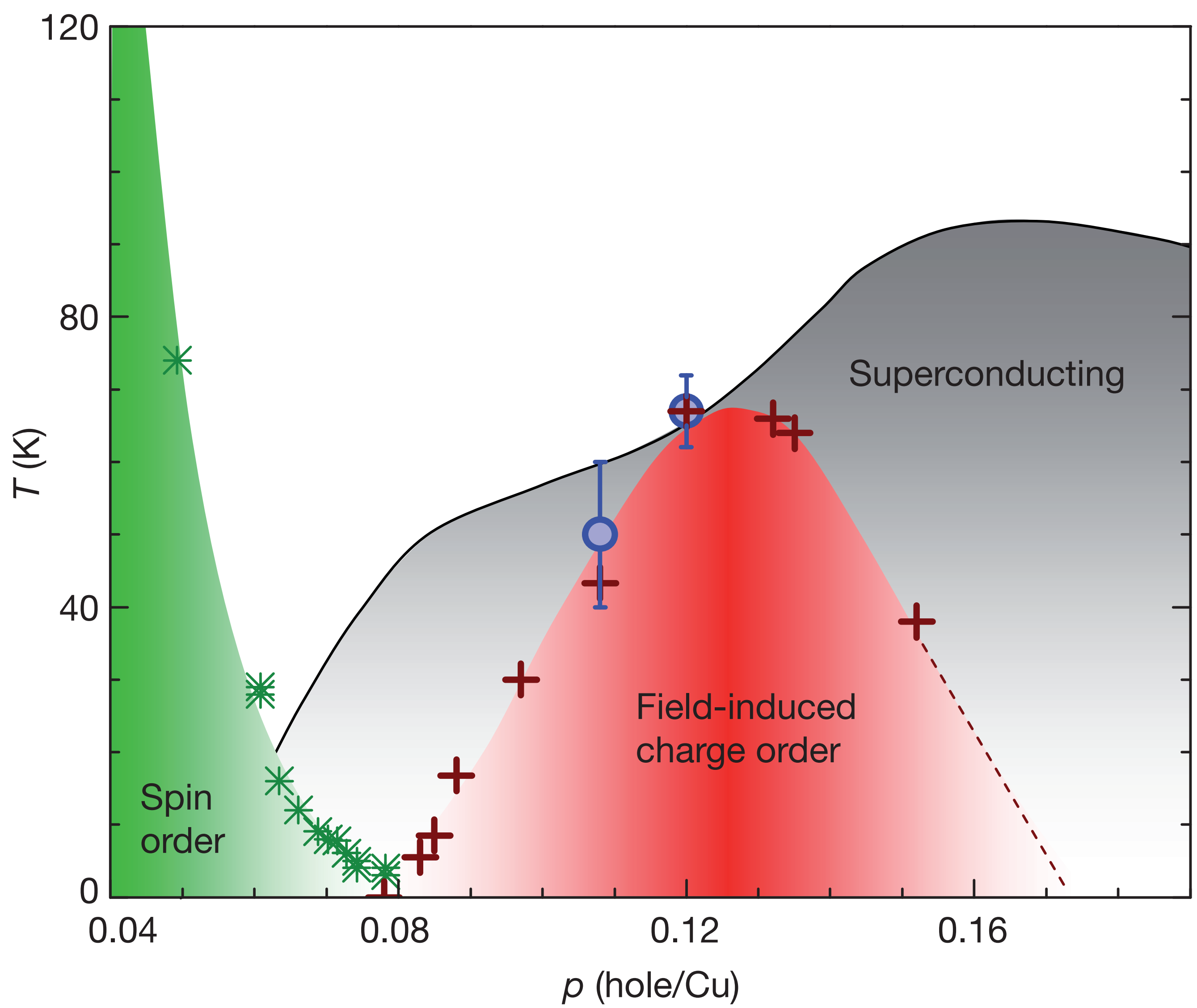
Suchitra E. Sebastian,[1*] N. Harrison,[2] F. F. Balakirev,[2] M. M. Altarawneh,[2,3]
Ruixing Liang,[4,5] D. A. Bonn,[4,5] W. N. Hardy,[4,5] G. G. Lonzarich,[1]

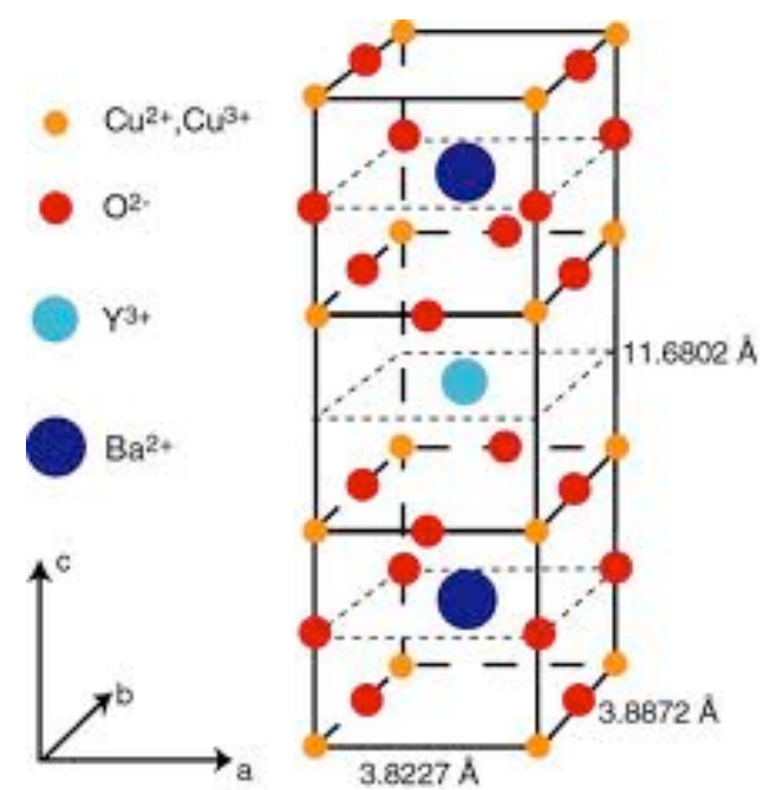
APS March meeting 2013
B2.00004

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

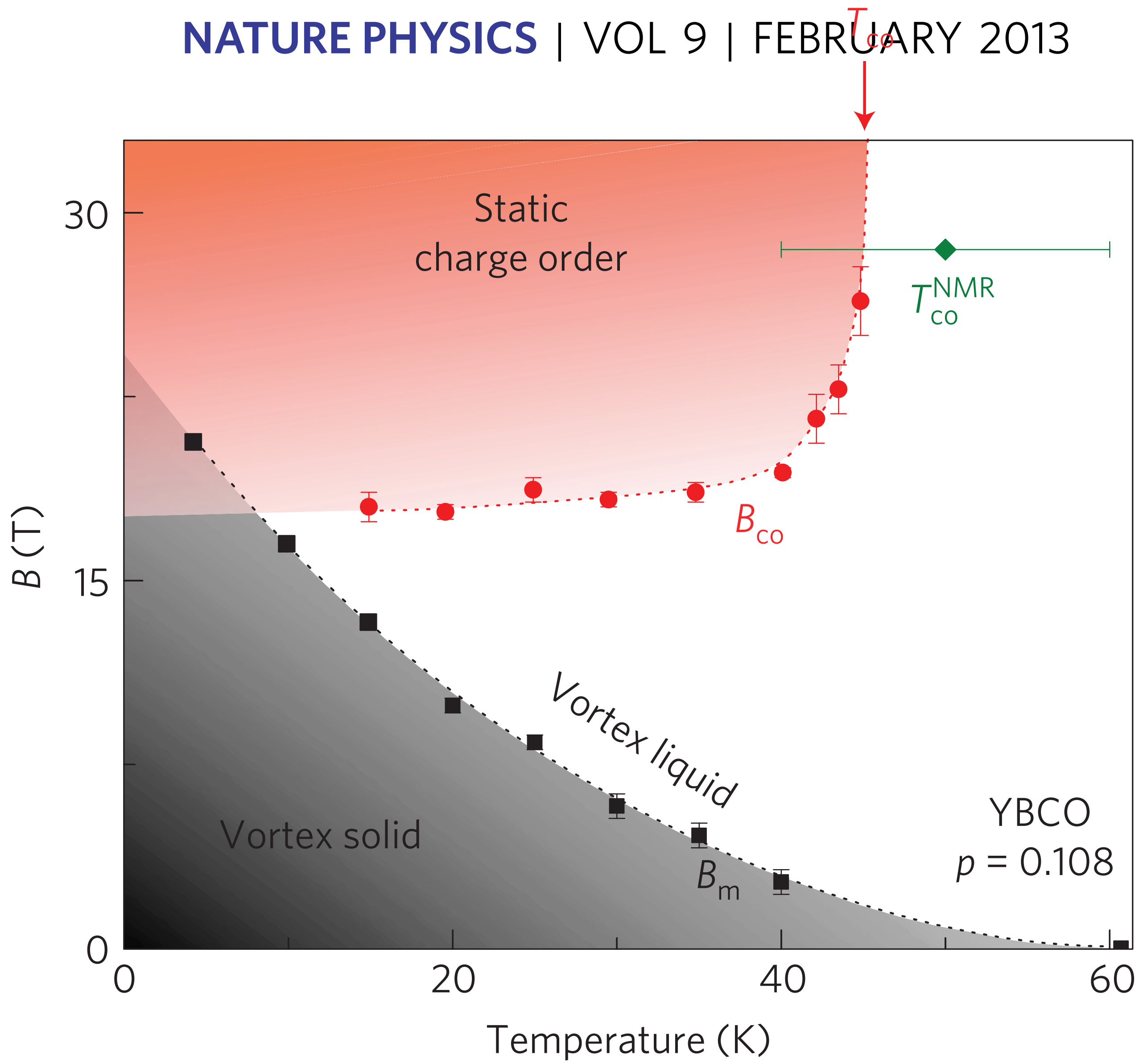




Thermodynamic phase diagram of static charge order in underdoped $YBa_2Cu_3O_y$

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

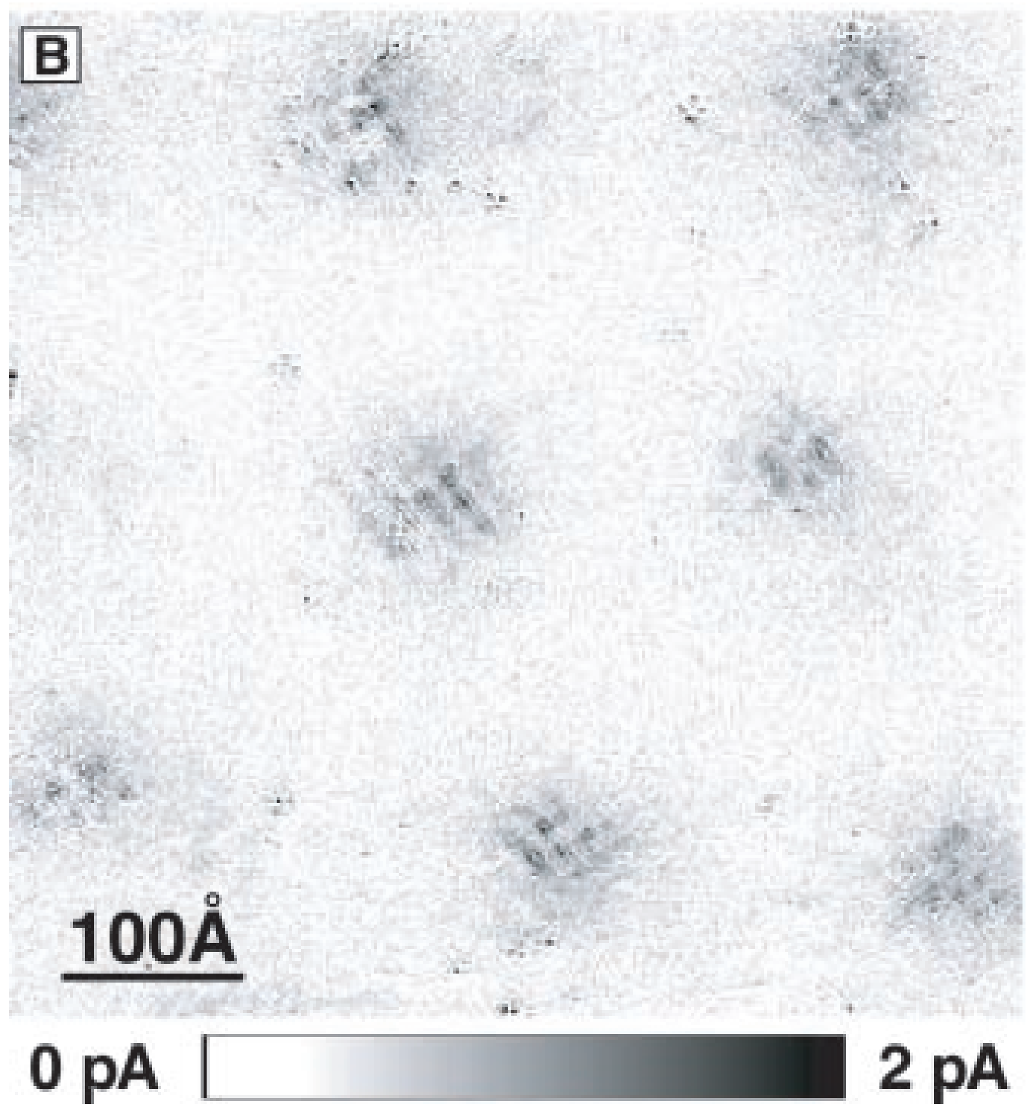


The comparison of different acoustic modes indicates that the charge modulation is biaxial, which differs from a uniaxial stripe charge order.

A Four Unit Cell Periodic Pattern of Quasi-Particle States Surrounding Vortex Cores in $Bi_2Sr_2CaCu_2O_{8+\delta}$

J. E. Hoffman,[1] E. W. Hudson,[1,2*] K. M. Lang,[1] V. Madhavan,[1]
H. Eisaki,[3†] S. Uchida,[3] J. C. Davis[1,2‡]

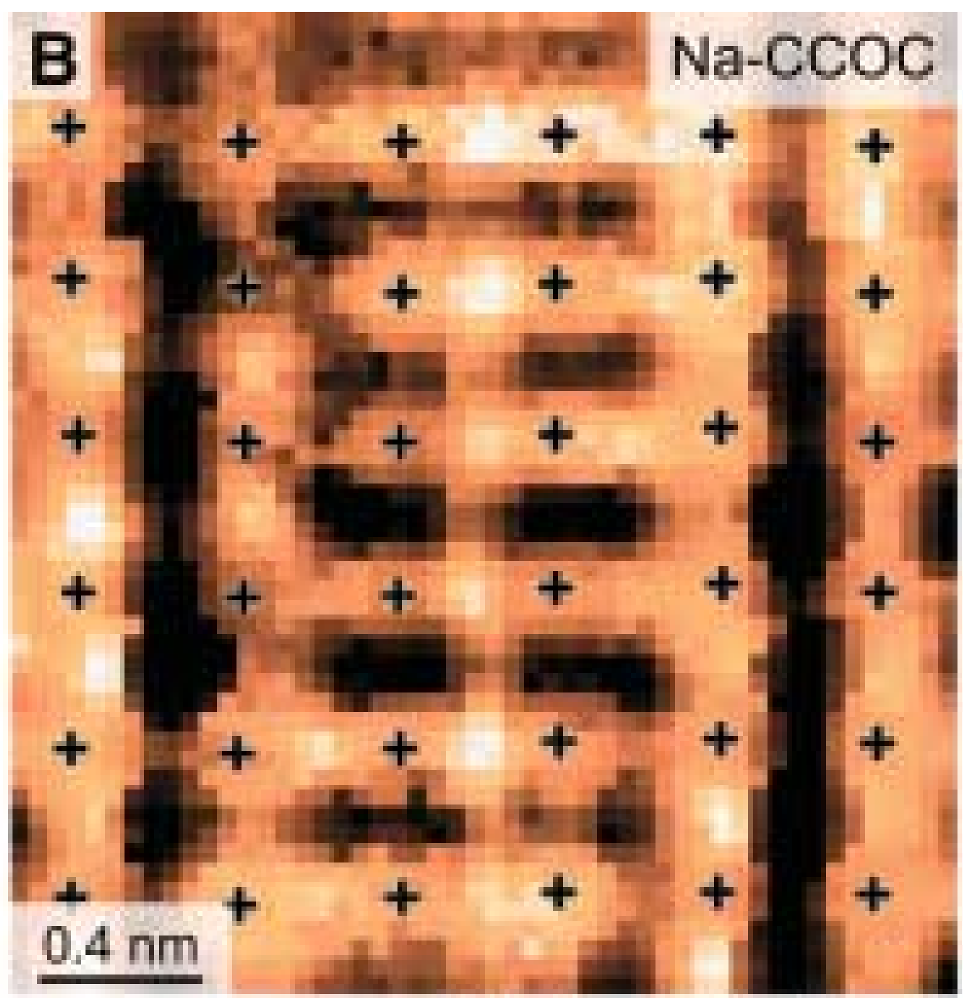
SCIENCE VOL 295 18 JANUARY 2002



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]*

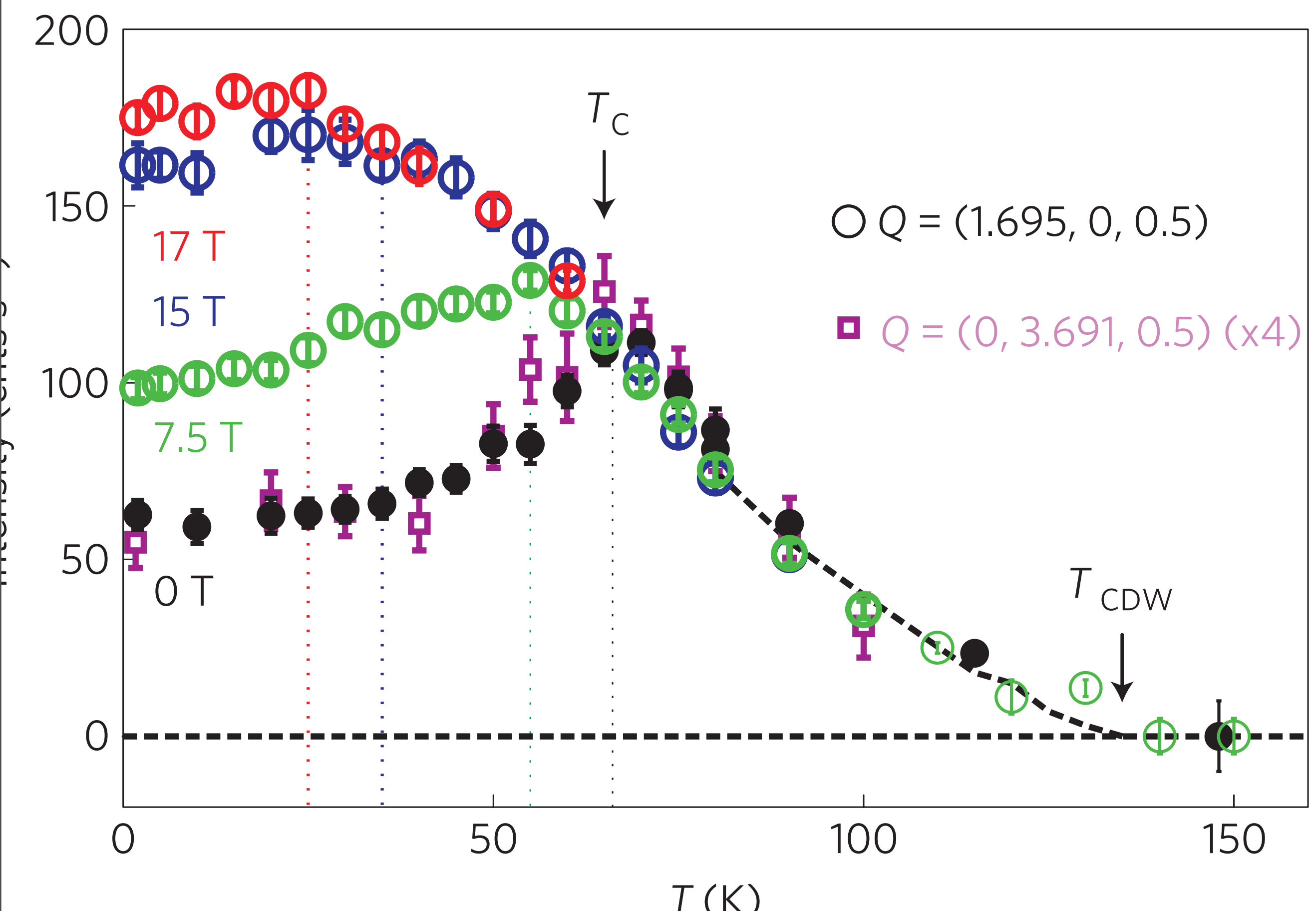
9 MARCH 2007 VOL 315 SCIENCE



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

NATURE PHYSICS | VOL 8 | DECEMBER 2012 |

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]



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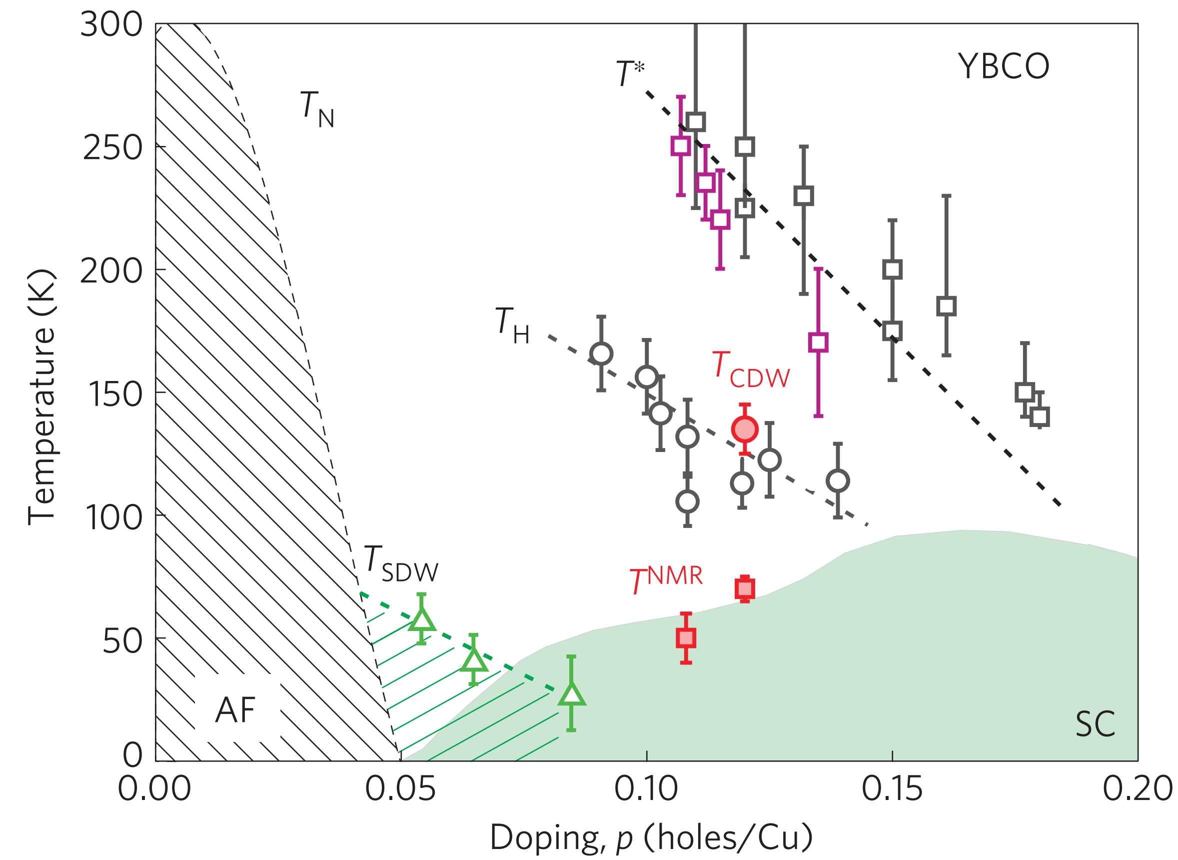
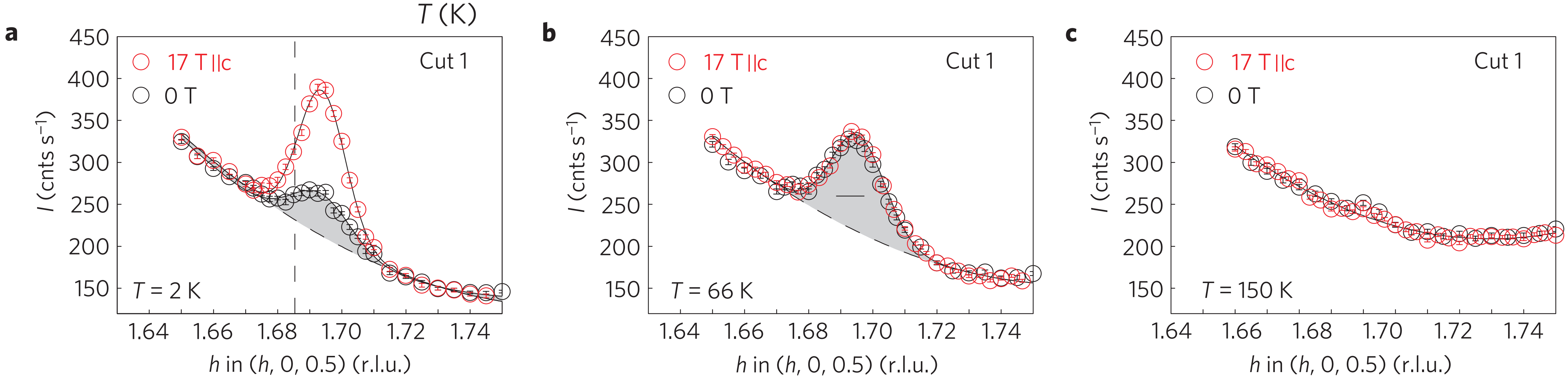
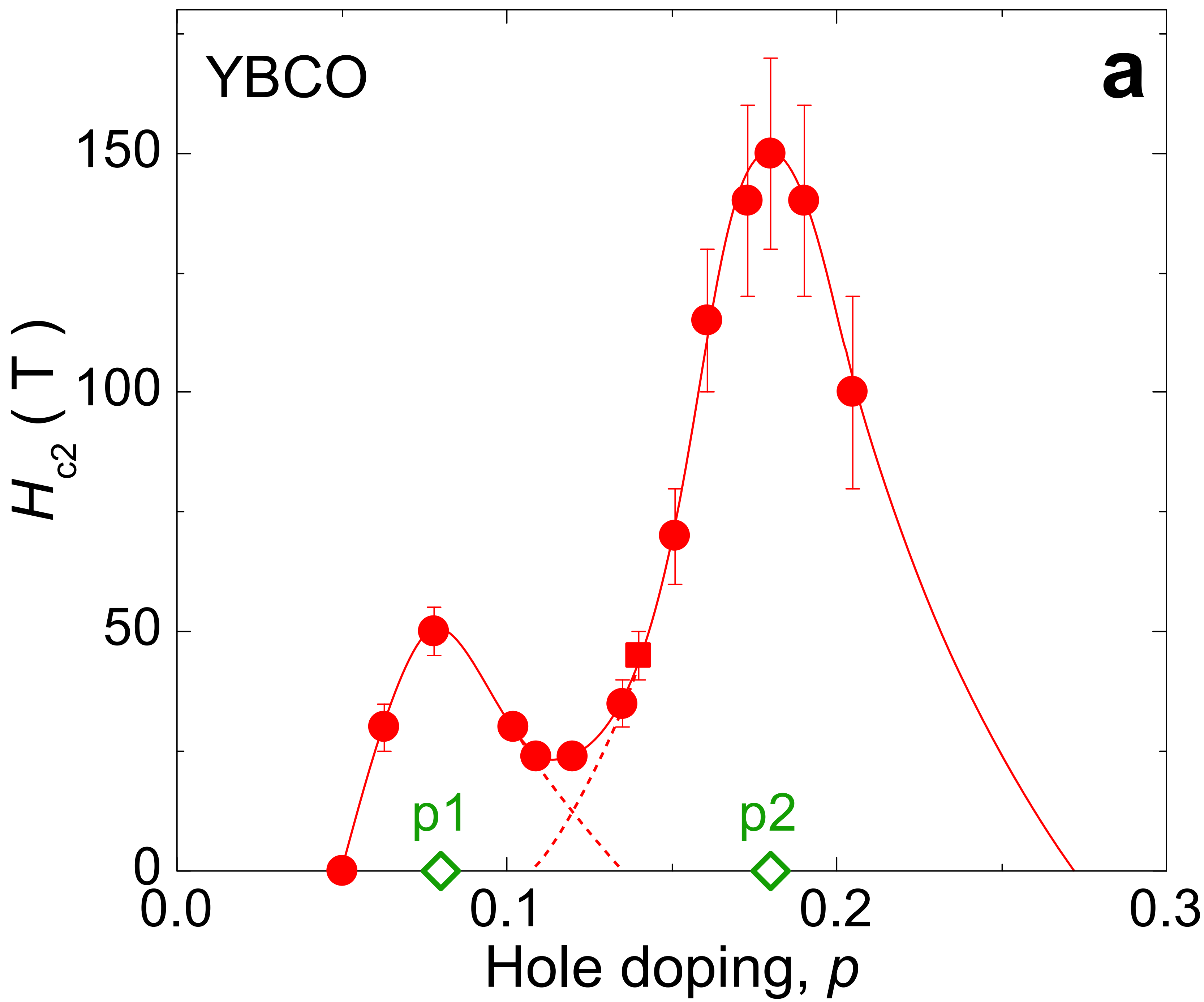
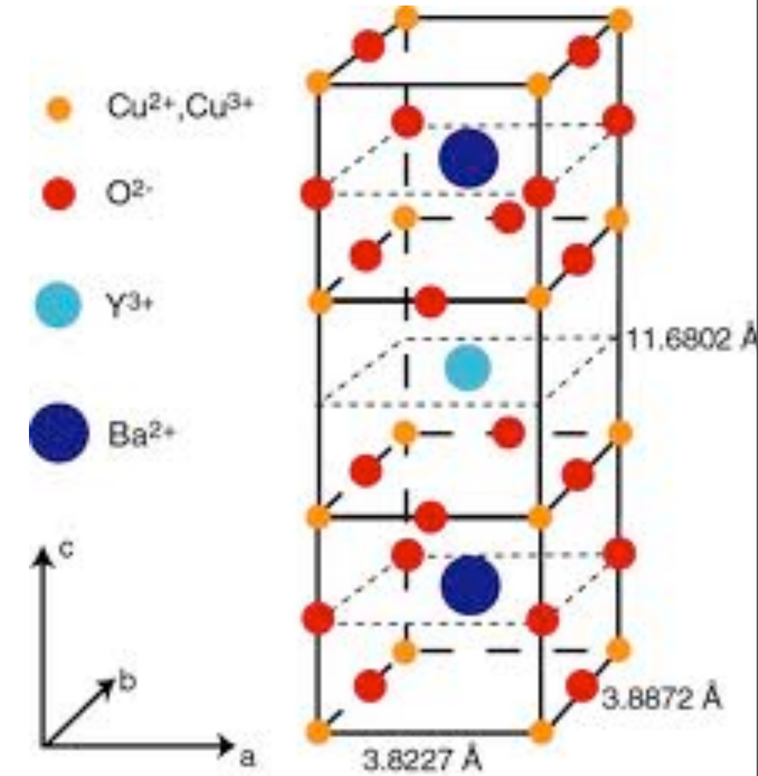




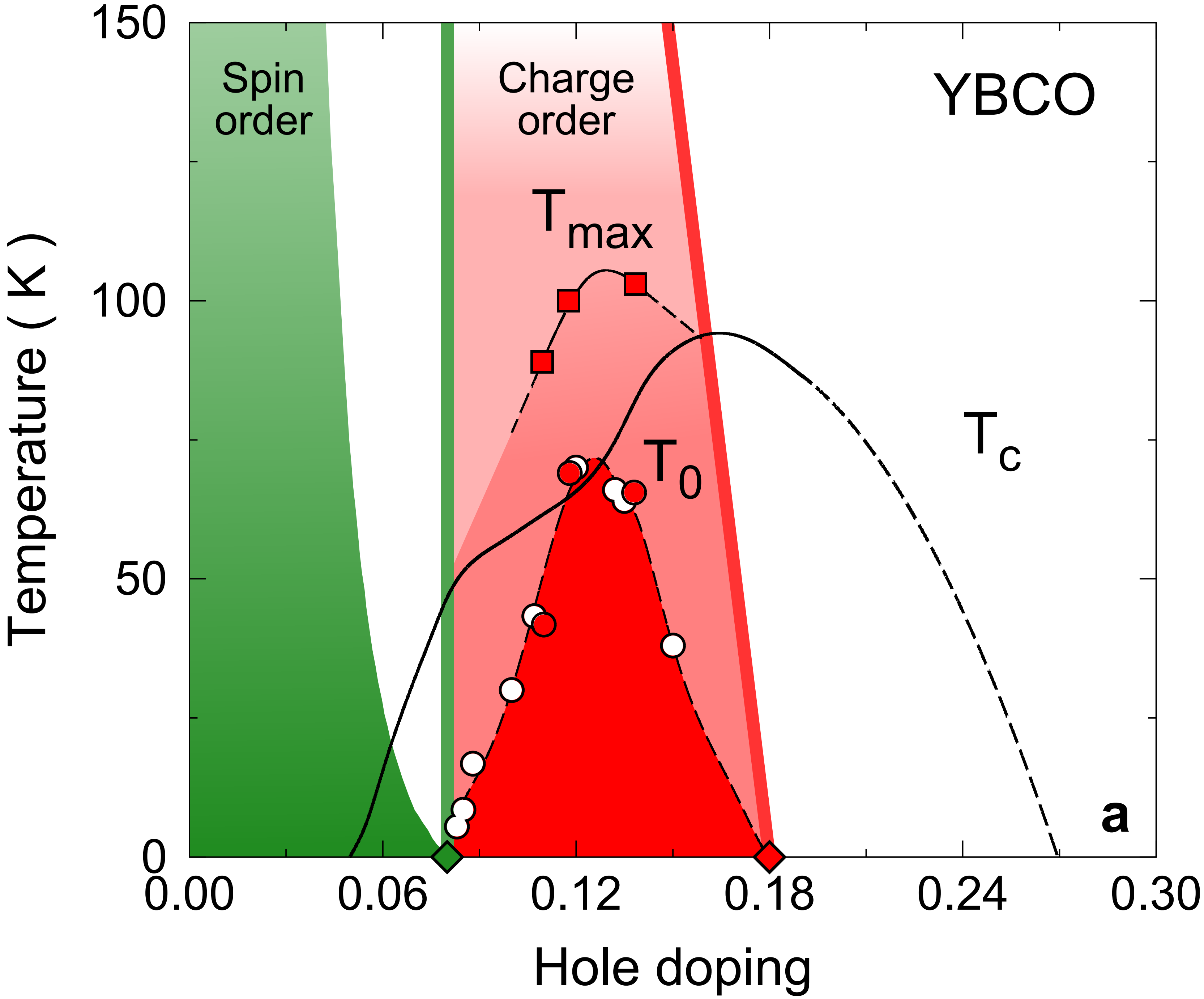
Saturday, March 23, 13

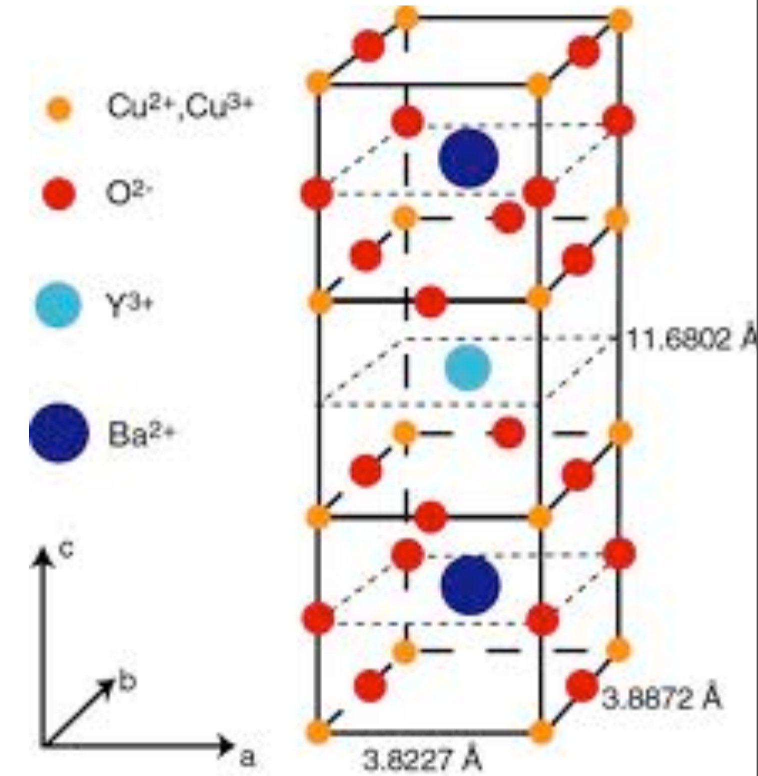




APS March meeting 2013 B36.00002

G. Grissonnanche, O. Cyr-Choinière, F. Laliberté, S. René de Cotret, A. Juneau-Fecteau, S. Dufour-Beauséjour, M.-È. Delage, D. LeBoeuf, J. Chang, B. J. Ramshaw, D. A. Bonn, W. N. Hardy, R. Liang, S. Adachi, N. E. Hussey, B. Vignolle, C. Proust, M. Sutherland, S. Krämer, J.-H. Park, D. Graf, N. Doiron-Leyraud & Louis Taillefer





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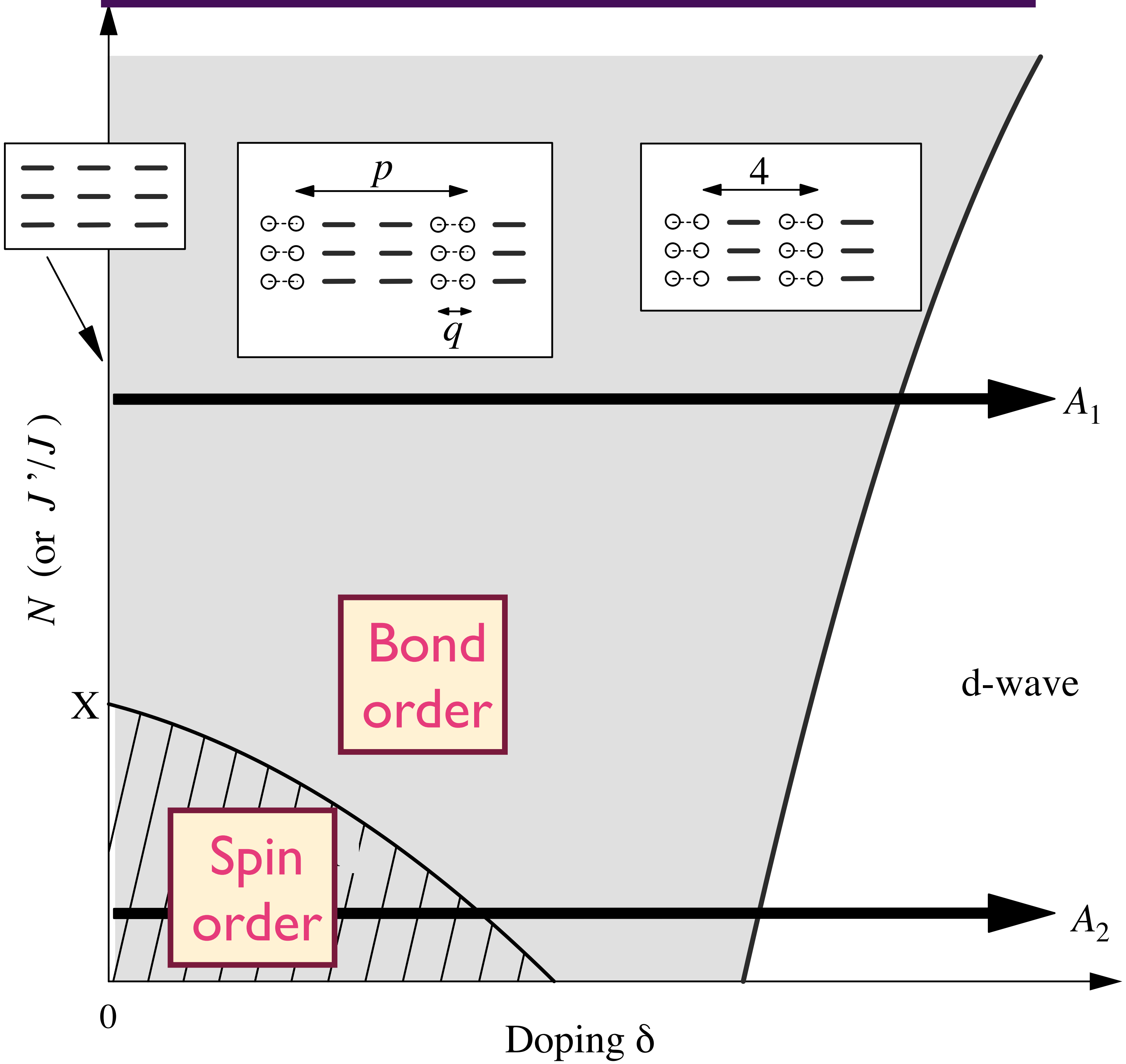
Low T phase diagram of a doped antiferromagnet



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

Outline

1. Update on cuprate experiments

2. Antiferromagnetism in metals:
   d-wave superconductivity

3. Low energy theory, emergent pseudospin
   symmetry, and bond order

4. Unrestricted Hartree-Fock-BCS

5. Quantum Monte Carlo
   without the sign problem

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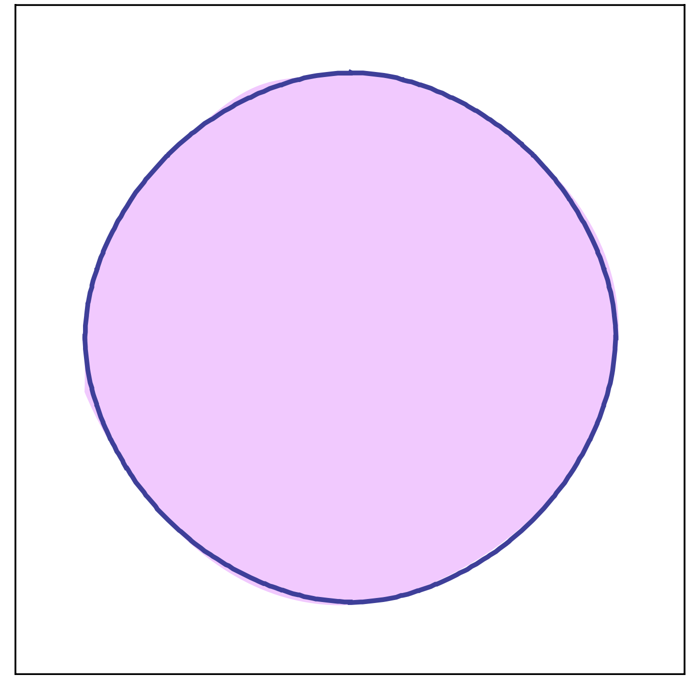
Fermi surface+antiferromagnetism

Metal with "large" Fermi surface



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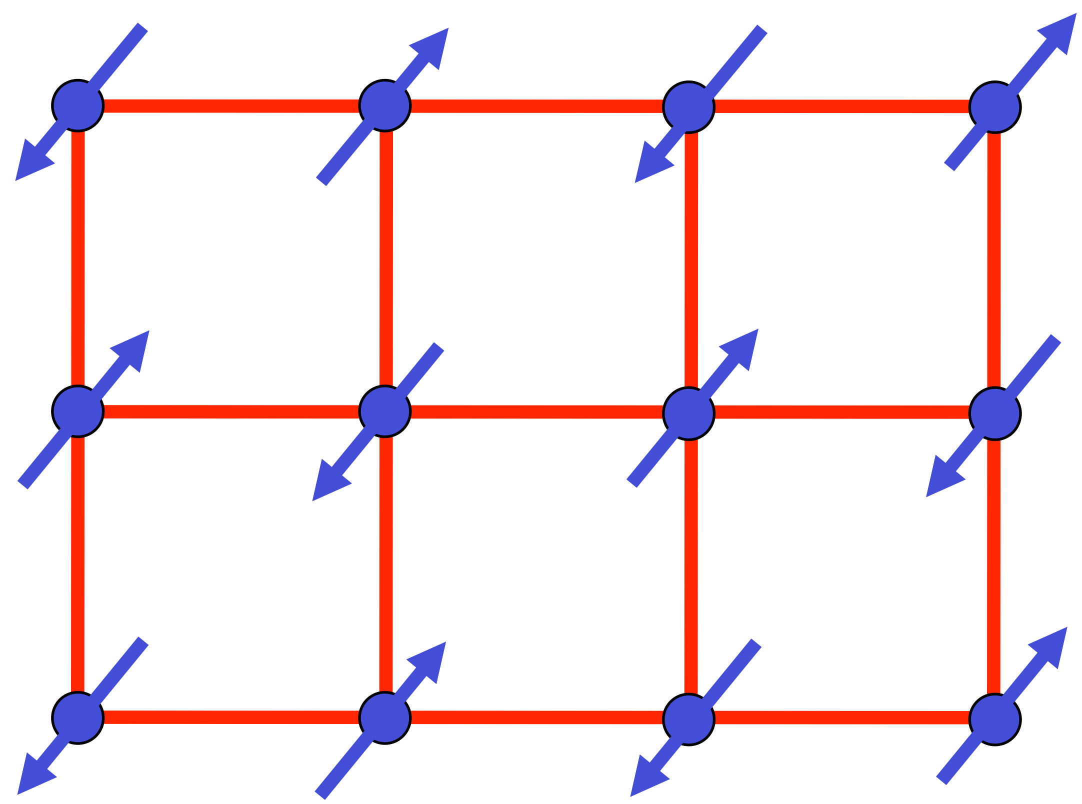
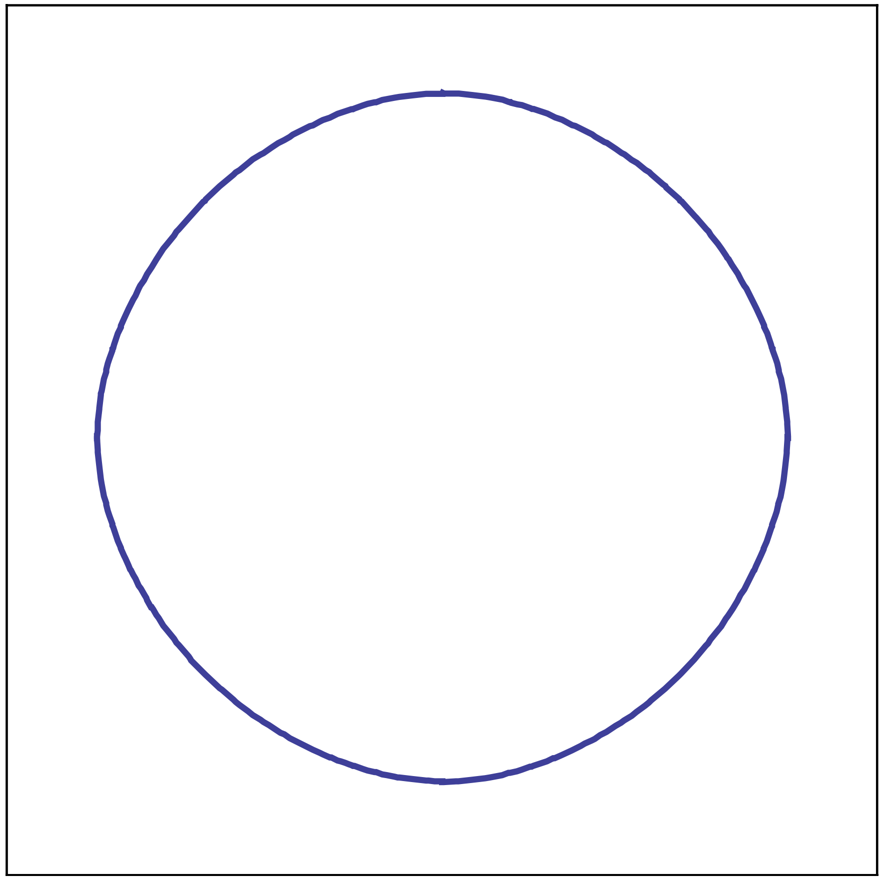


The electron spin polarization obeys

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

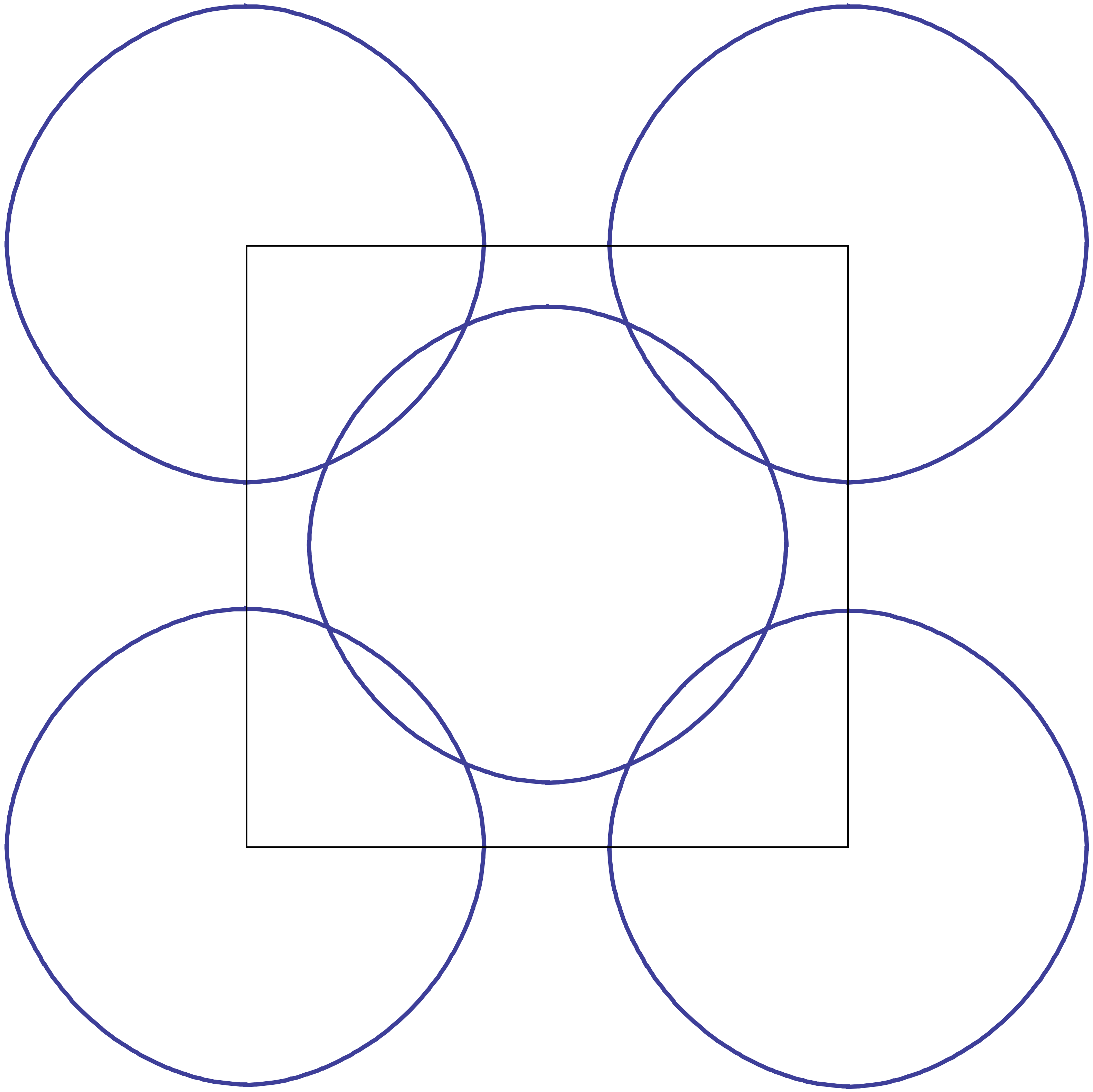
where $\mathbf{K}$ is the ordering wavevector.

Fermi surface+antiferromagnetism



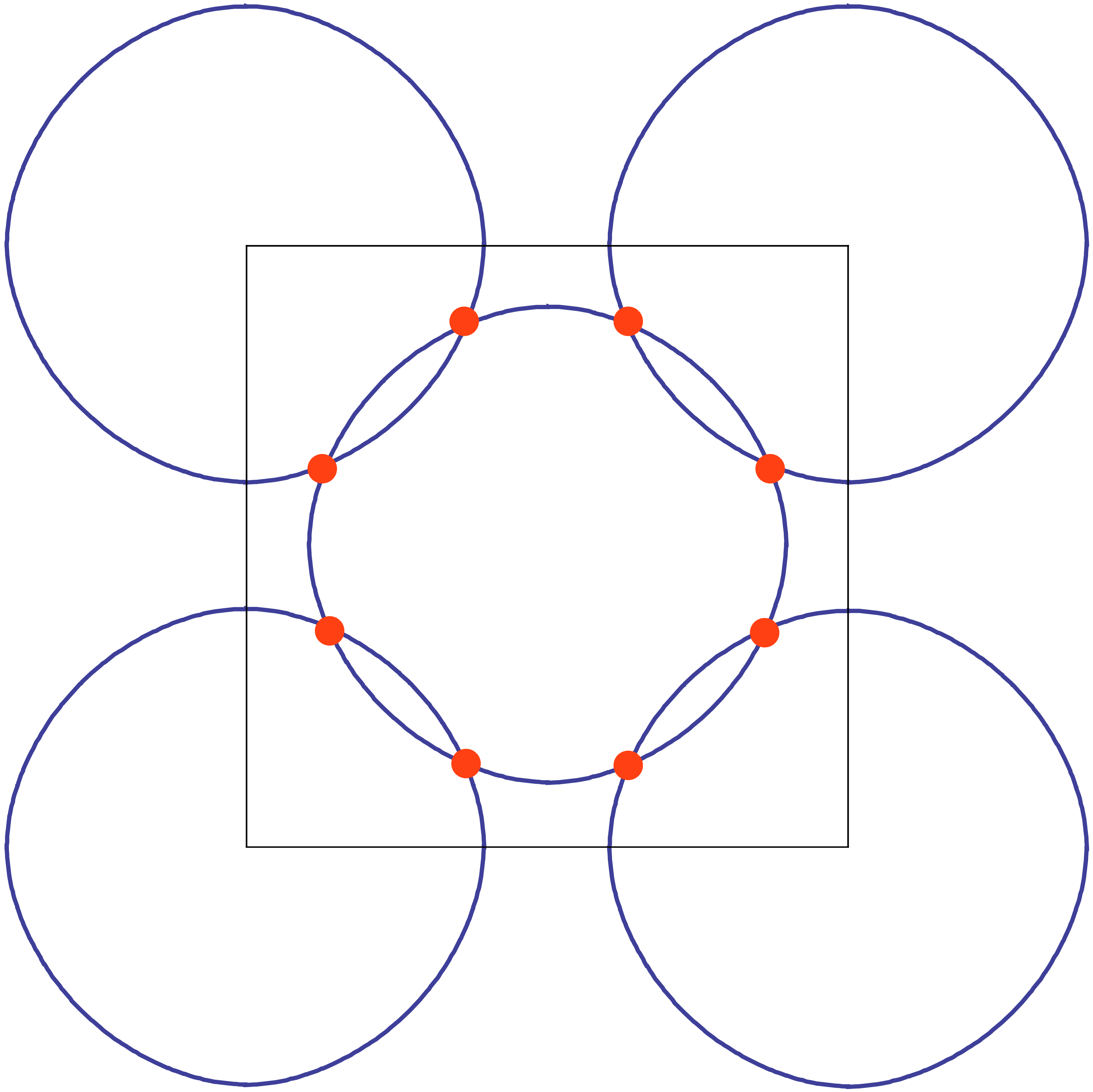
Metal with “large” Fermi surface

Fermi surface+antiferromagnetism



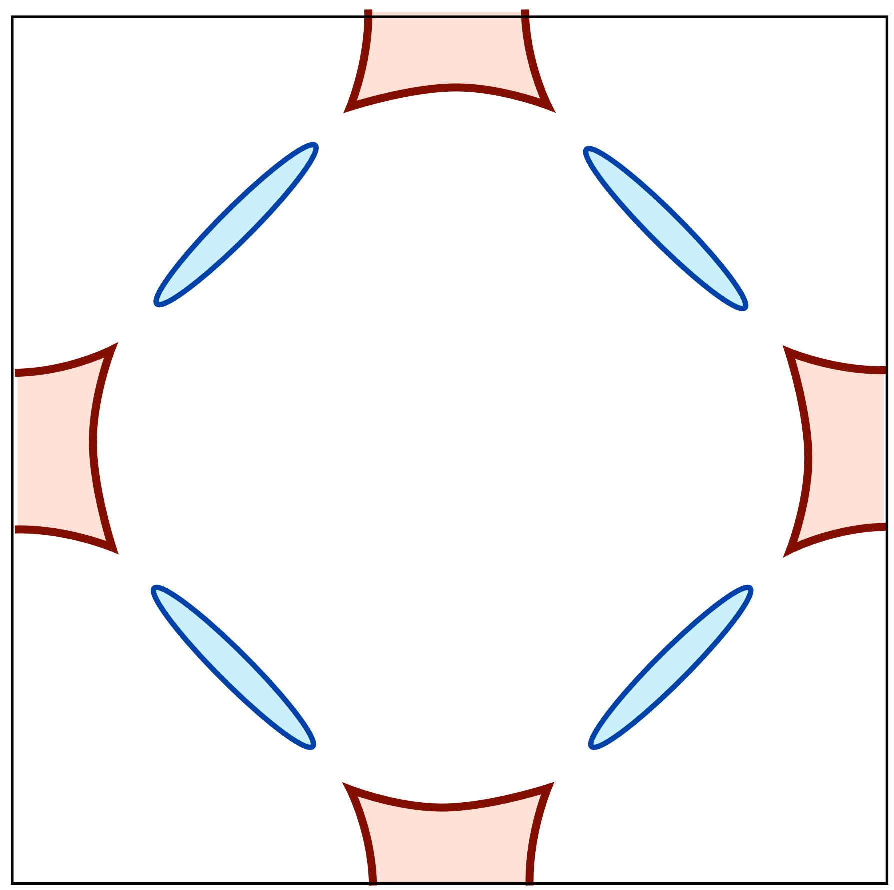
Fermi surfaces translated by $\mathbf{K} = (\pi, \pi)$.

Fermi surface+antiferromagnetism



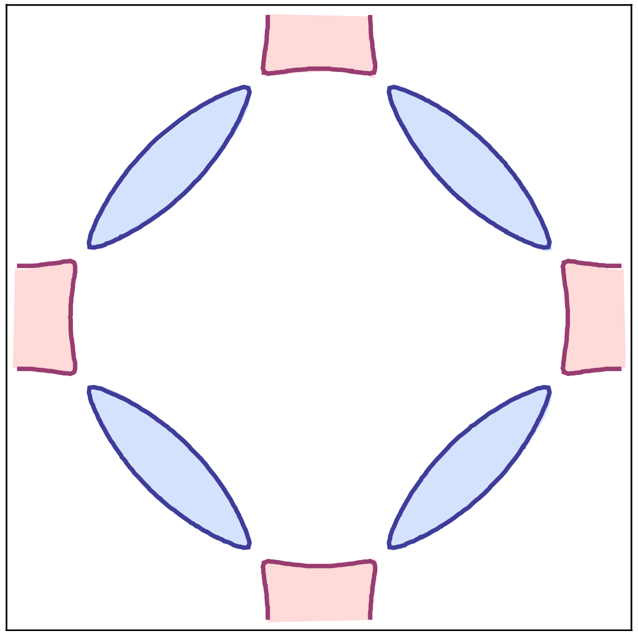
"Hot" spots

Fermi surface+antiferromagnetism



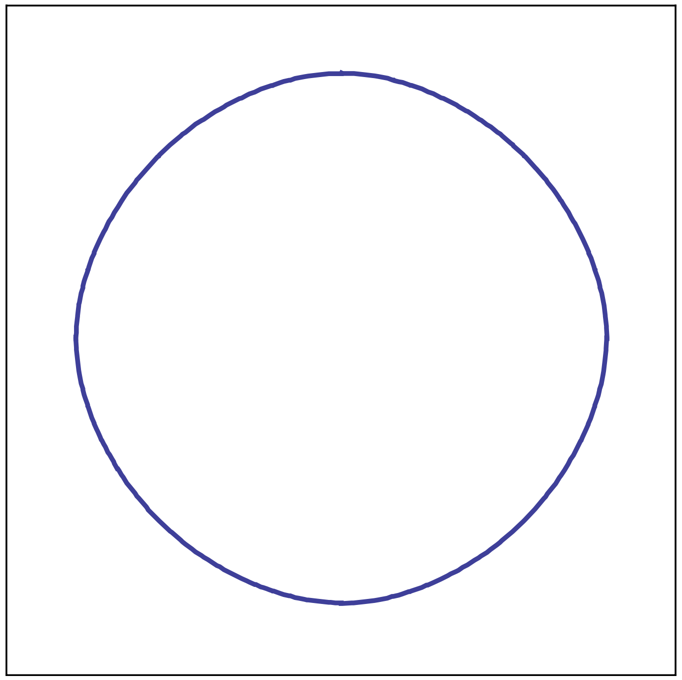
Electron and hole pockets in
antiferromagnetic phase
with antiferromagnetic order parameter $\langle \vec{\varphi} \rangle \neq 0$

Fermi surface+antiferromagnetism



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

Metal with electron and hole pockets



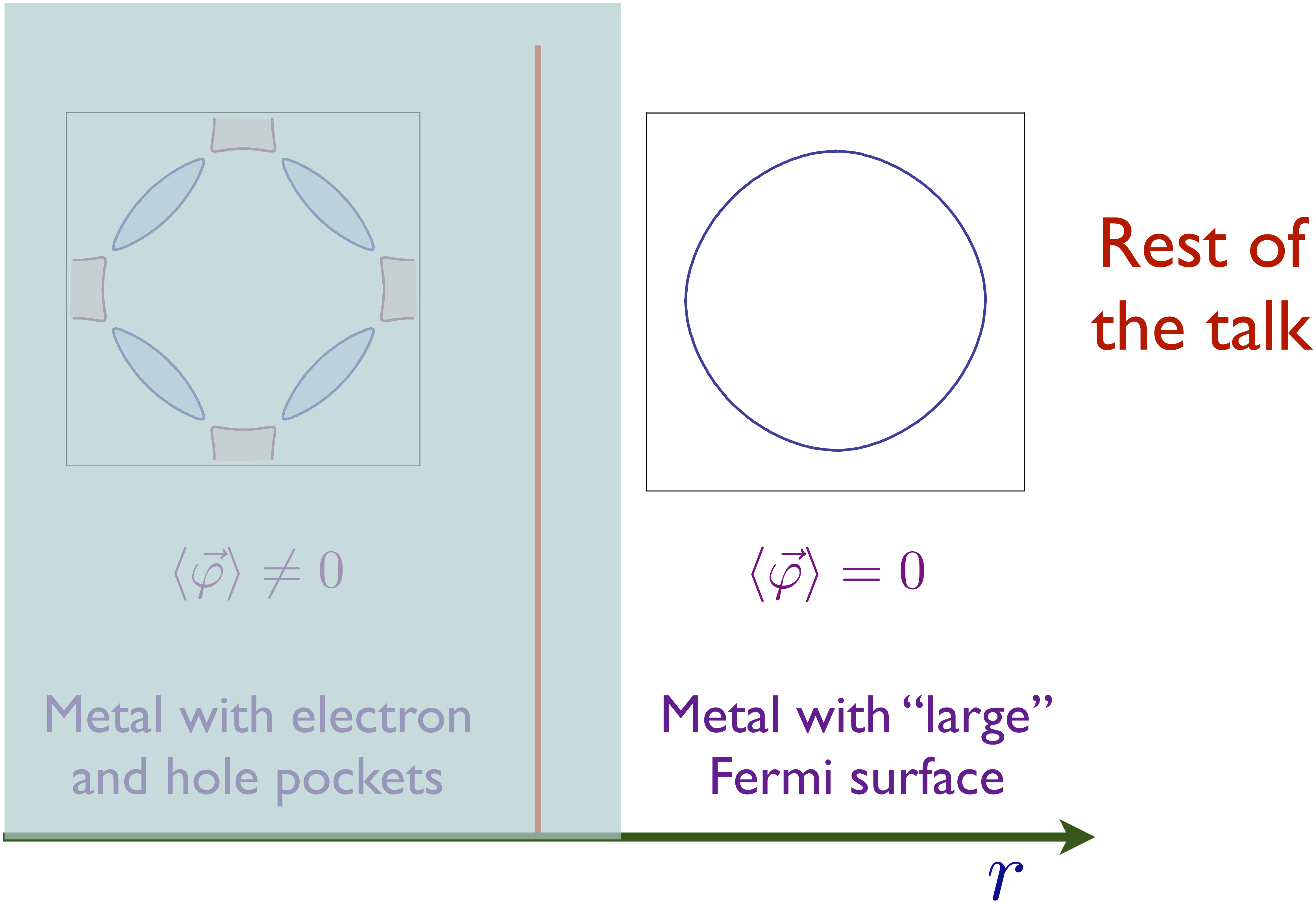
$\langle \vec{\varphi} \rangle = 0$

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



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).

Pairing by SDW fluctuation exchange

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

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

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

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

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.

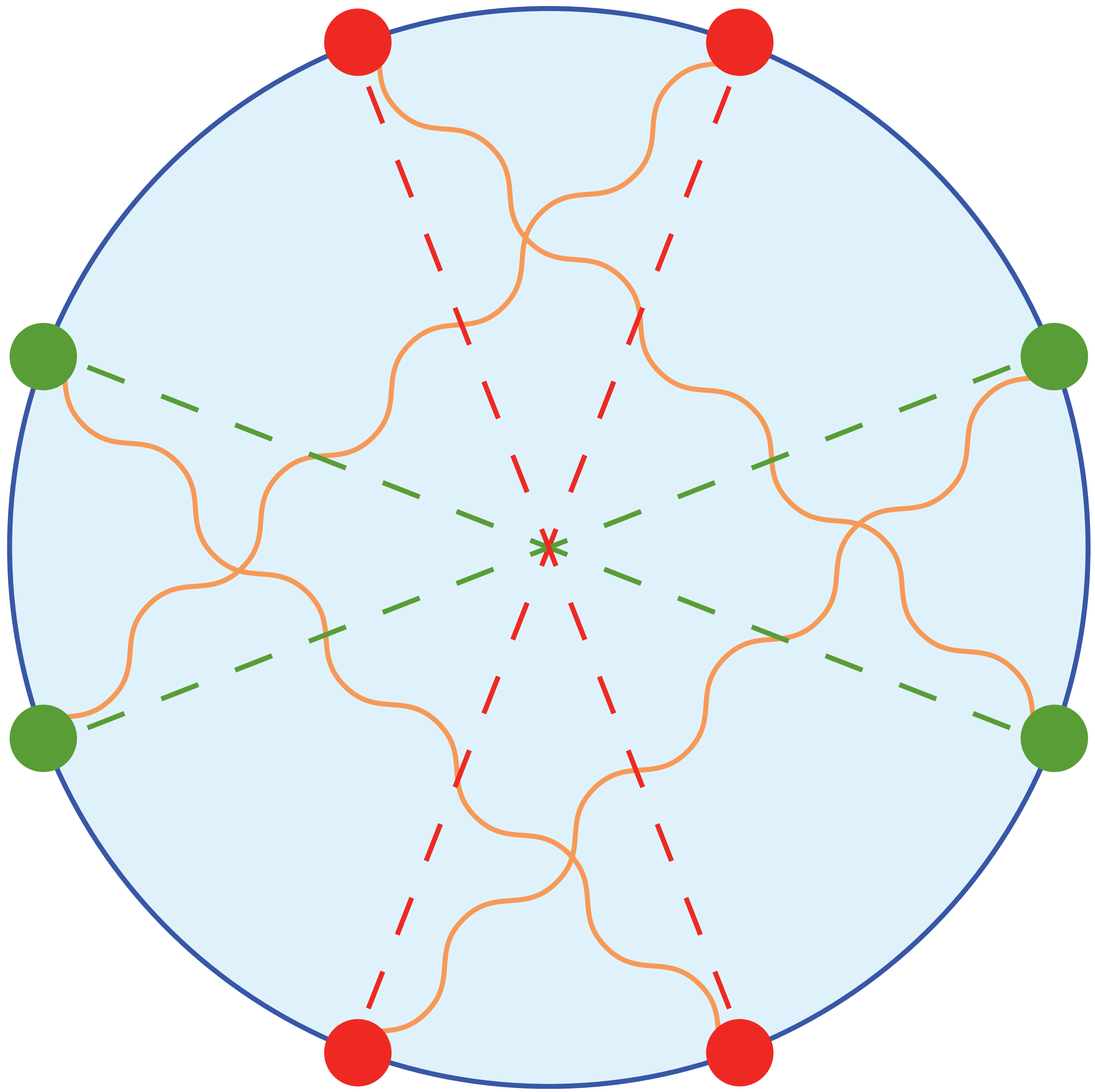
BCS Gap equation

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

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

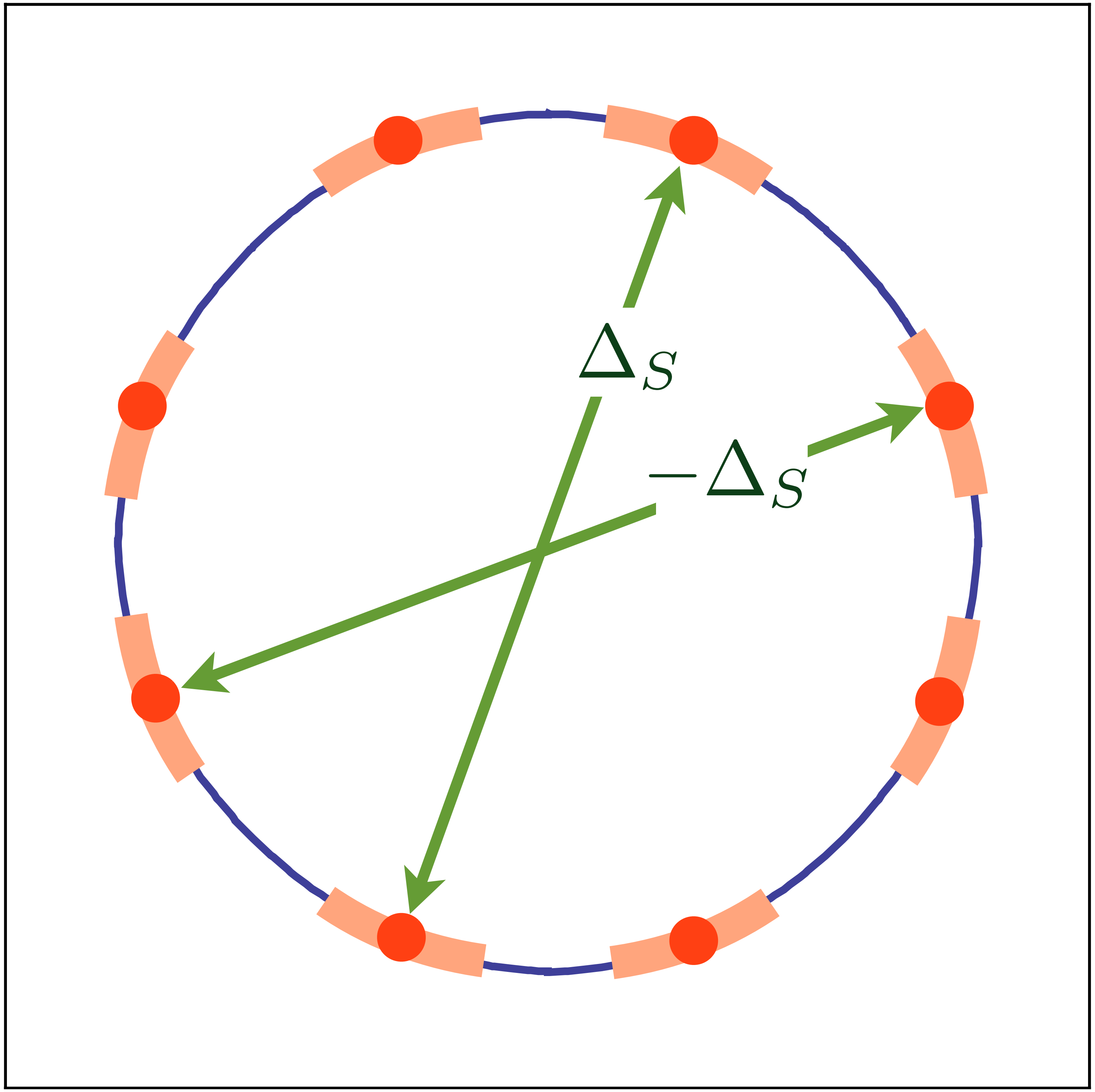
Non-zero solutions of this equation require that $\Delta_{\mathbf{k}}$ and $\Delta_{\mathbf{p}}$ have opposite signs when $\mathbf{p} - \mathbf{k} \approx \mathbf{K}$.

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

Outline

1. The "modern era" of cuprate experiments

2. Antiferromagnetism in metals:
   d-wave superconductivity

3. Low energy theory, emergent pseudospin
   symmetry, and bond order

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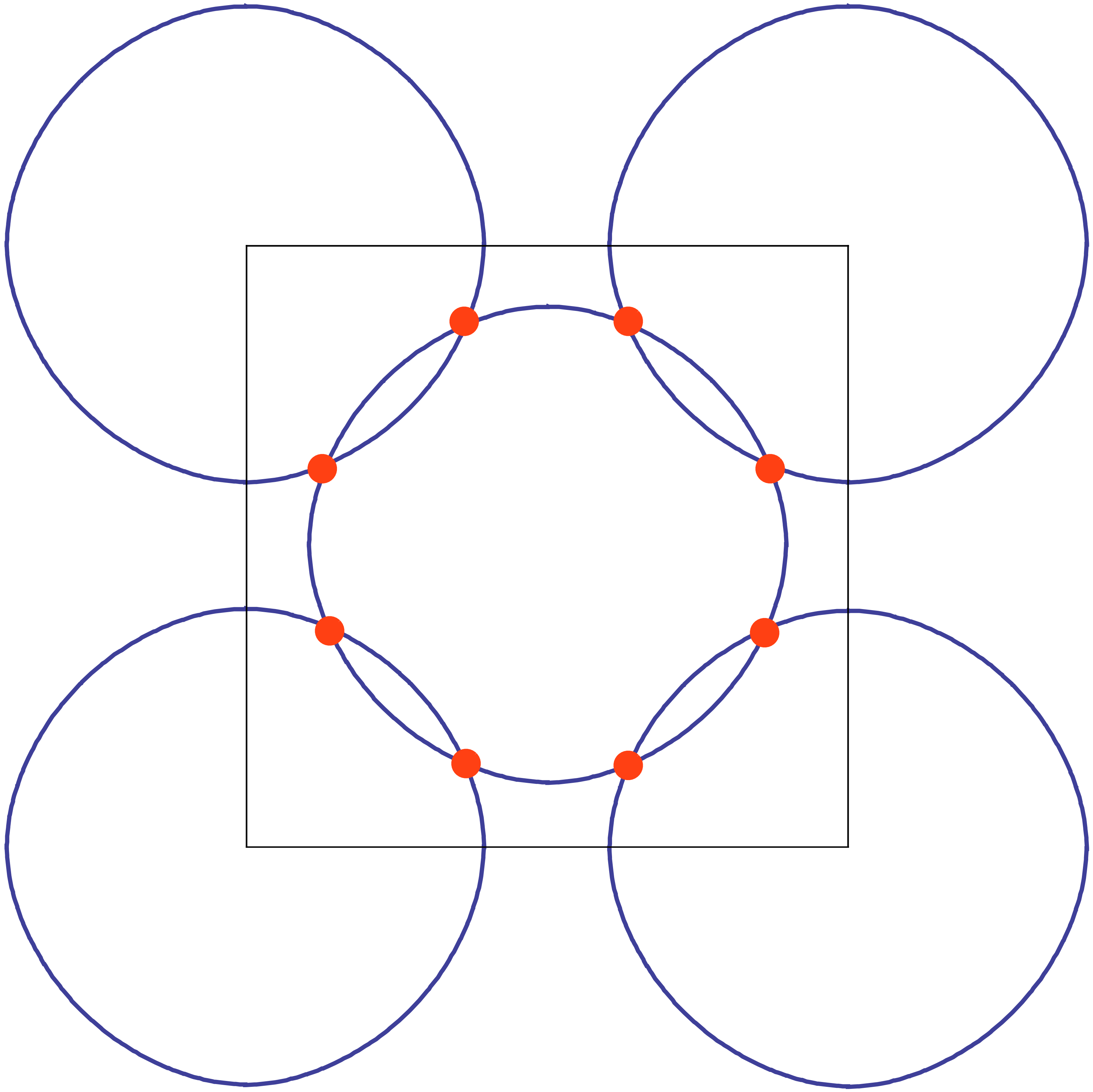
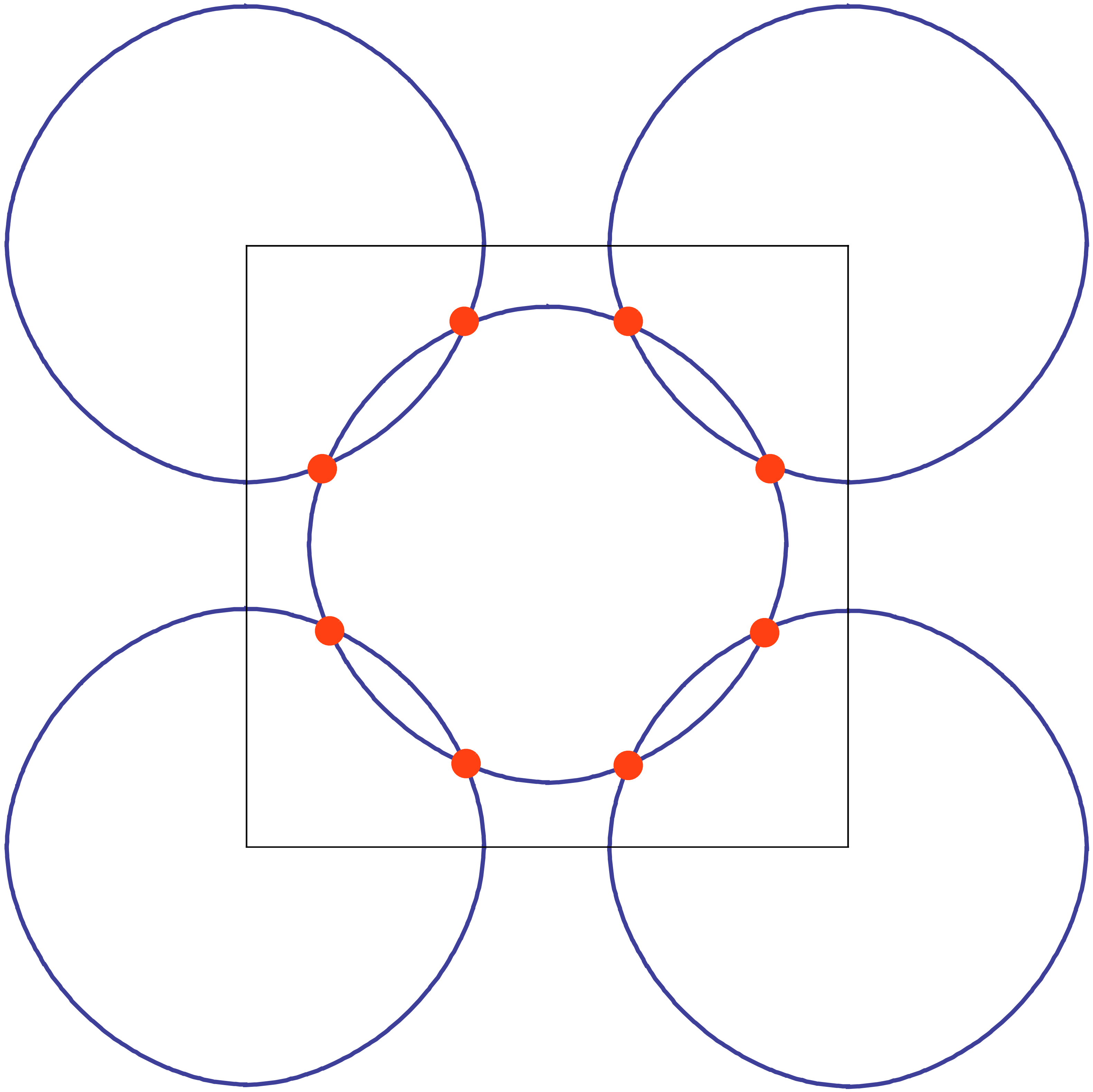
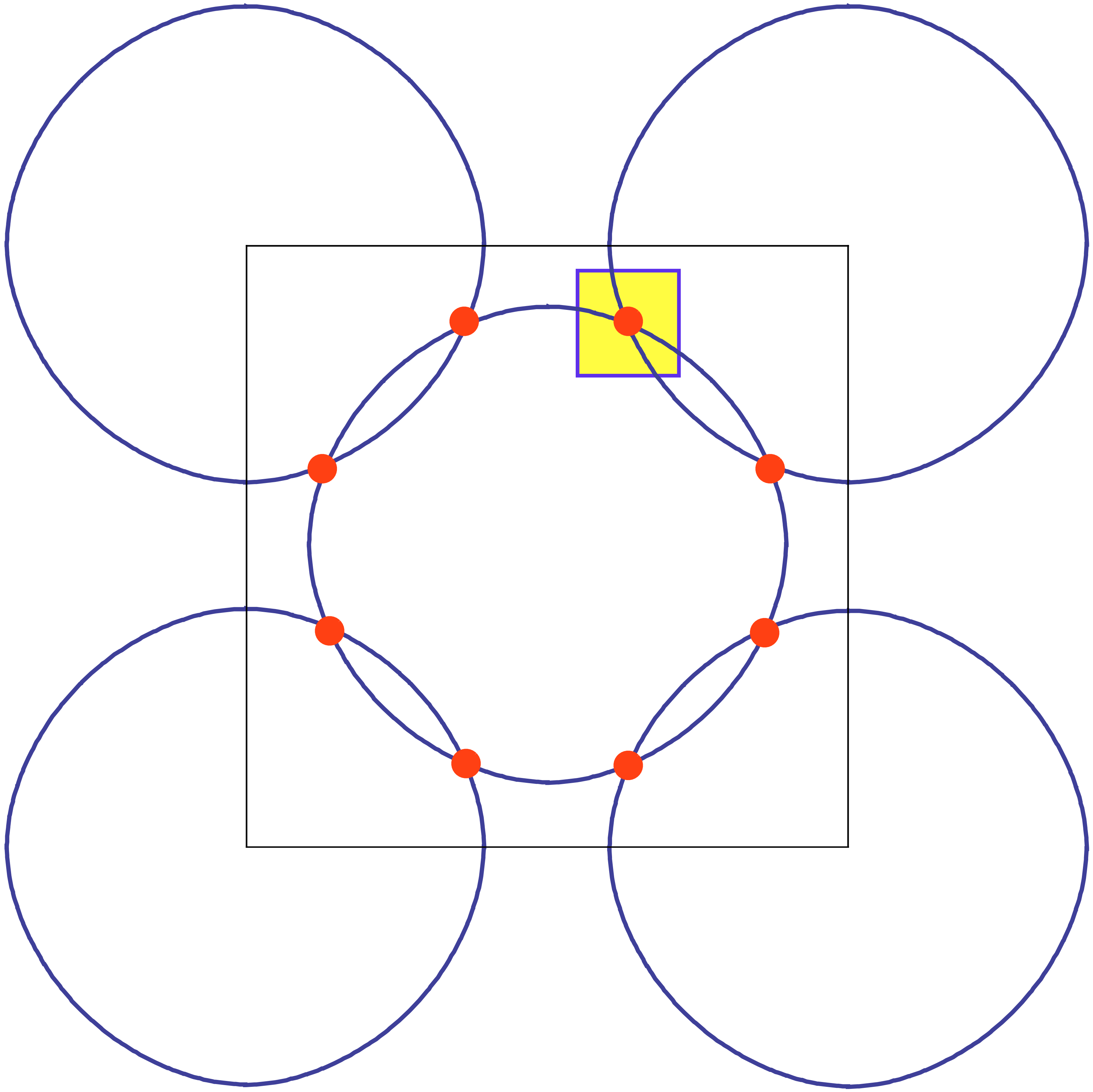


“Hot” spots

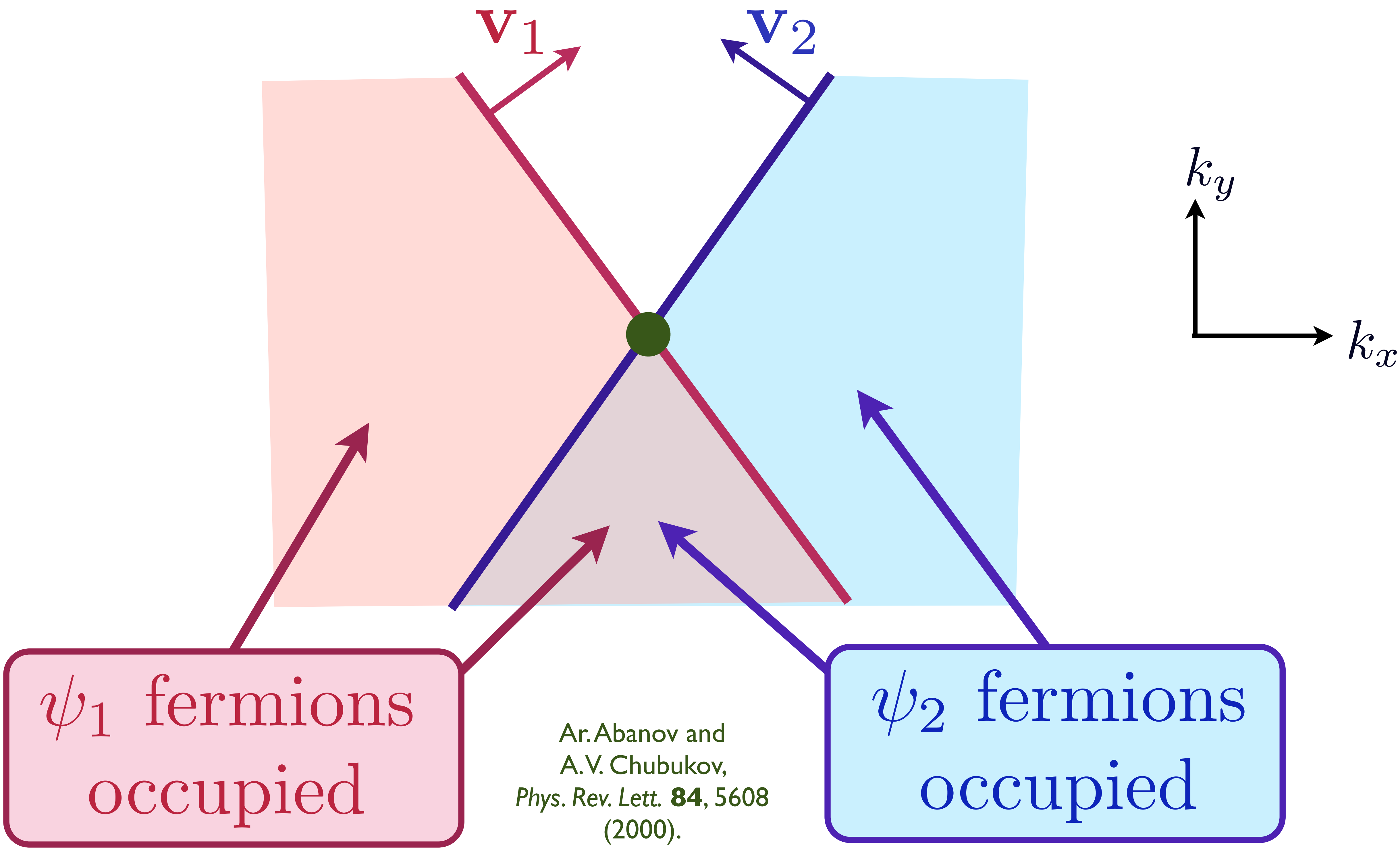


Low energy theory for critical point near hot spots



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



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

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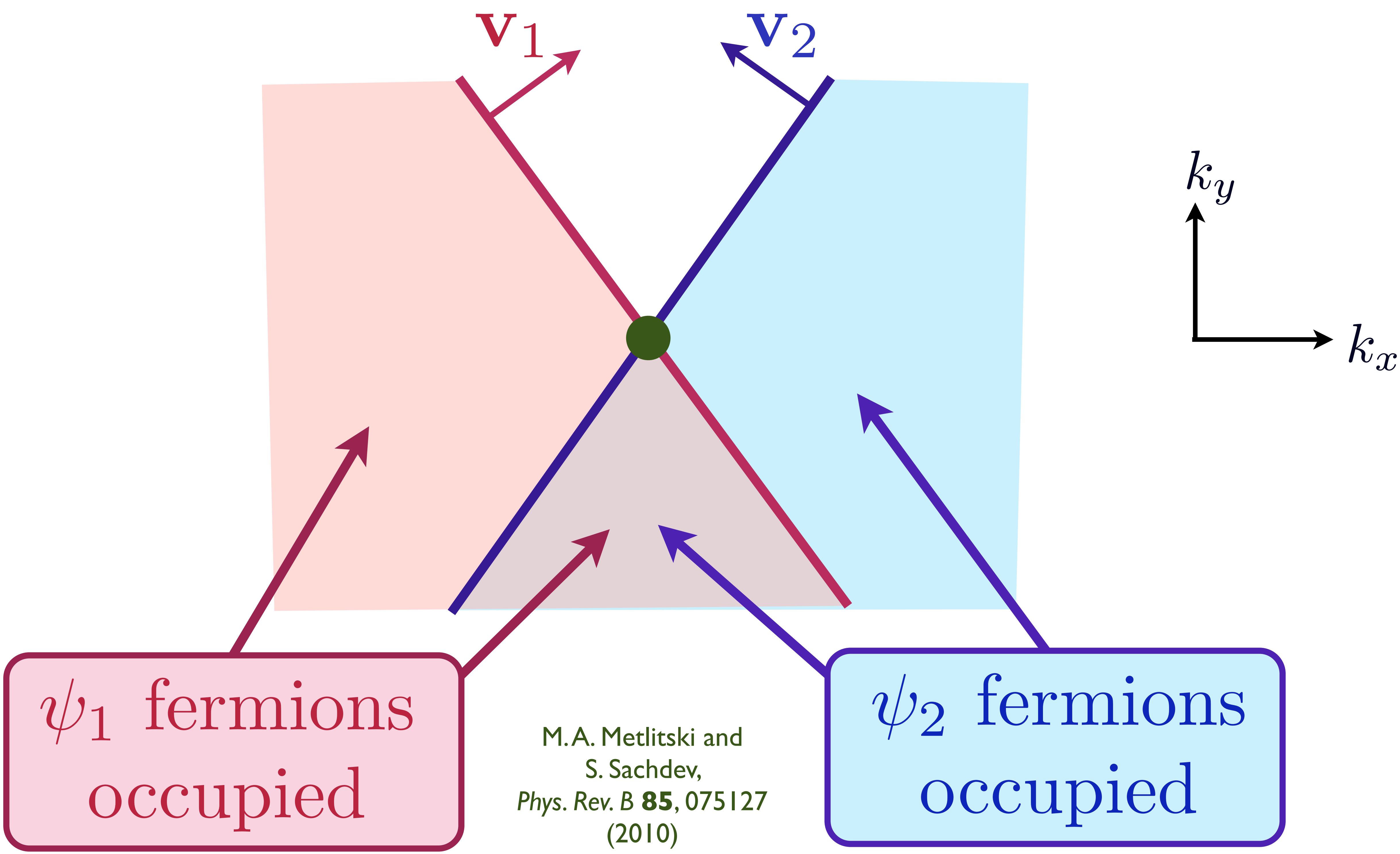
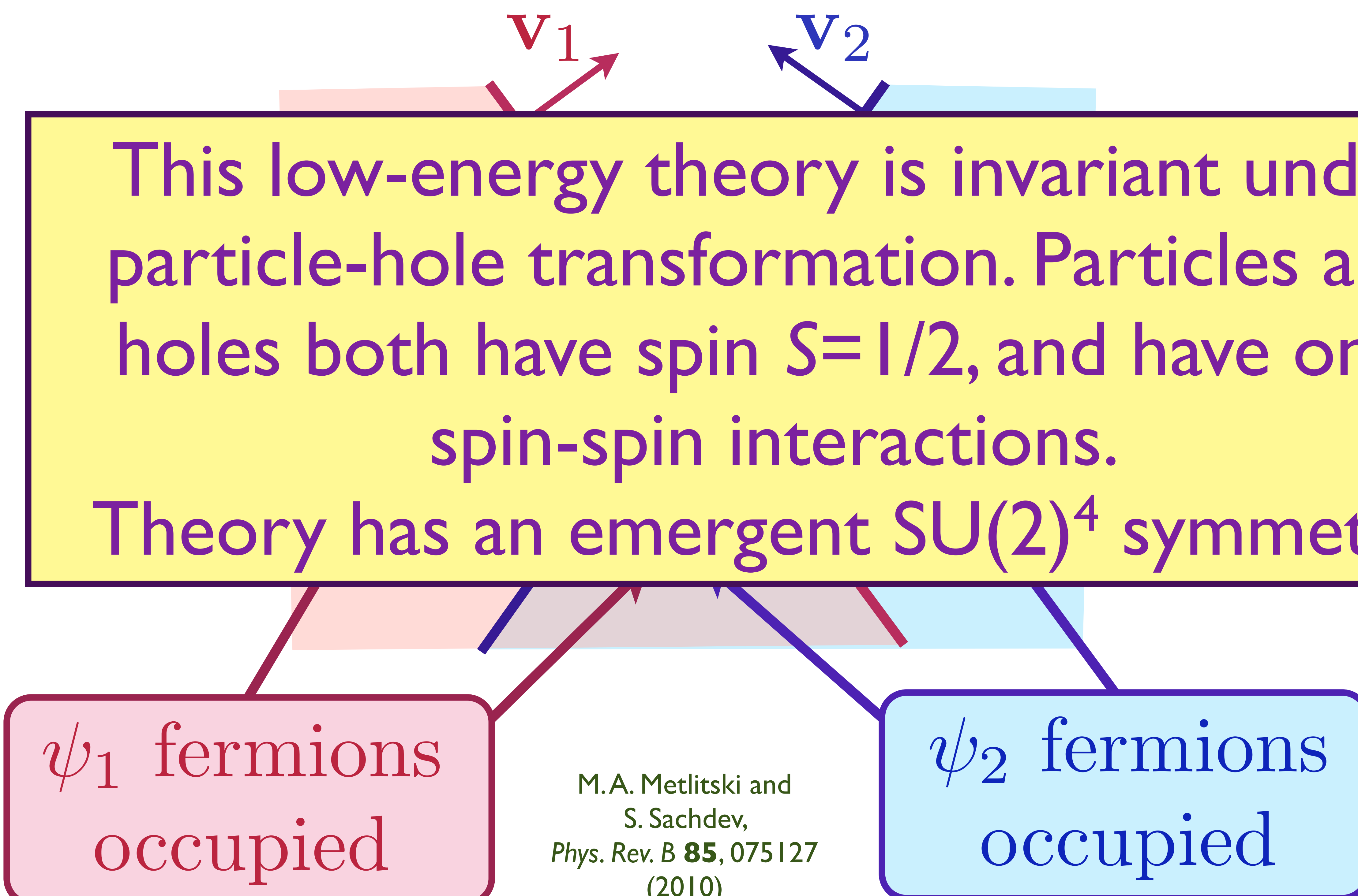


M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)

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

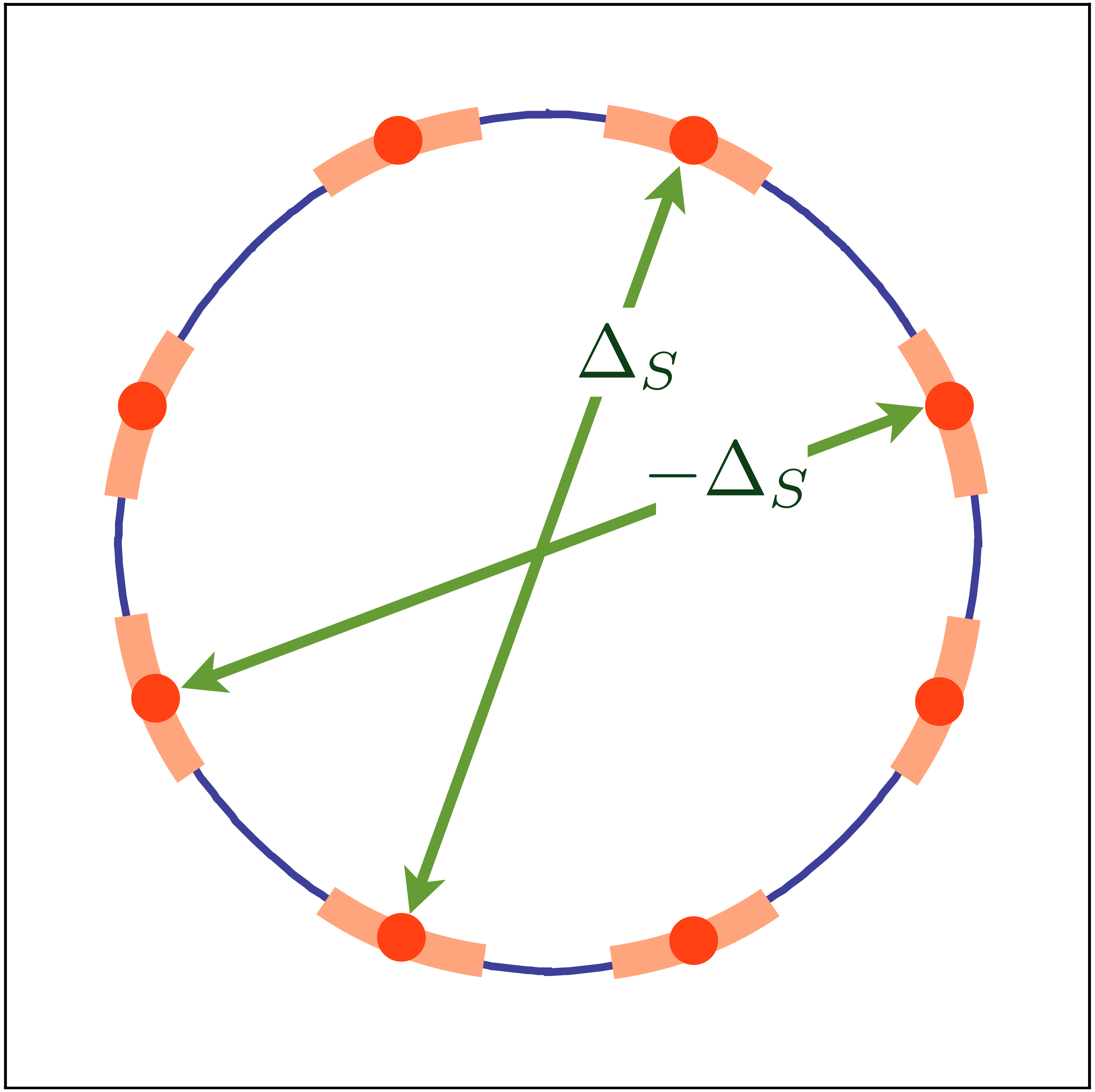


This low-energy theory is invariant under particle-hole transformation. Particles and holes both have spin S=1/2, and have only spin-spin interactions.

Theory has an emergent $SU(2)^4$ symmetry.

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

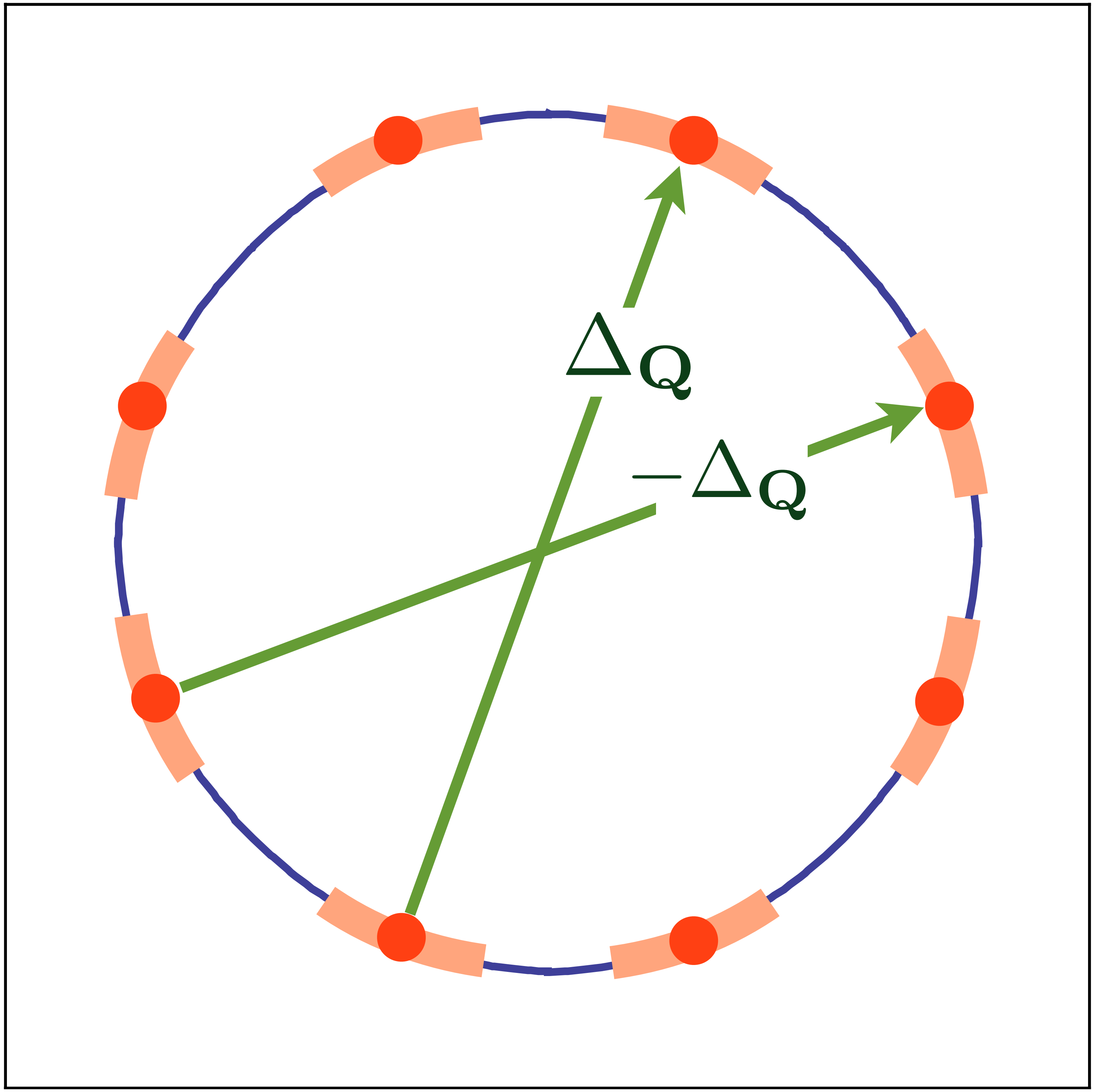
$$\left\langle c^{\dagger}_{\mathbf{k}\alpha} c^{\dagger}_{-\mathbf{k}\beta} \right\rangle = \varepsilon_{\alpha\beta} \Delta_S (\cos k_x - \cos k_y)$$



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)

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

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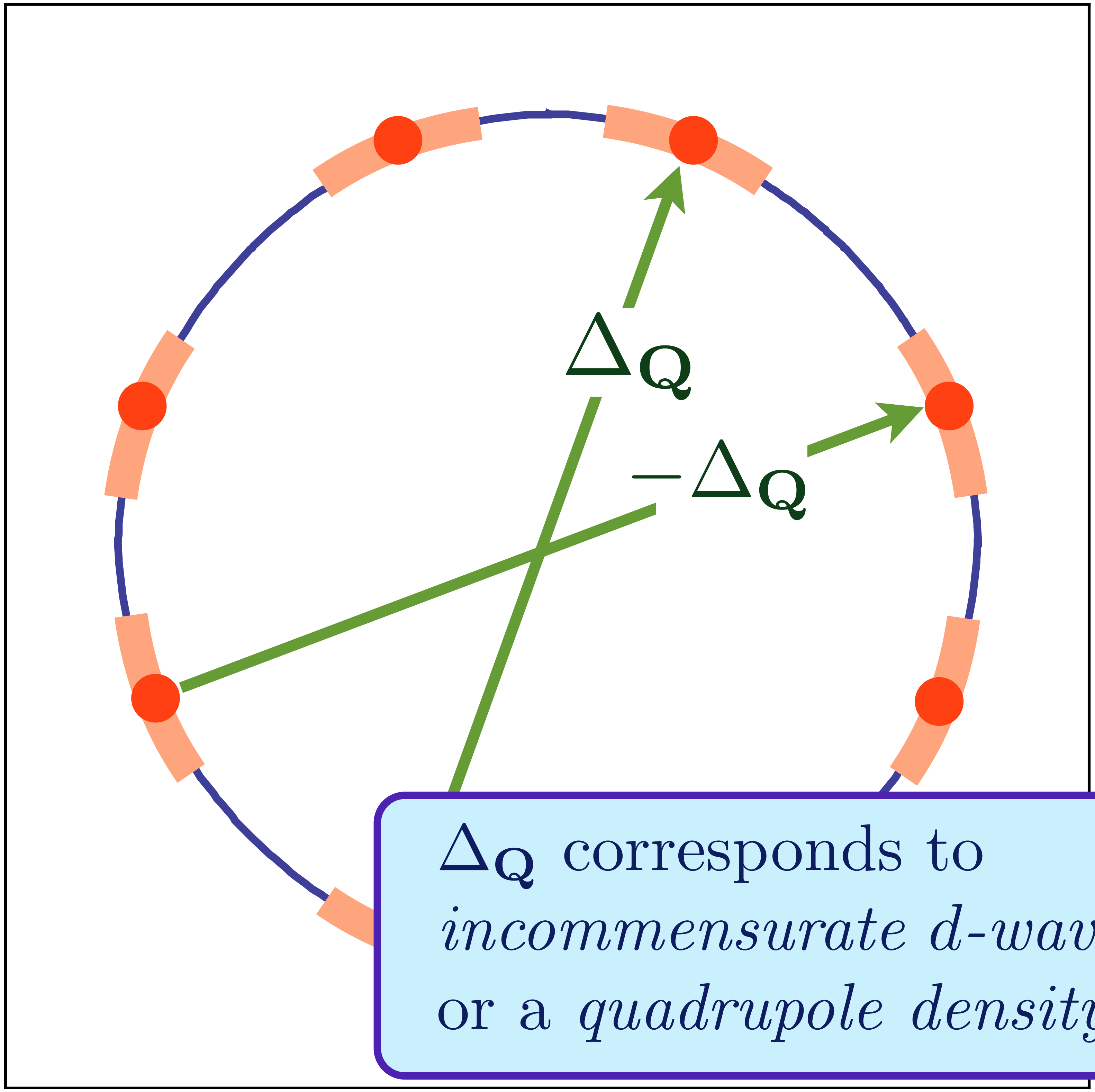


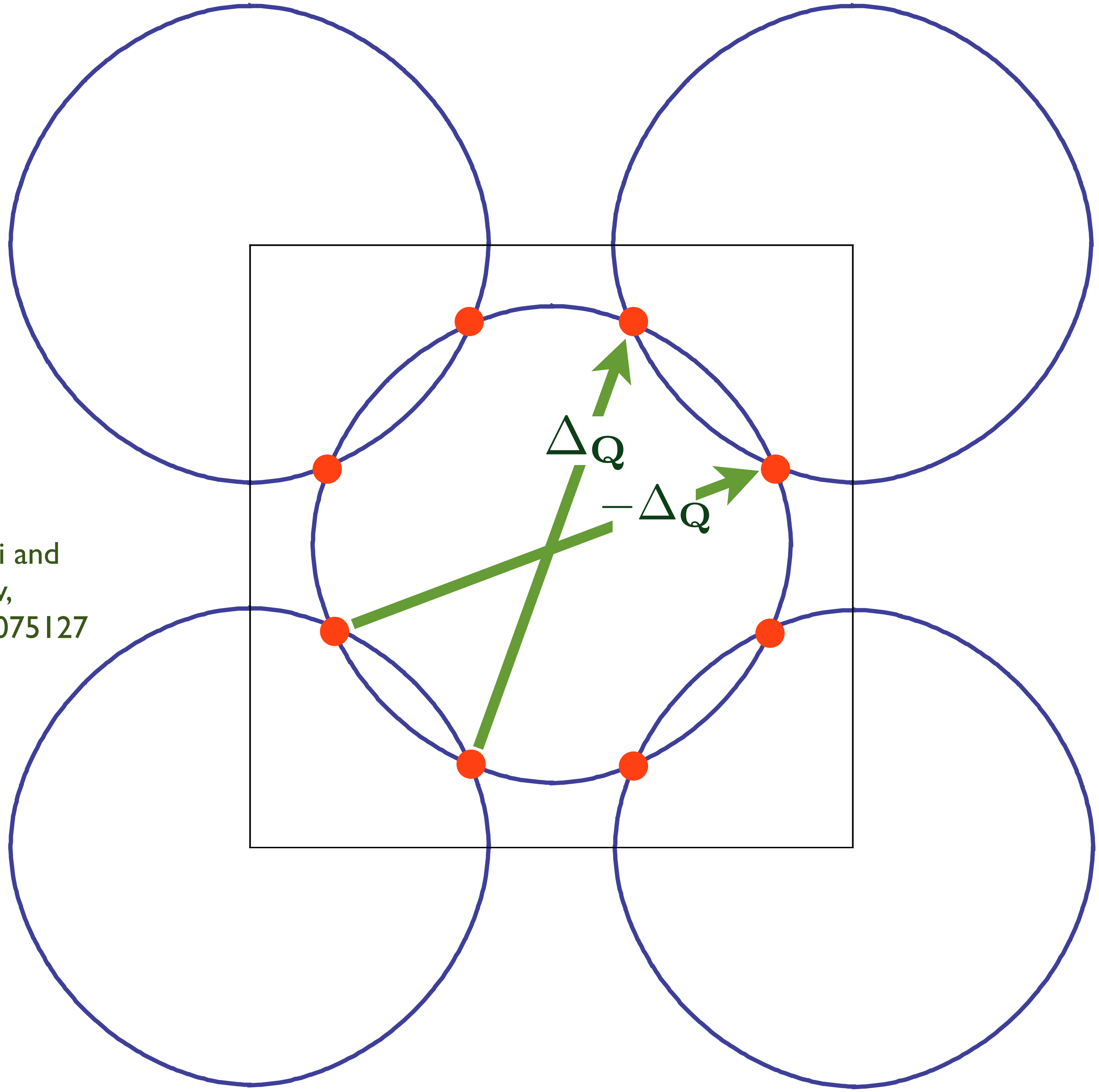
$\mathbf{Q}$ is '$2k_F$' wavevector

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

$\Delta_{\mathbf{Q}}$ corresponds to *incommensurate d-wave bond order* or a *quadrupole density wave*

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

Incommensurate *d*-wave bond order



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

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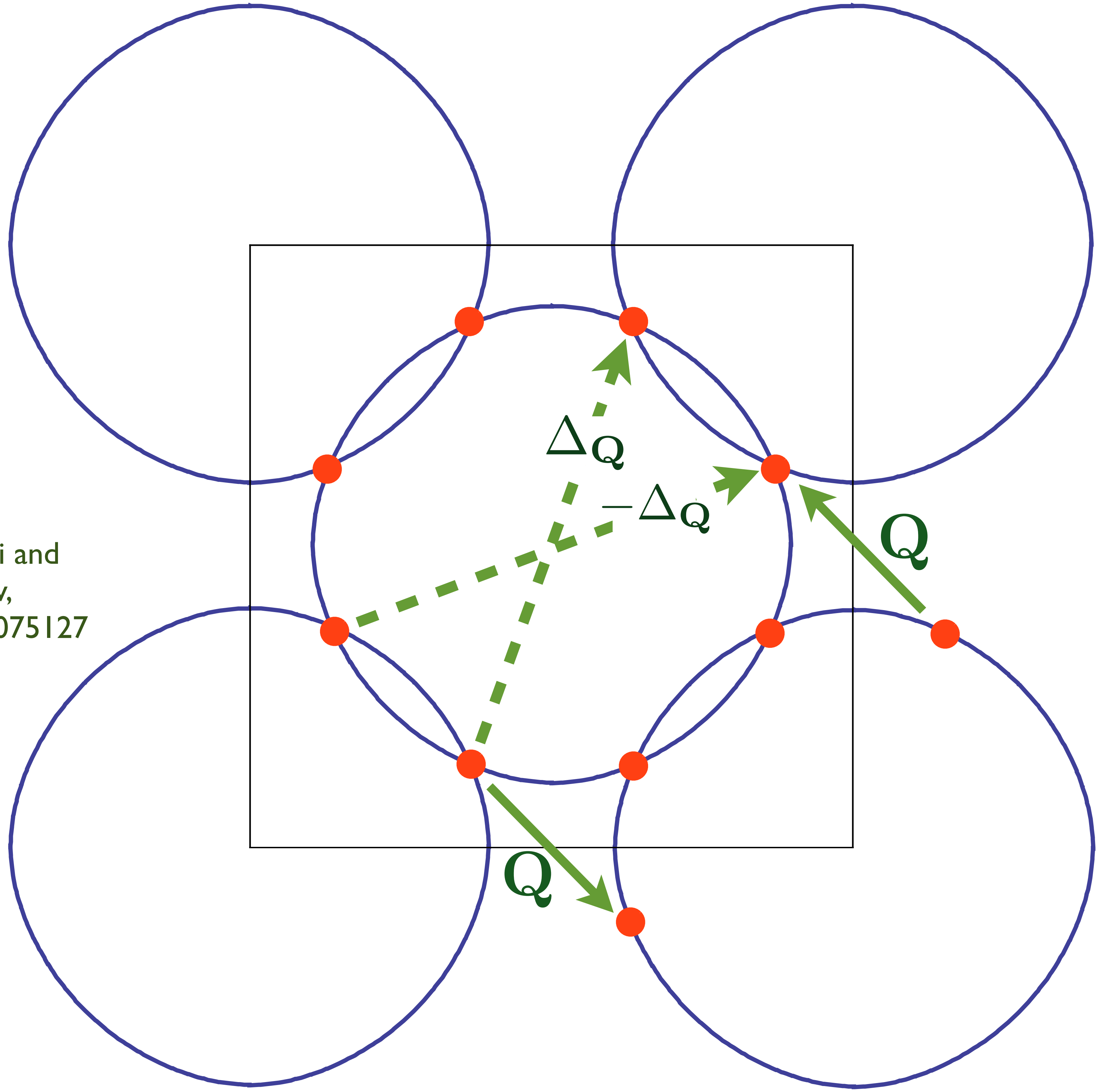
Incommensurate *d*-wave bond order



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

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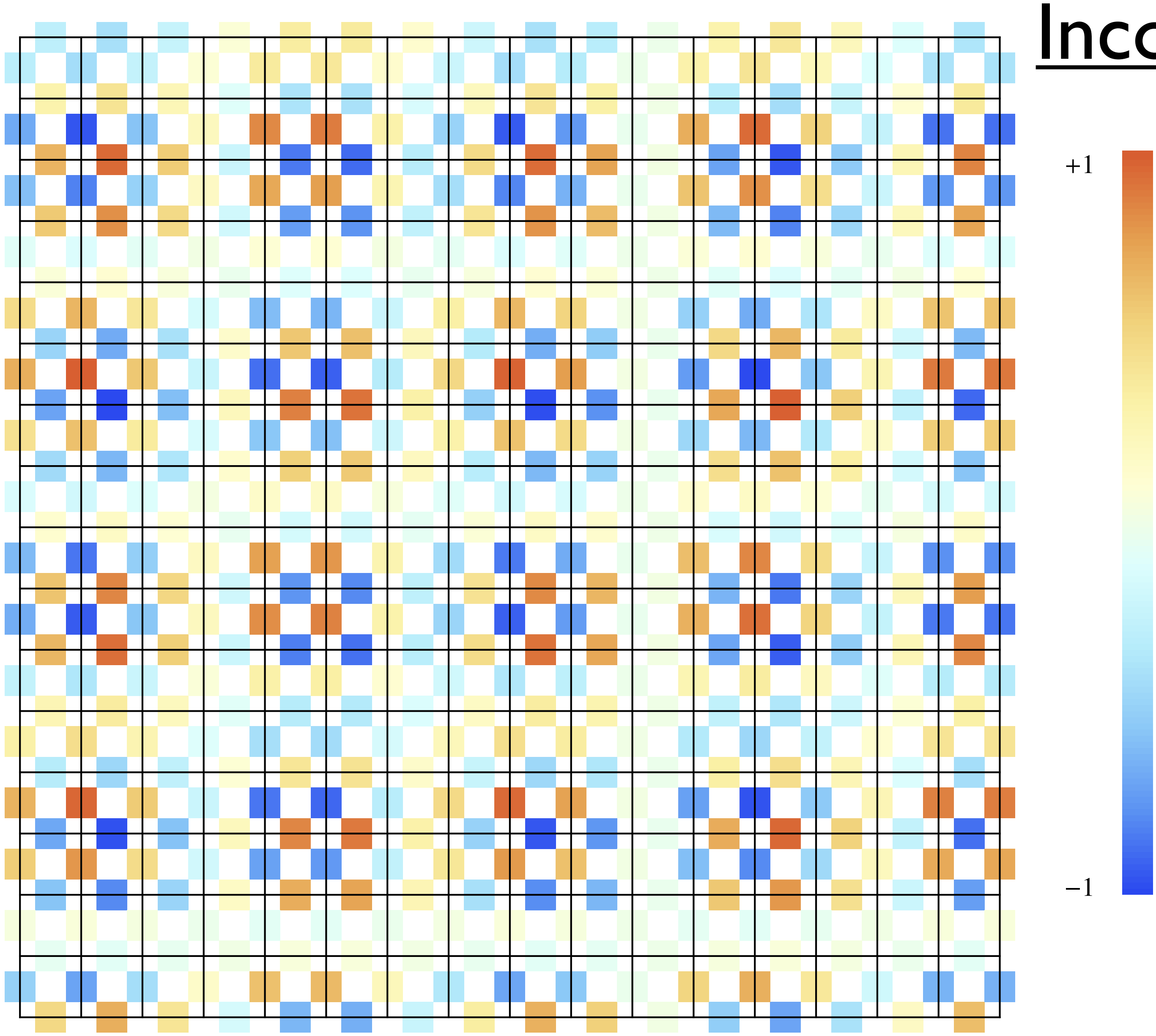
Incommensurate *d*-wave bond order



"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)

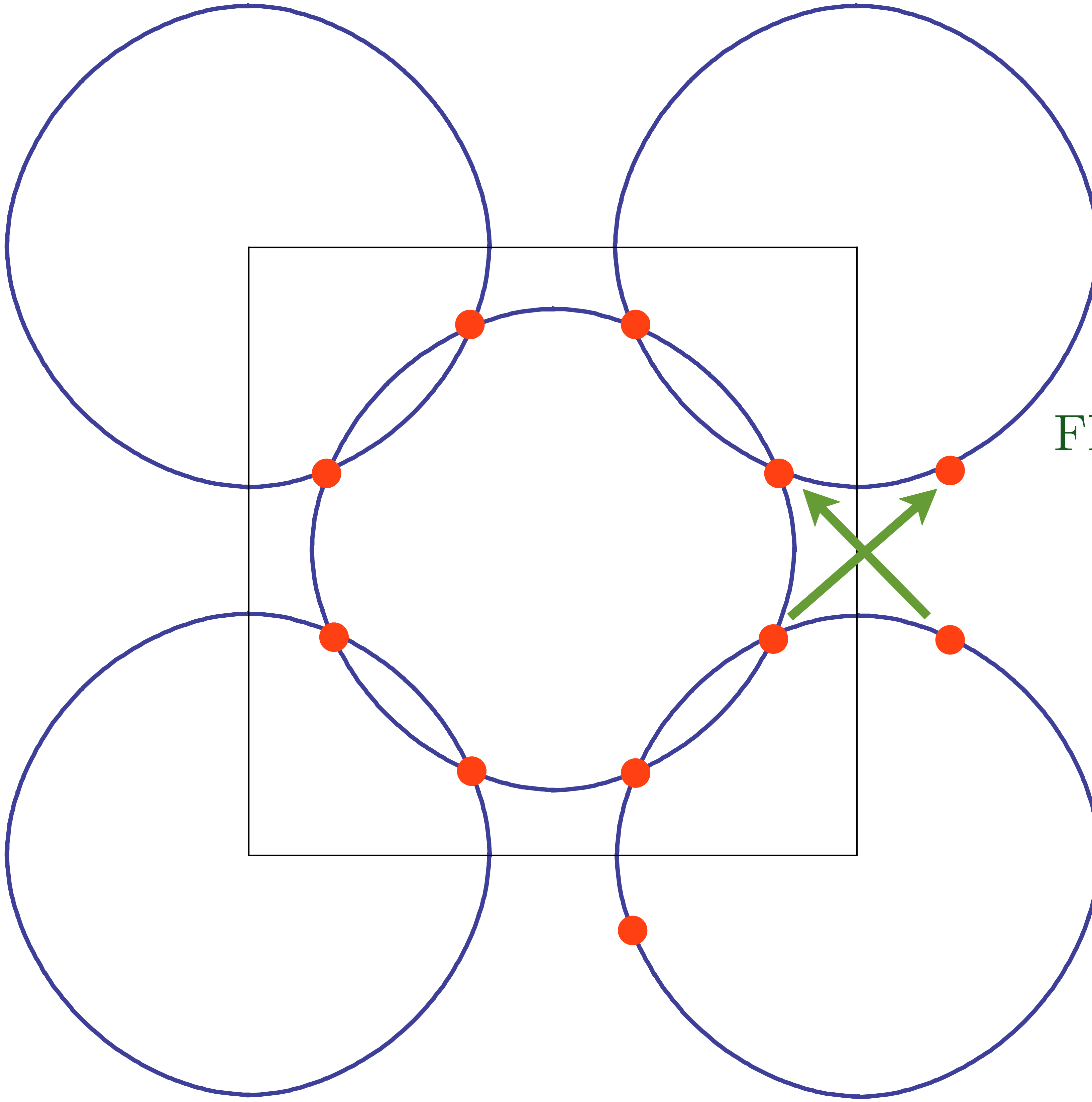
$$\left\langle c_{\mathbf{r}\alpha}^{\dagger} c_{\mathbf{s}\alpha} \right\rangle = \sum_{\mathbf{Q}} \sum_{\mathbf{k}} e^{i\mathbf{Q}\cdot(\mathbf{r}+\mathbf{s})/2} e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{s})} \left\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^{\dagger} c_{\mathbf{k}+\mathbf{Q}/2,\alpha}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

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.

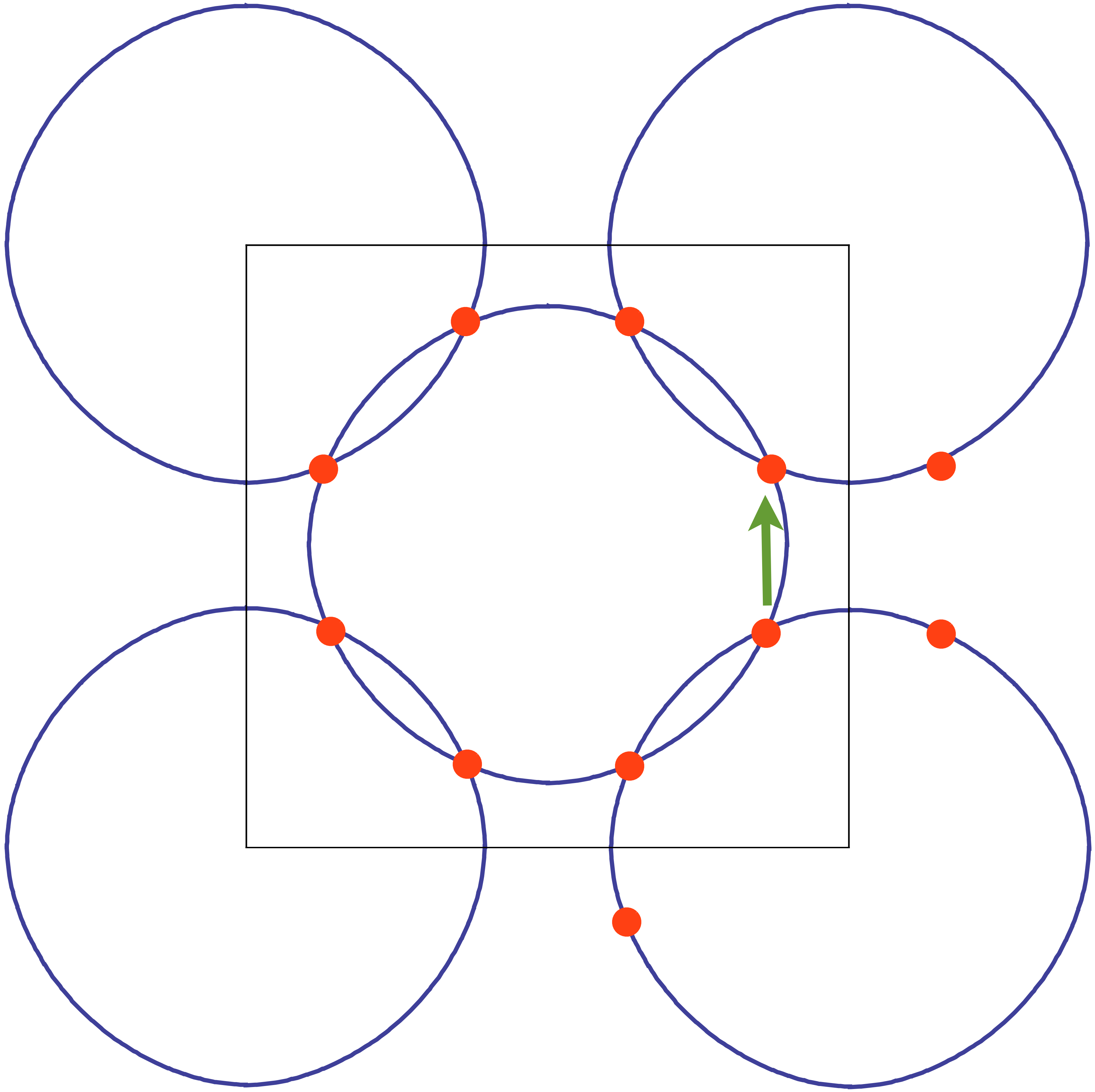
Incommensurate *d*-wave bond order



High T pseudogap: Fluctuating composite order parameter of nearly degenerate d-wave pairing and incommensurate d-wave bond order

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

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



Observed
low T ordering

Outline

1. The “modern era” of cuprate experiments

2. Antiferromagnetism in metals:
   d-wave superconductivity

3. Low energy theory, emergent pseudospin
   symmetry, and bond order

4. Unrestricted Hartree-Fock-BCS

5. Quantum Monte Carlo
   without the sign problem

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

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

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

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

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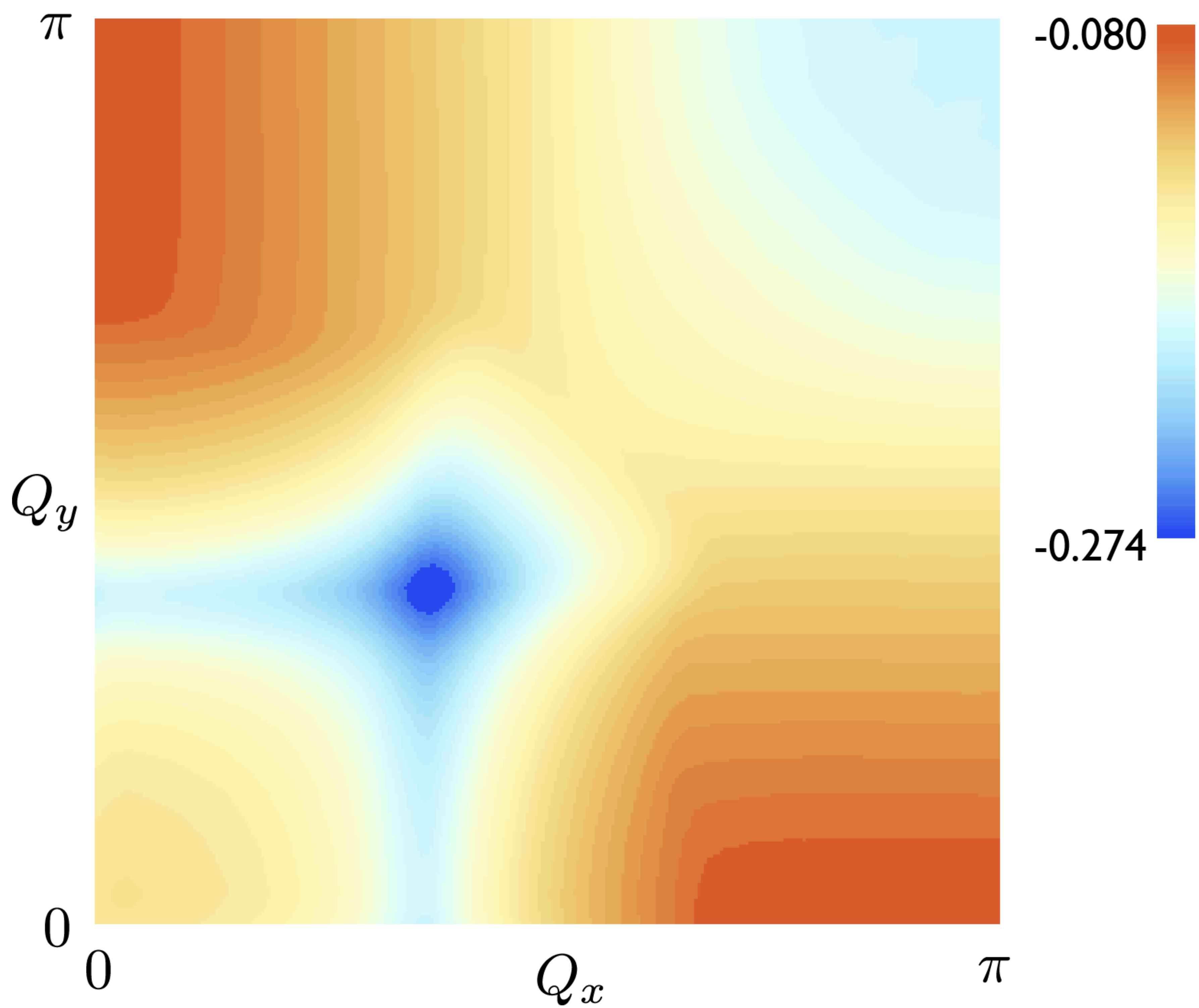
$$+ \sum_{\boldsymbol{Q}} \Delta_{\boldsymbol{Q}}(\boldsymbol{k})\, c^{\dagger}_{\boldsymbol{k}+\boldsymbol{Q}/2,\alpha} c_{\boldsymbol{k}-\boldsymbol{Q}/2,\alpha} \Bigg],$$

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

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

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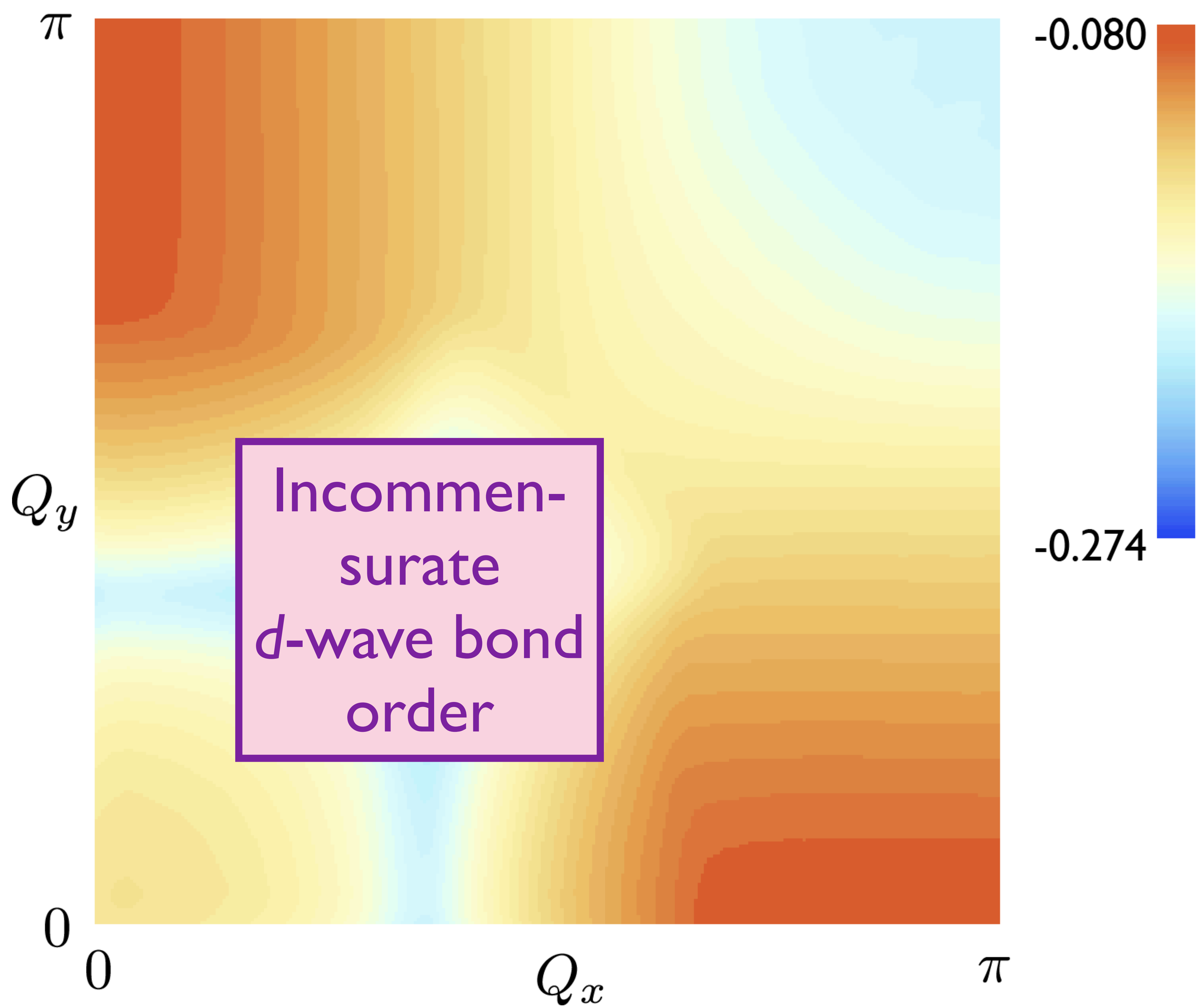

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S. Sachdev and R. La Placa, arXiv:1303.2114

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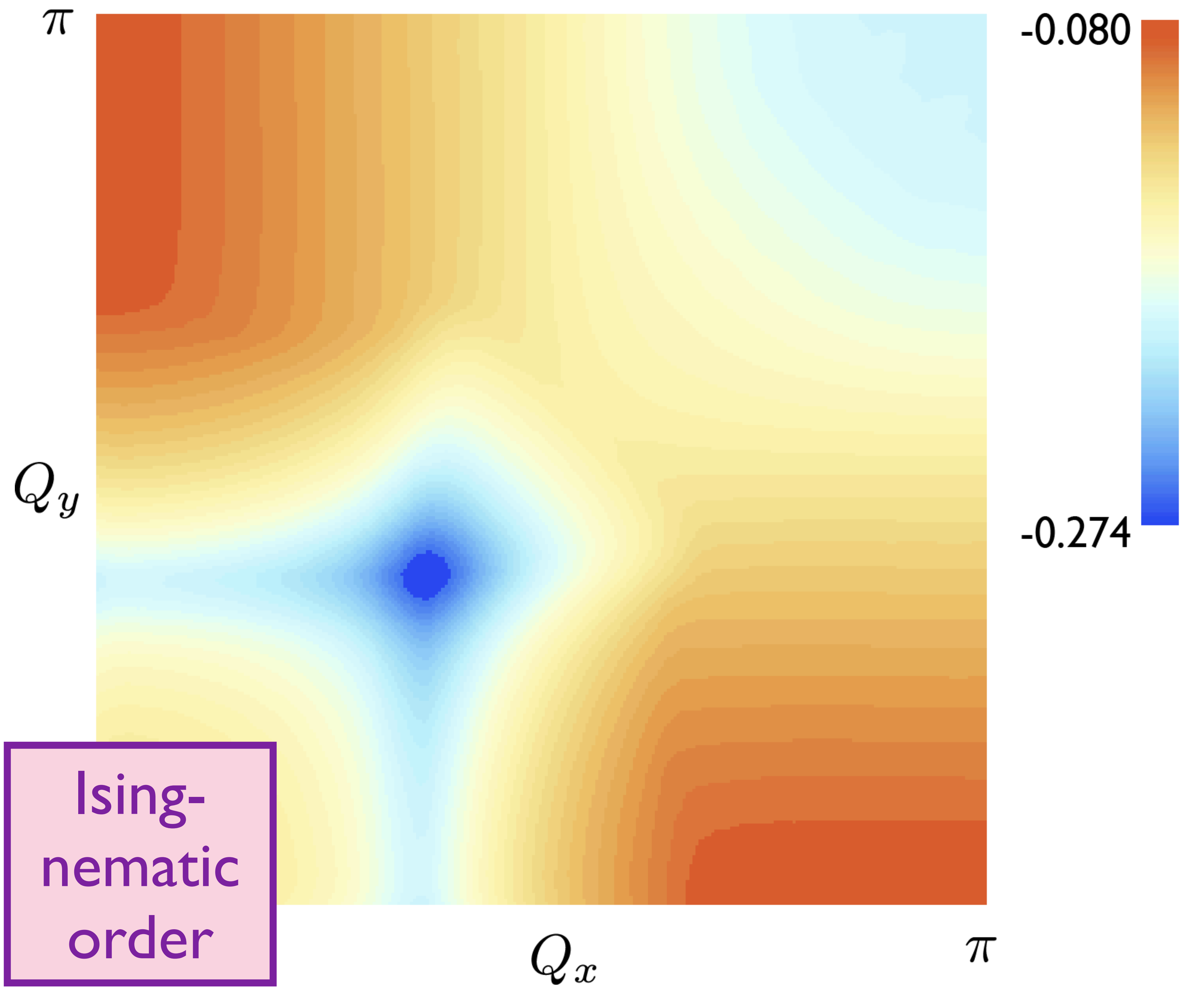

Ising-nematic order

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

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

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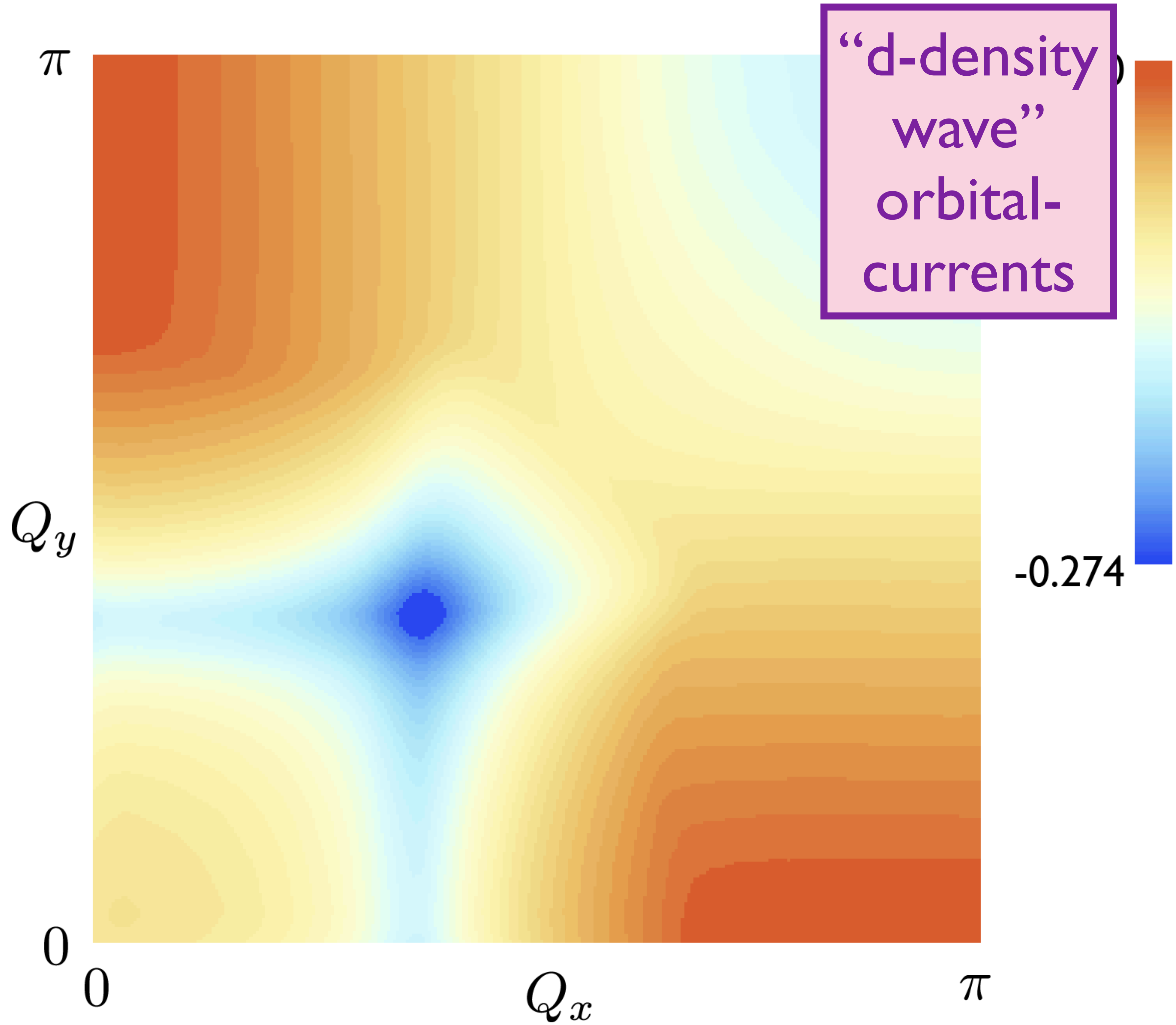

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S. Sachdev and R. La Placa, arXiv:1303.2114

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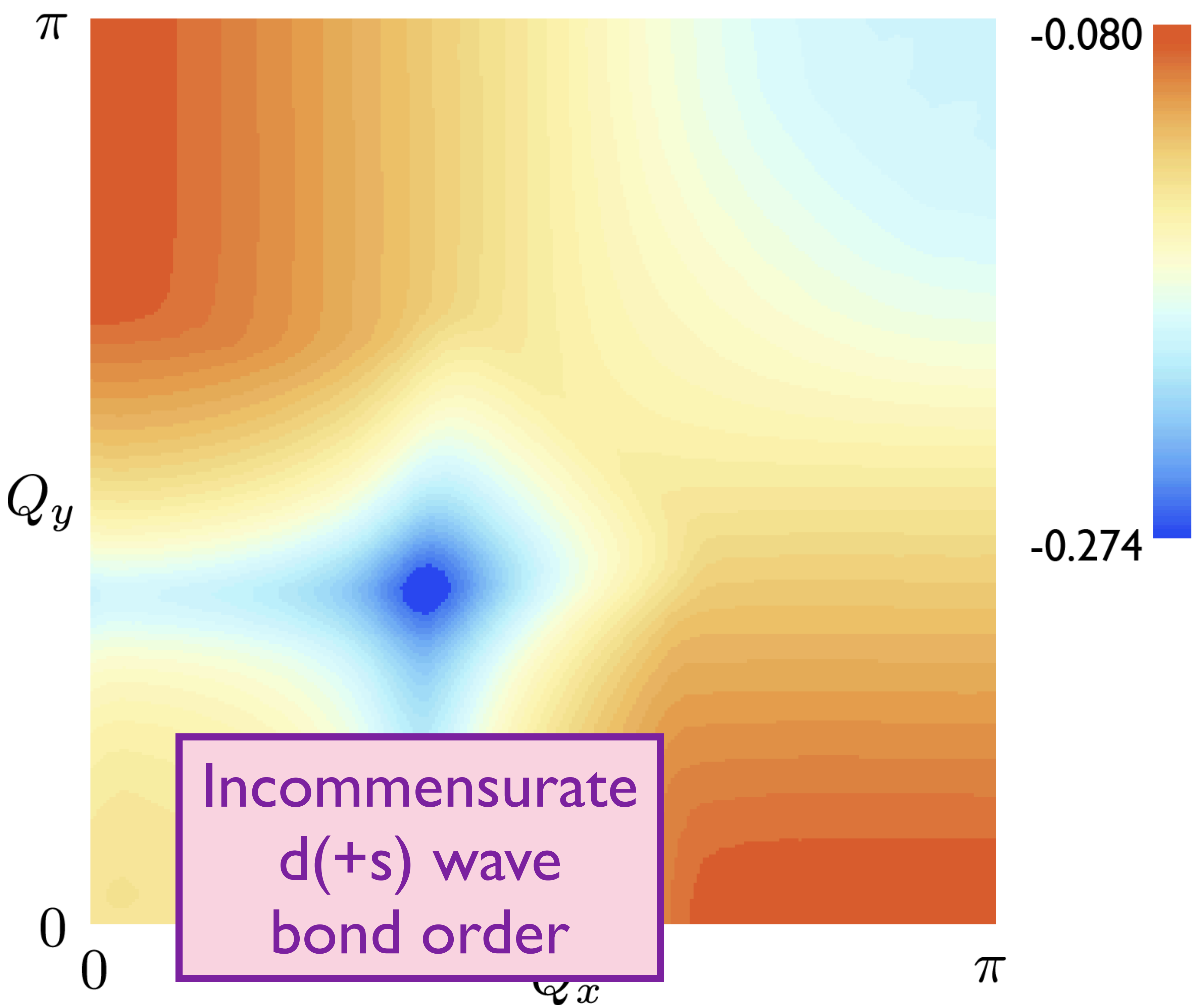
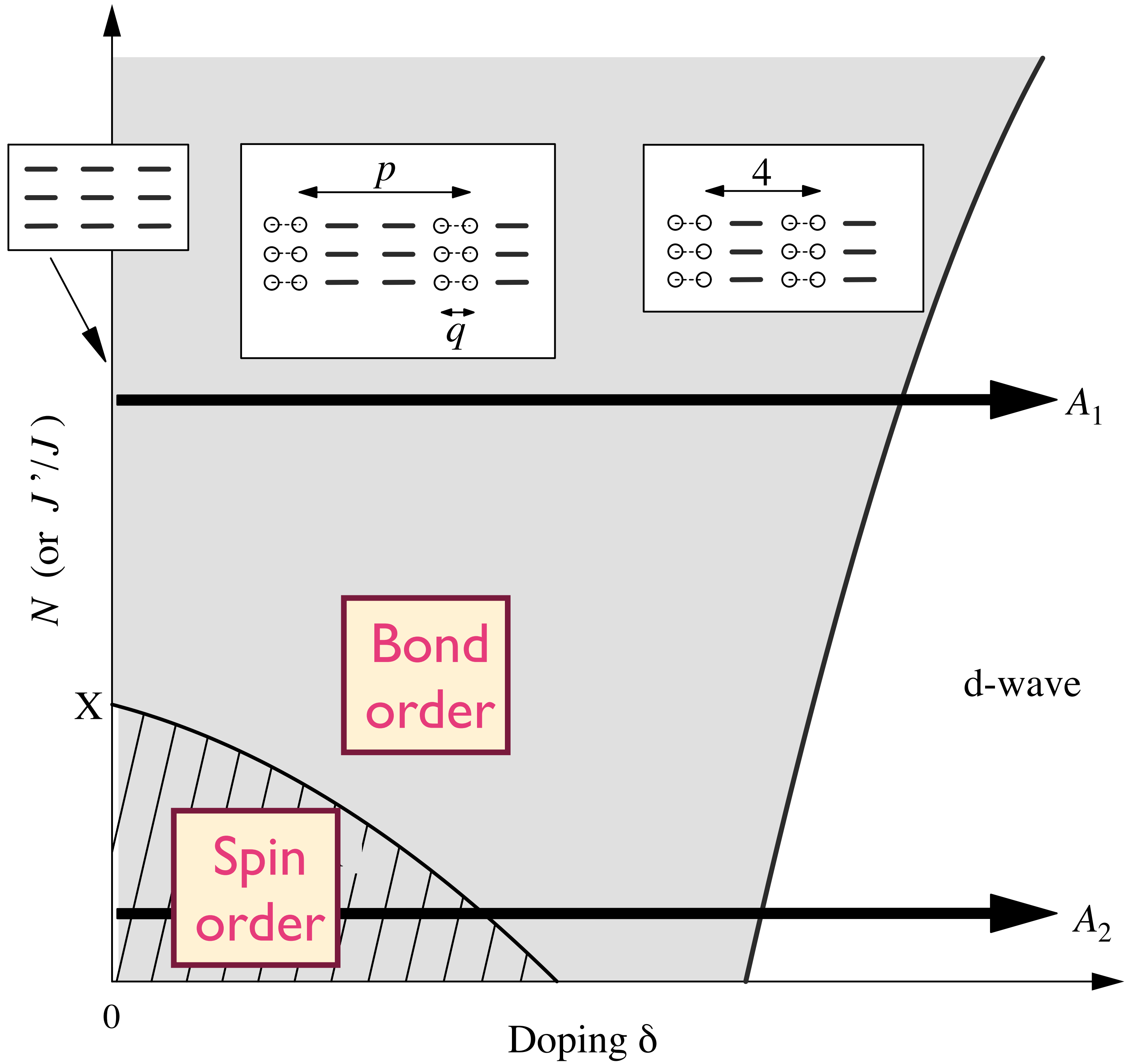


Charge-ordering eigenvalue $\lambda_{\mathbf{Q}}$.

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

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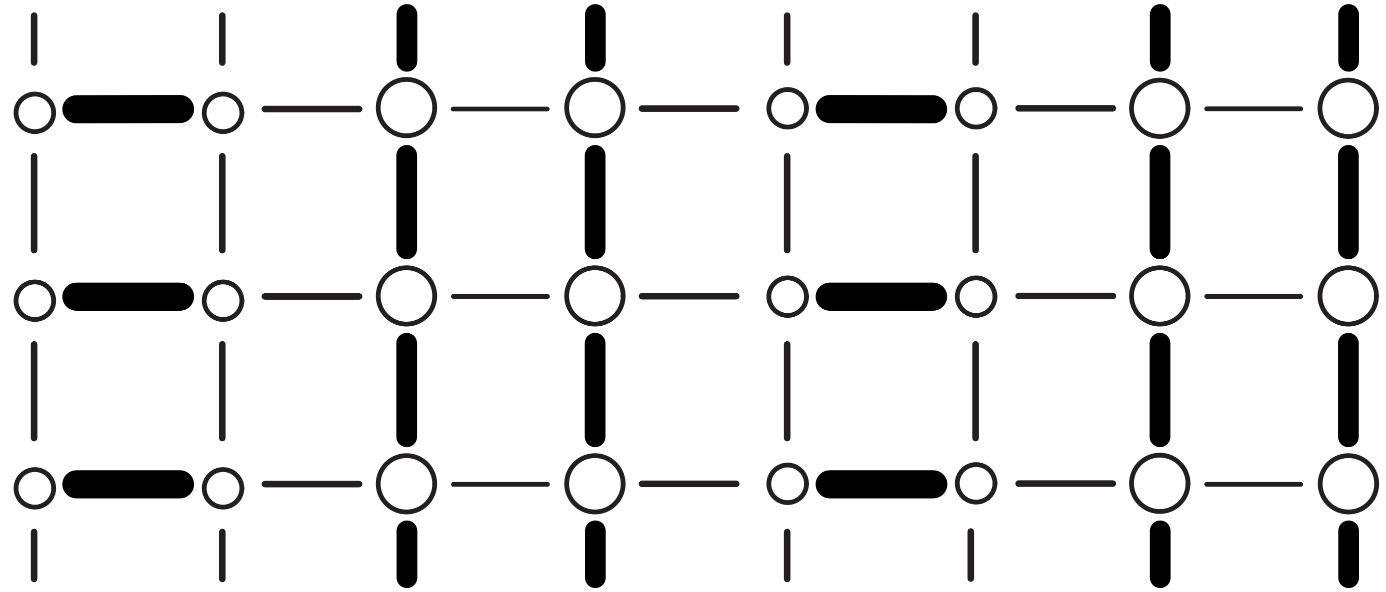
PHYSICAL REVIEW B **77**, 094504 (2008)

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

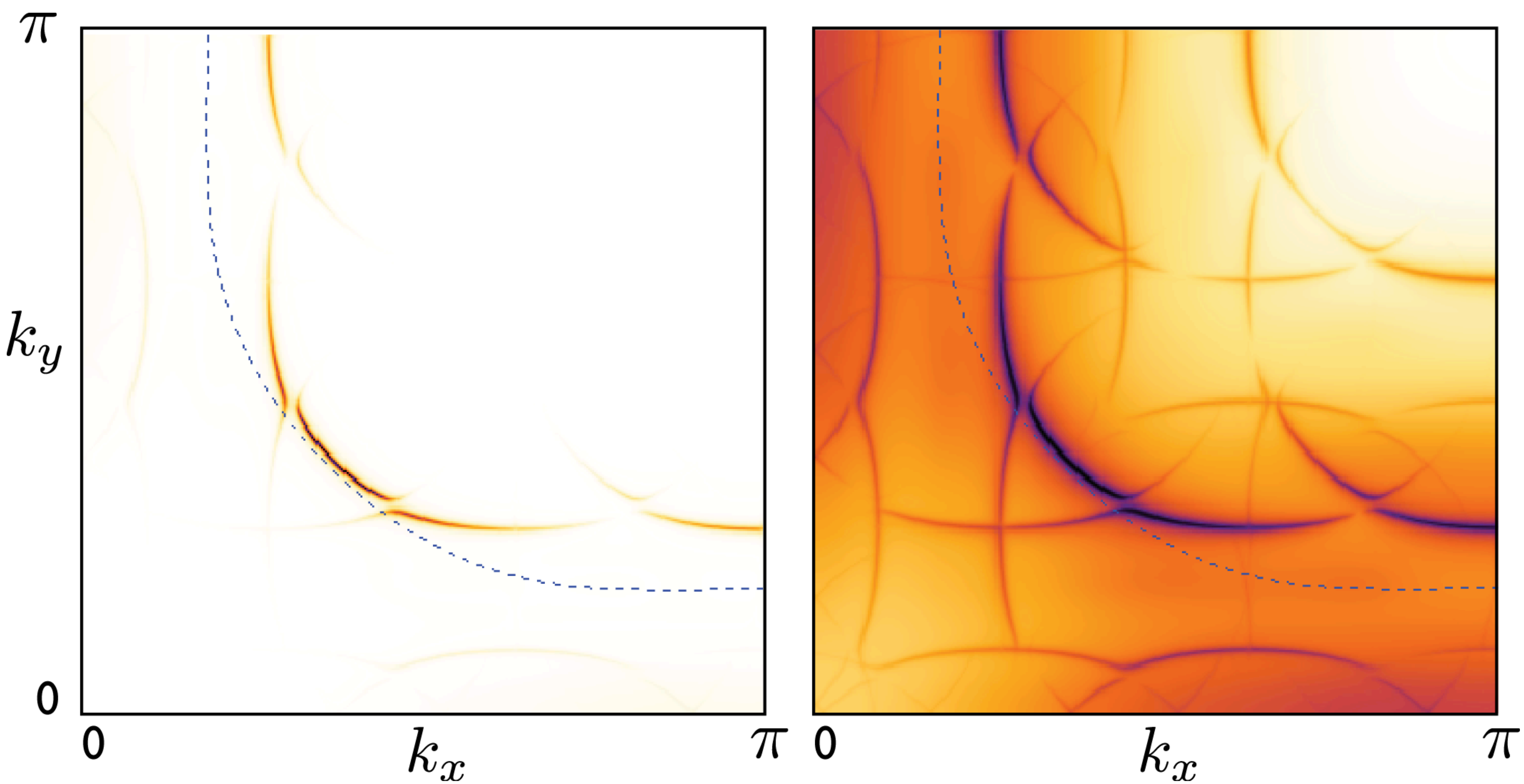
Matthias Vojta and Oliver Rösch
Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany
(Received 8 January 2008; revised manuscript received 10 January 2008; published 6 March 2008)

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. The resulting bond-charge-density wave, coexisting with superconductivity, is compatible with recent photoemission and tunneling data and as well as neutron-scattering measurements, once long-range order is destroyed by slow fluctuations or glassy disorder. In particular, the real-space structure of *d*-wave stripes is consistent with the scanning-tunneling-microscopy measurements on both underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ and $Ca_{2-x}Na_xCuO_2Cl_2$ of Kohsaka *et al.* [Science **315**, 1380 (2007)].



Saturday, March 23, 13

Electron spectral function



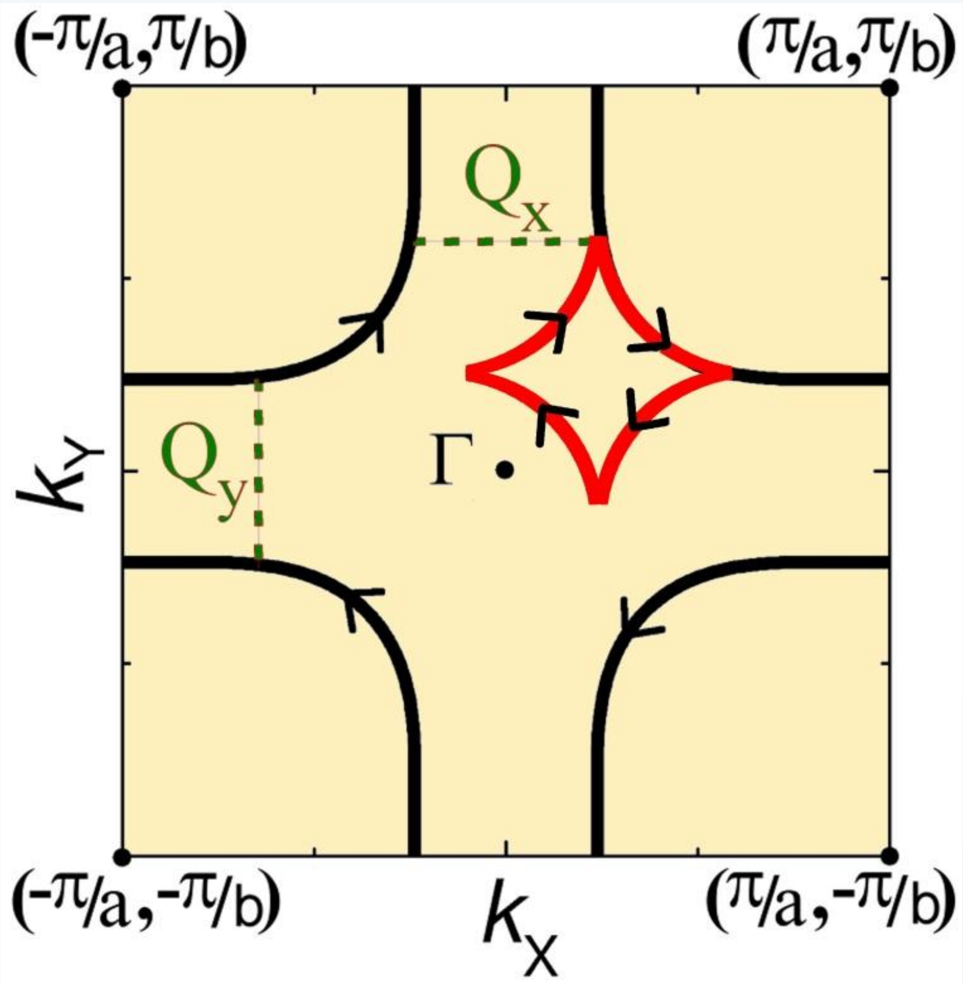
$\text{Im}G(\mathbf{k}, \omega + i\eta)$ $\log \text{Im}G(\mathbf{k}, \omega + i\eta)$

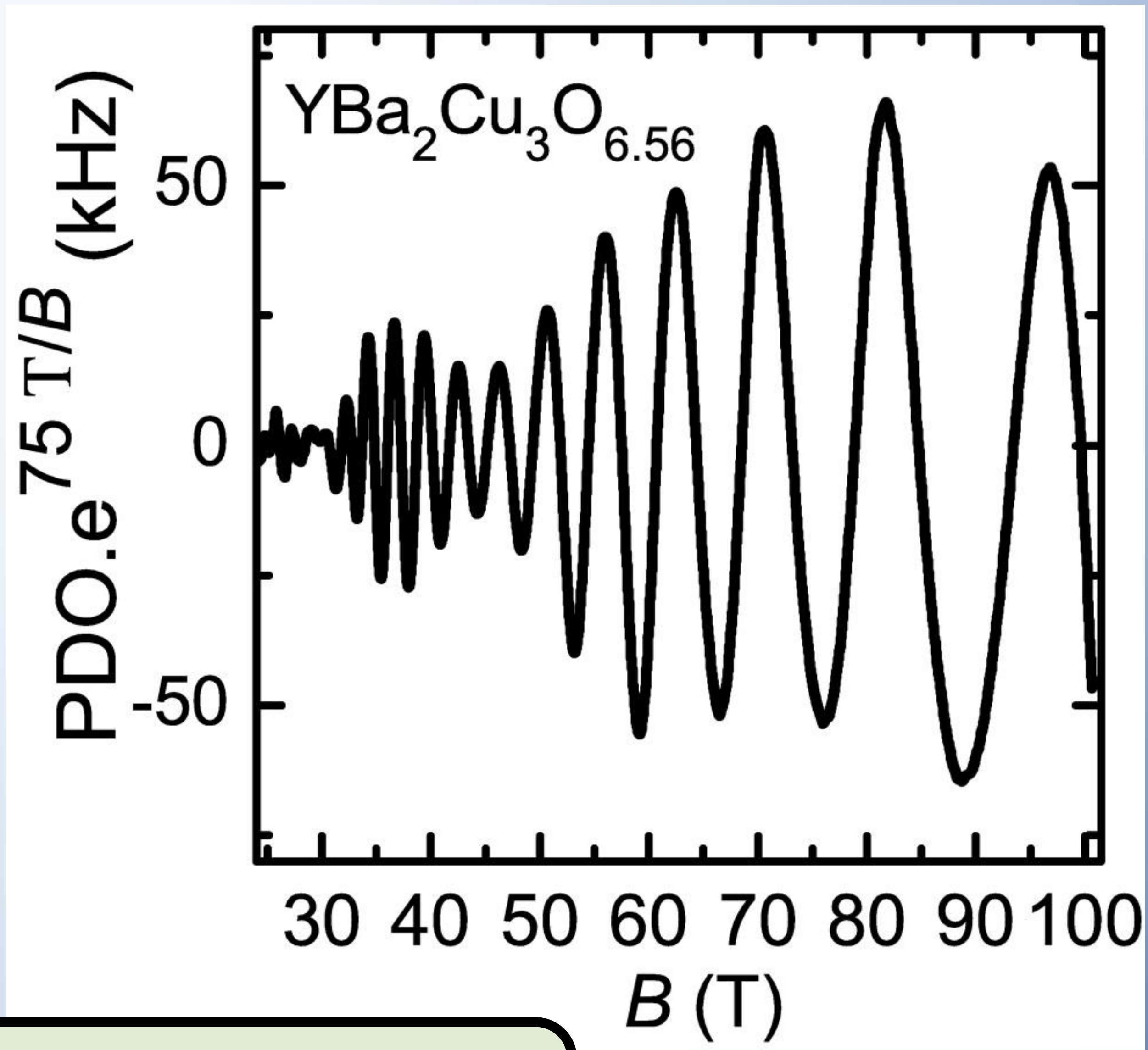
$$\left\langle c^{\dagger}_{\boldsymbol{k}-\boldsymbol{Q}/2,\alpha} c_{\boldsymbol{k}+\boldsymbol{Q}/2,\alpha} \right\rangle \propto \Delta_{\boldsymbol{Q}}(\boldsymbol{k}) = \begin{cases} \Delta_s + \Delta_d(\cos k_x - \cos k_y) & , \quad \boldsymbol{Q} = (\pm Q_0, 0) \\ \Delta_s - \Delta_d(\cos k_x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

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

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

Do we finally have a resolution to the low energy electronic structure of underdoped YBCO?





N. Harrison and S. E. Sebastian
Phys. Rev. Lett. **106**, 226402 (2011).

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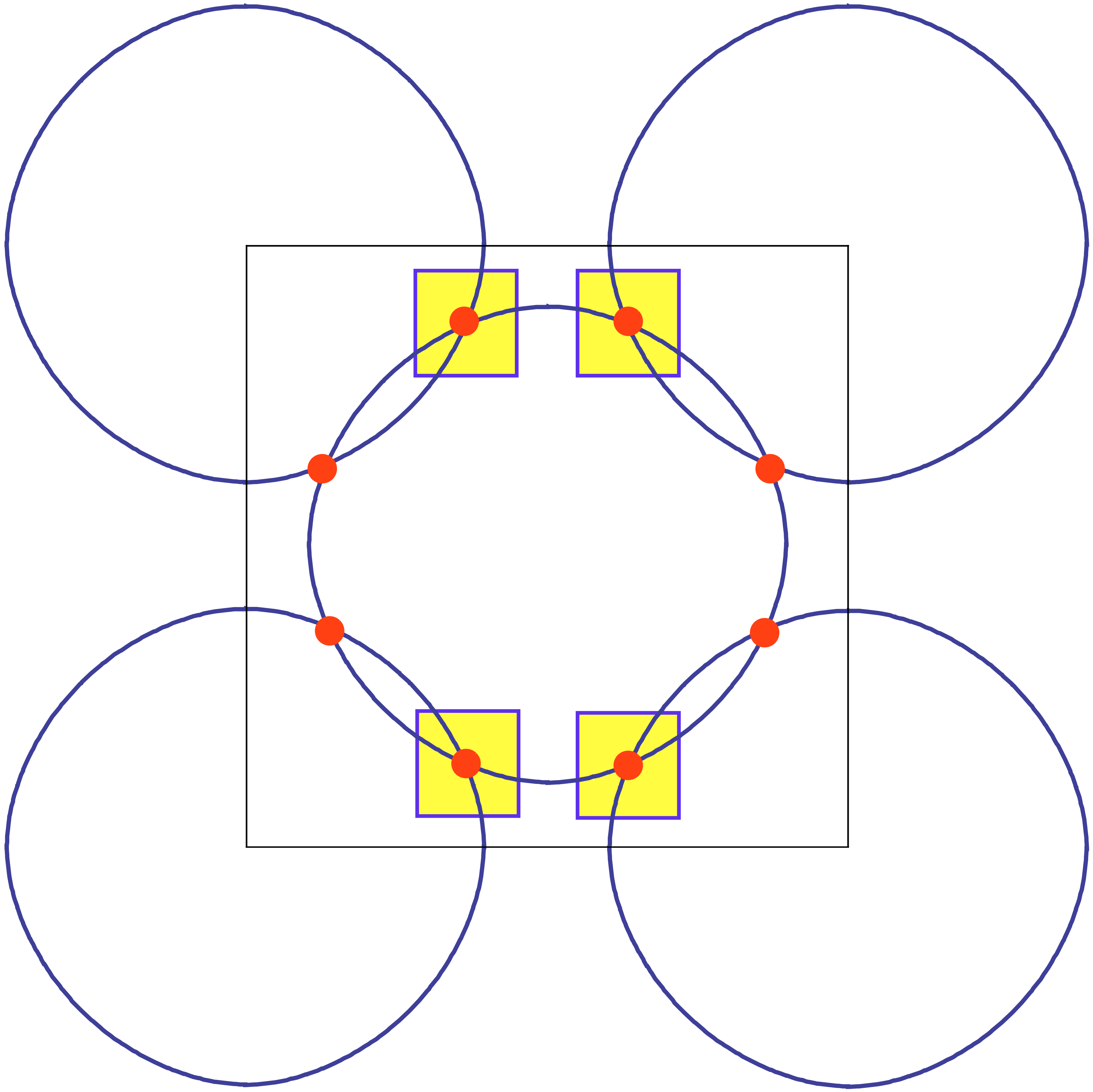
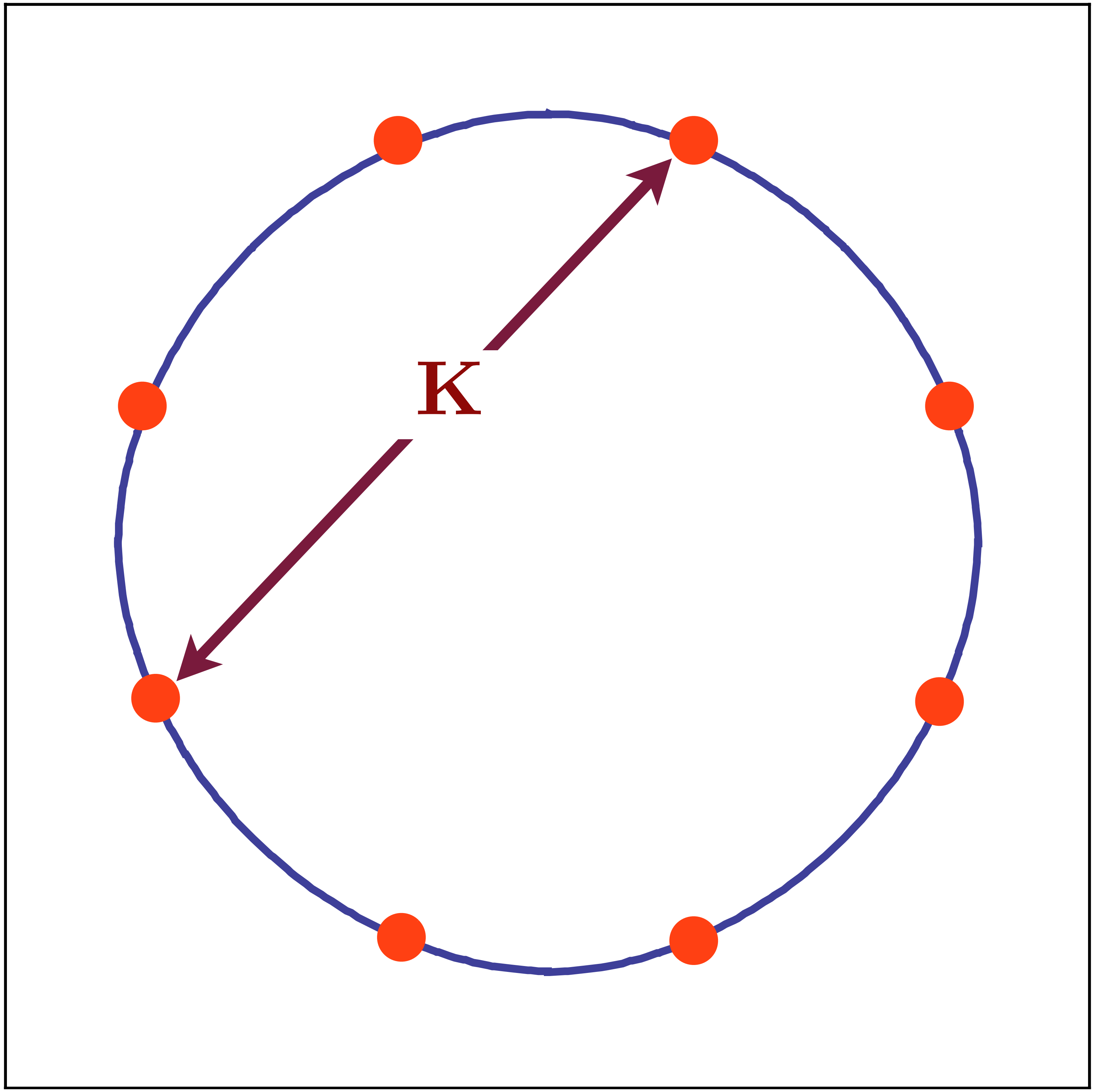


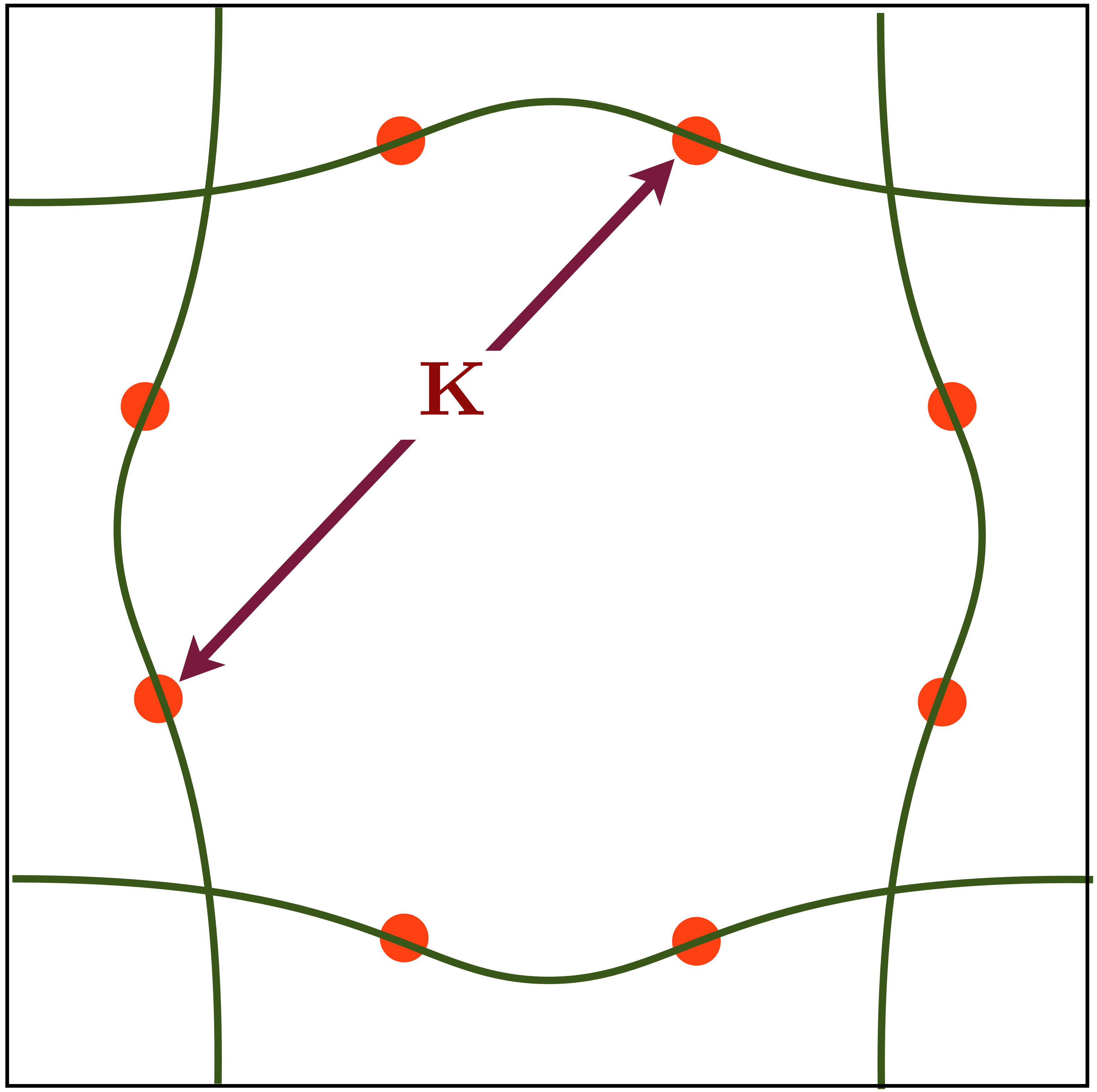
Low energy theory for critical point near hot spots

QMC for the onset of antiferromagnetism



Hot spots in a single band model

QMC for the onset of antiferromagnetism

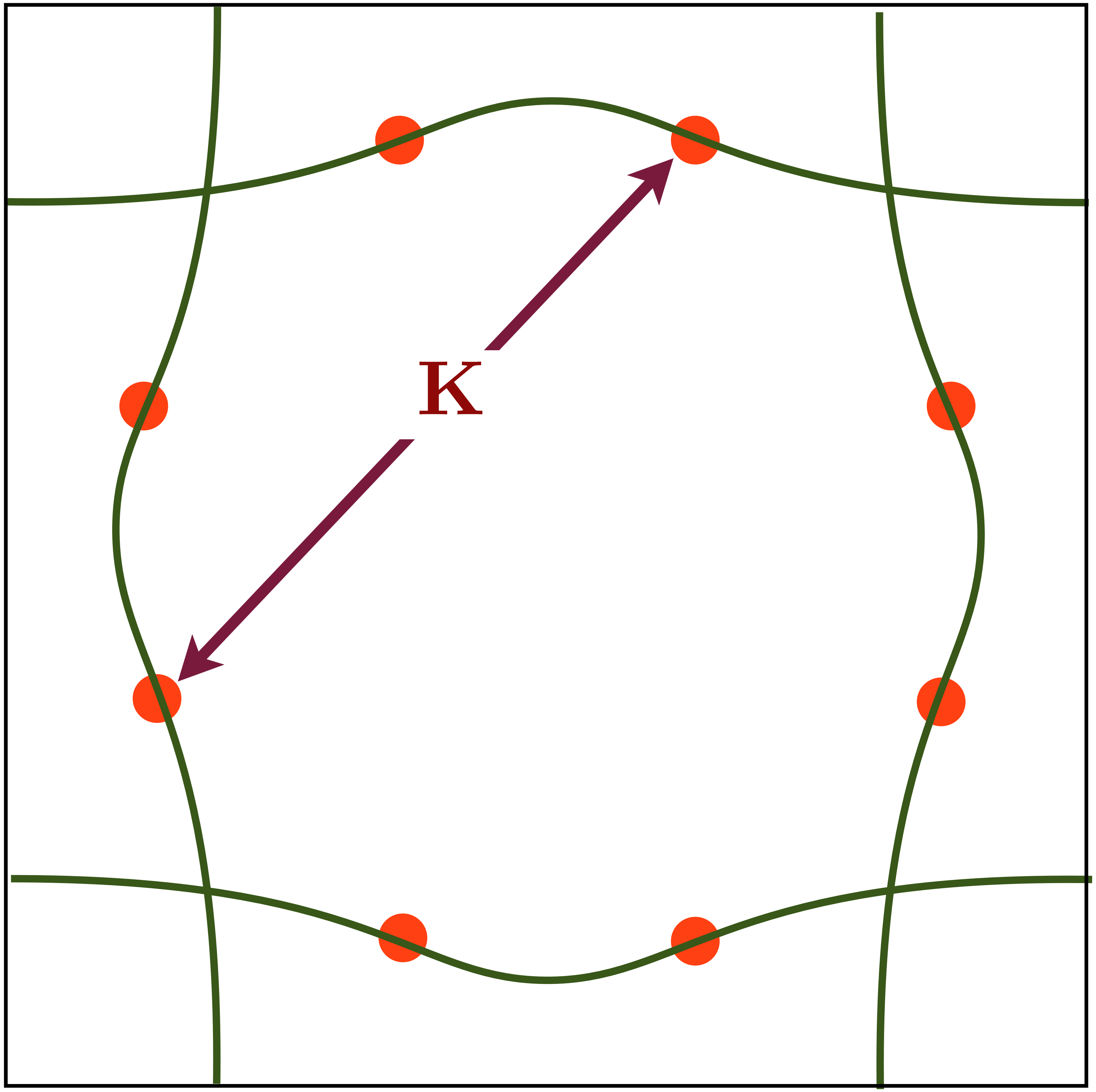


E. Berg,
M. Metlitski, and
S. Sachdev,
Science **338**, 1606
(2012).

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 antiferro-magnetism.



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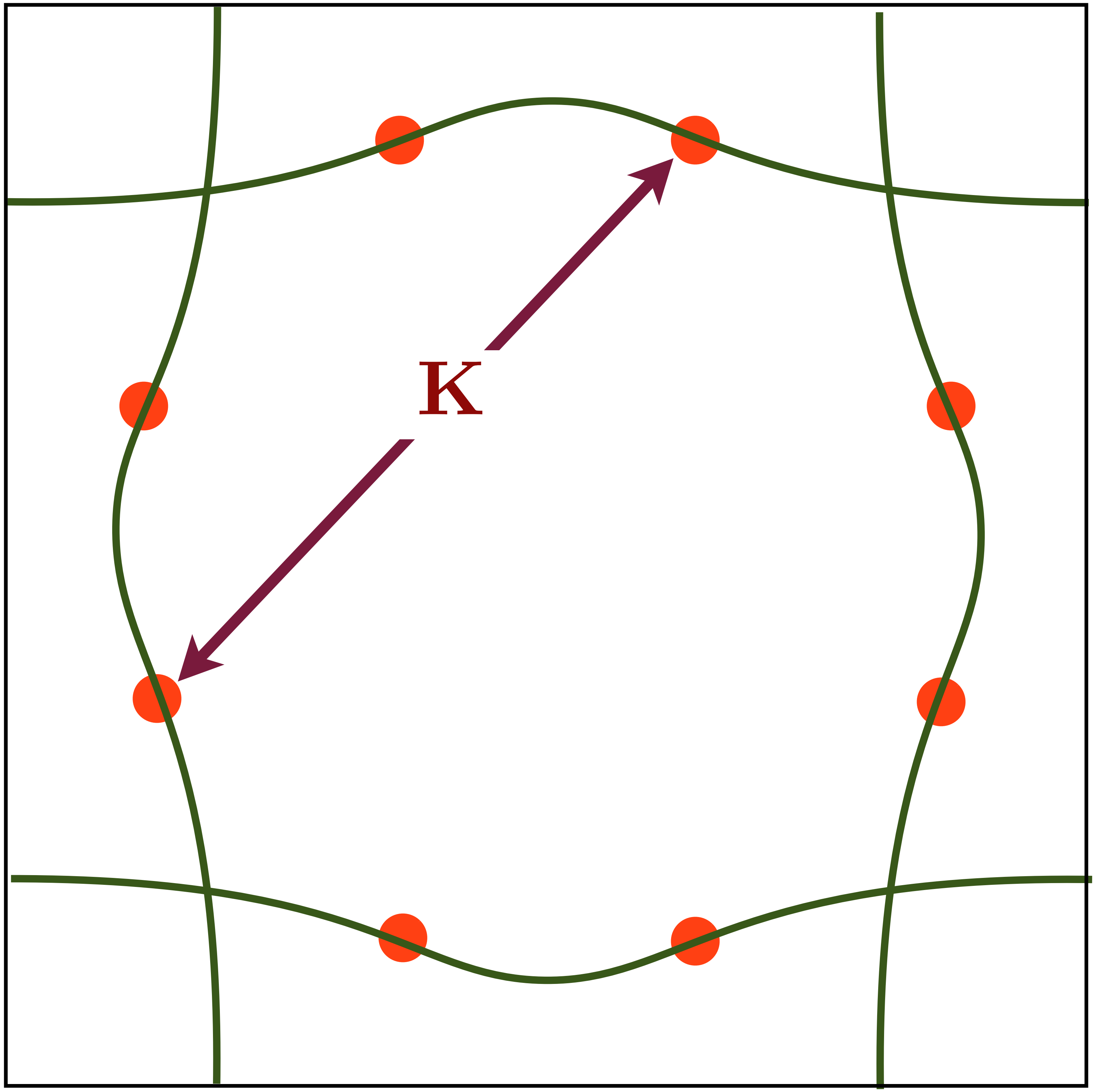

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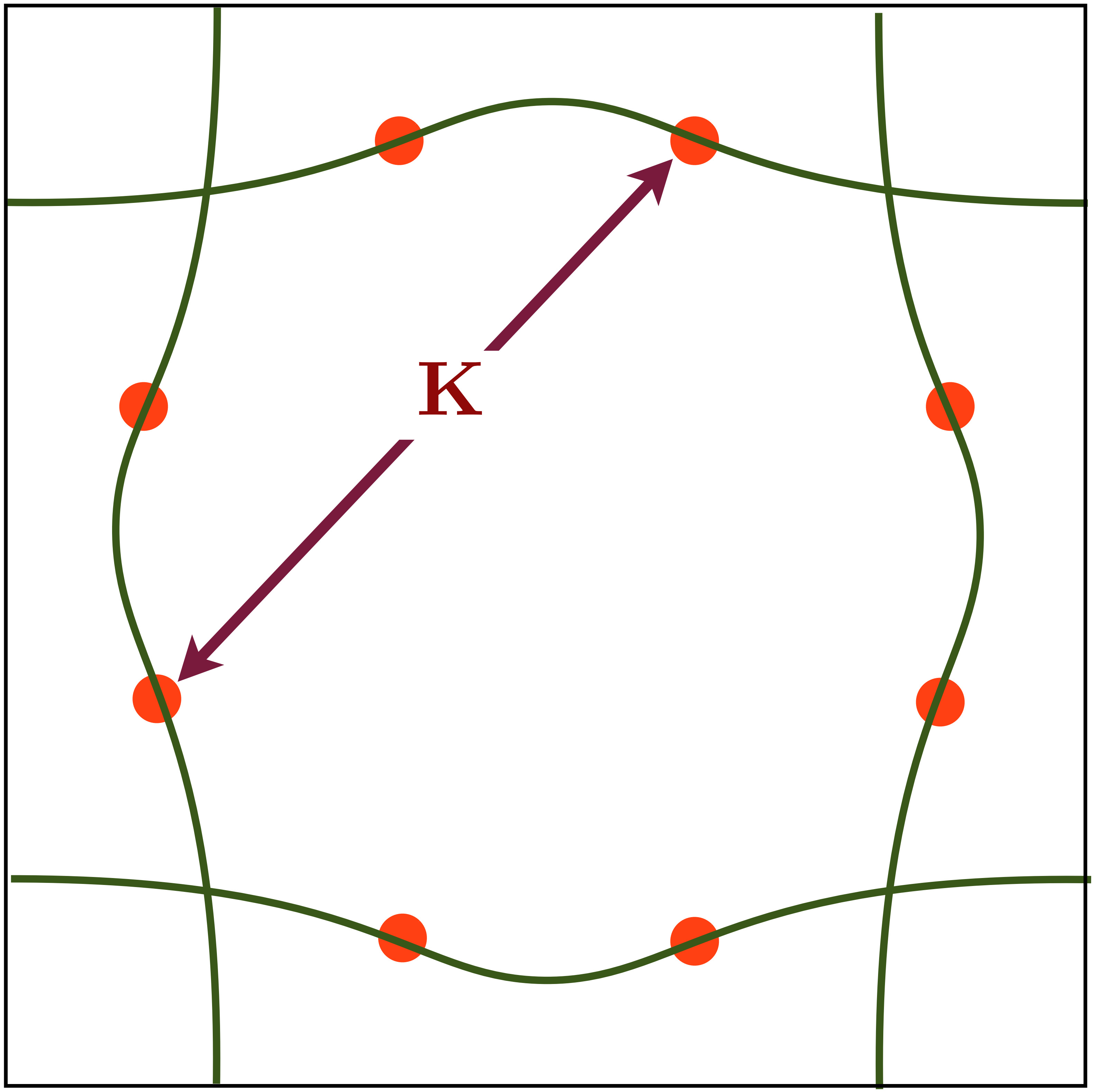

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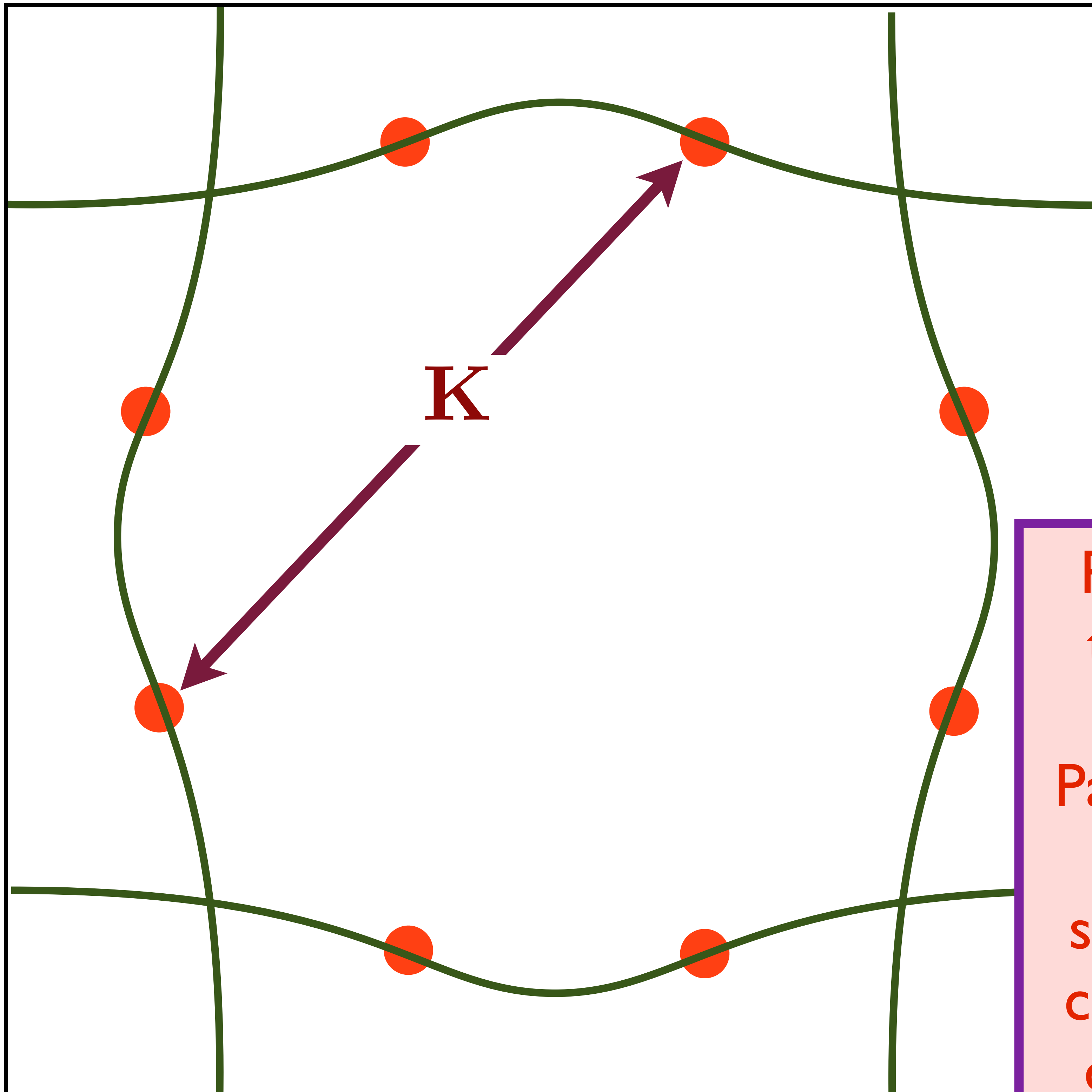

Hot spots in a two band model

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

Requires only time-reversal symmetry. 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 $\vec{\varphi}$.

$$\mathcal{Z} = \int \mathcal{D}c_\alpha \mathcal{D}\vec{\varphi} \exp\left(-\mathcal{S}\right)$$

$$\mathcal{S} = \int d\tau \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} \left(\frac{\partial}{\partial\tau} - \varepsilon_{\mathbf{k}}\right) c_{\mathbf{k}\alpha}$$

$$+ \int d\tau d^2x \left[\frac{1}{2}\left(\boldsymbol{\nabla}_x \vec{\varphi}\right)^2 + \frac{r}{2}\vec{\varphi}^2 + \ldots\right]$$

$$- \lambda \int d\tau \sum_i \vec{\varphi}_i \cdot (-1)^{\mathbf{x}_i} c^\dagger_{i\alpha} \vec{\sigma}_{\alpha\beta} c_{i\beta}$$

QMC for the onset of antiferromagnetism

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

No sign problem !

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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

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 $\vec{\varphi}$.

$$\mathcal{Z} = \int \mathcal{D}c_\alpha^{(x)} \mathcal{D}c_\alpha^{(y)} \mathcal{D}\vec{\varphi} \exp\left(-\mathcal{S}\right)$$

$$\mathcal{S} = \int d\tau \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^{(x)\dagger} \left(\frac{\partial}{\partial \tau} - \varepsilon_{\mathbf{k}}^{(x)} \right) c_{\mathbf{k}\alpha}^{(x)}$$

$$+ \int d\tau \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^{(y)\dagger} \left(\frac{\partial}{\partial \tau} - \varepsilon_{\mathbf{k}}^{(y)} \right) c_{\mathbf{k}\alpha}^{(y)}$$

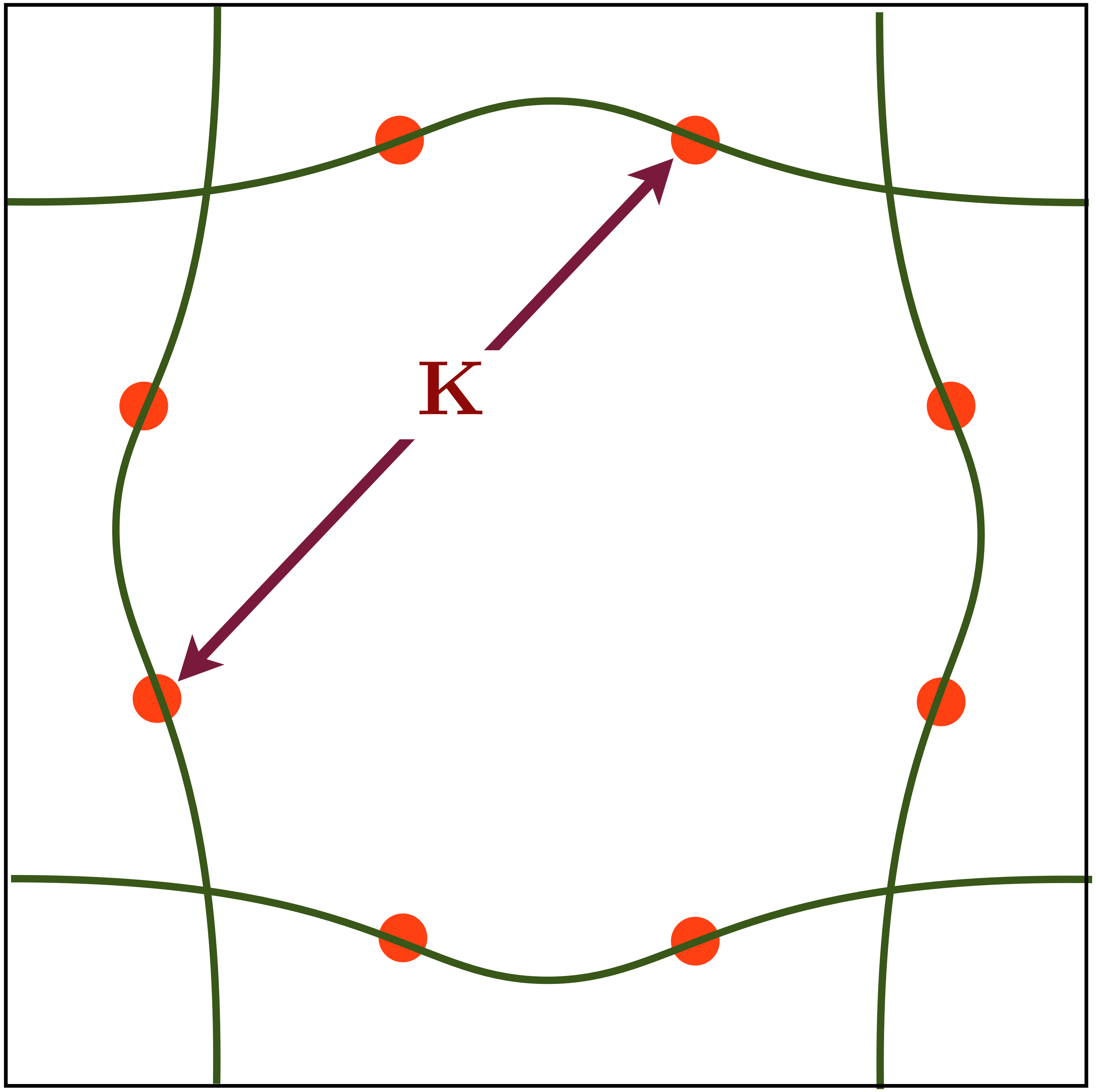
$$+ \int d\tau d^2 x \left[\frac{1}{2} \left(\boldsymbol{\nabla}_x \vec{\varphi} \right)^2 + \frac{r}{2} \vec{\varphi}^2 + \ldots \right]$$

$$- \lambda \int d\tau \sum_i \vec{\varphi}_i \cdot (-1)^{\mathbf{x}_i} c_{i\alpha}^{(x)\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta}^{(y)} + \text{H.c.}$$

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



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Hot spots in a two band model

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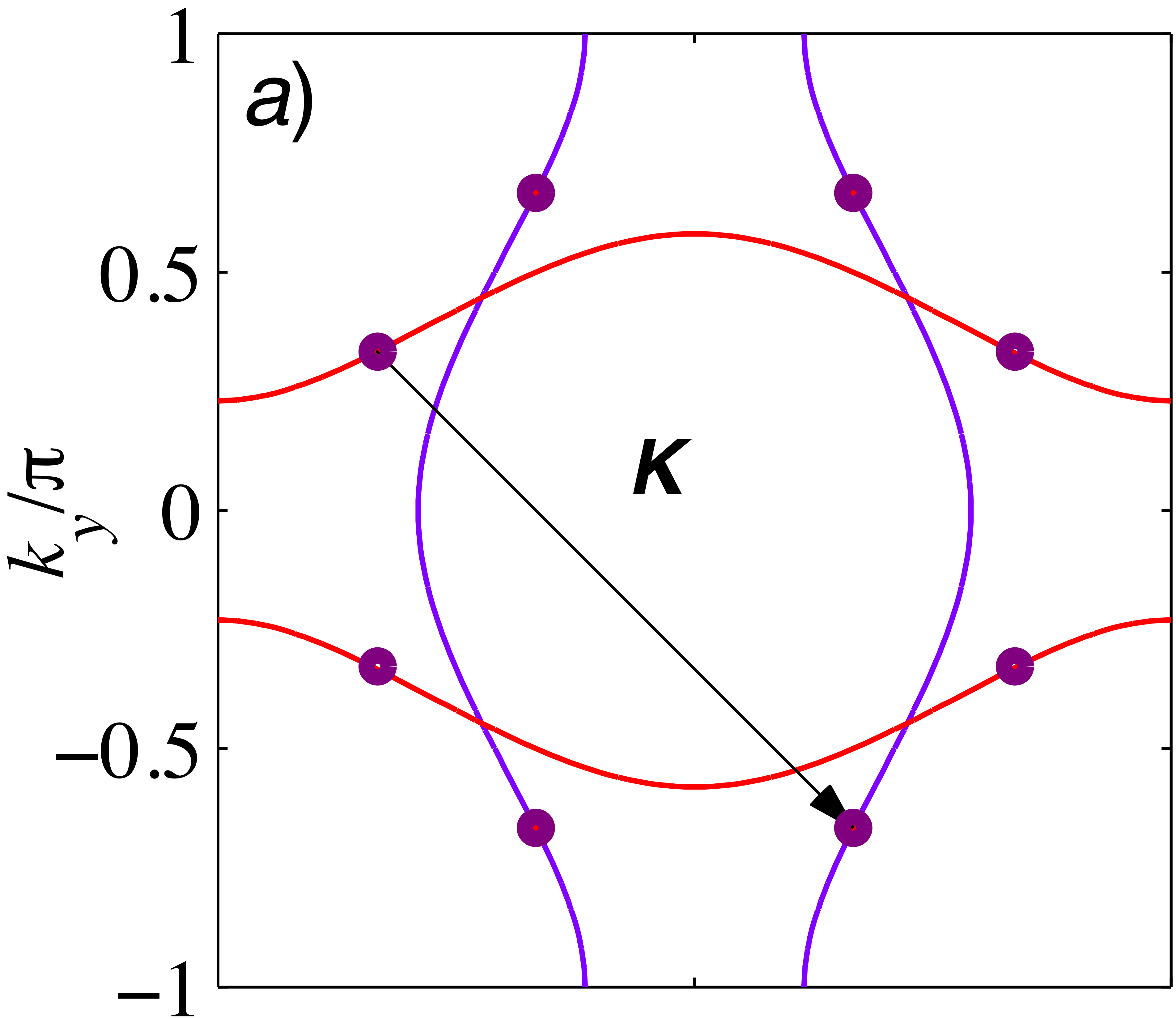

Center Brillouin zone at (π,π,)

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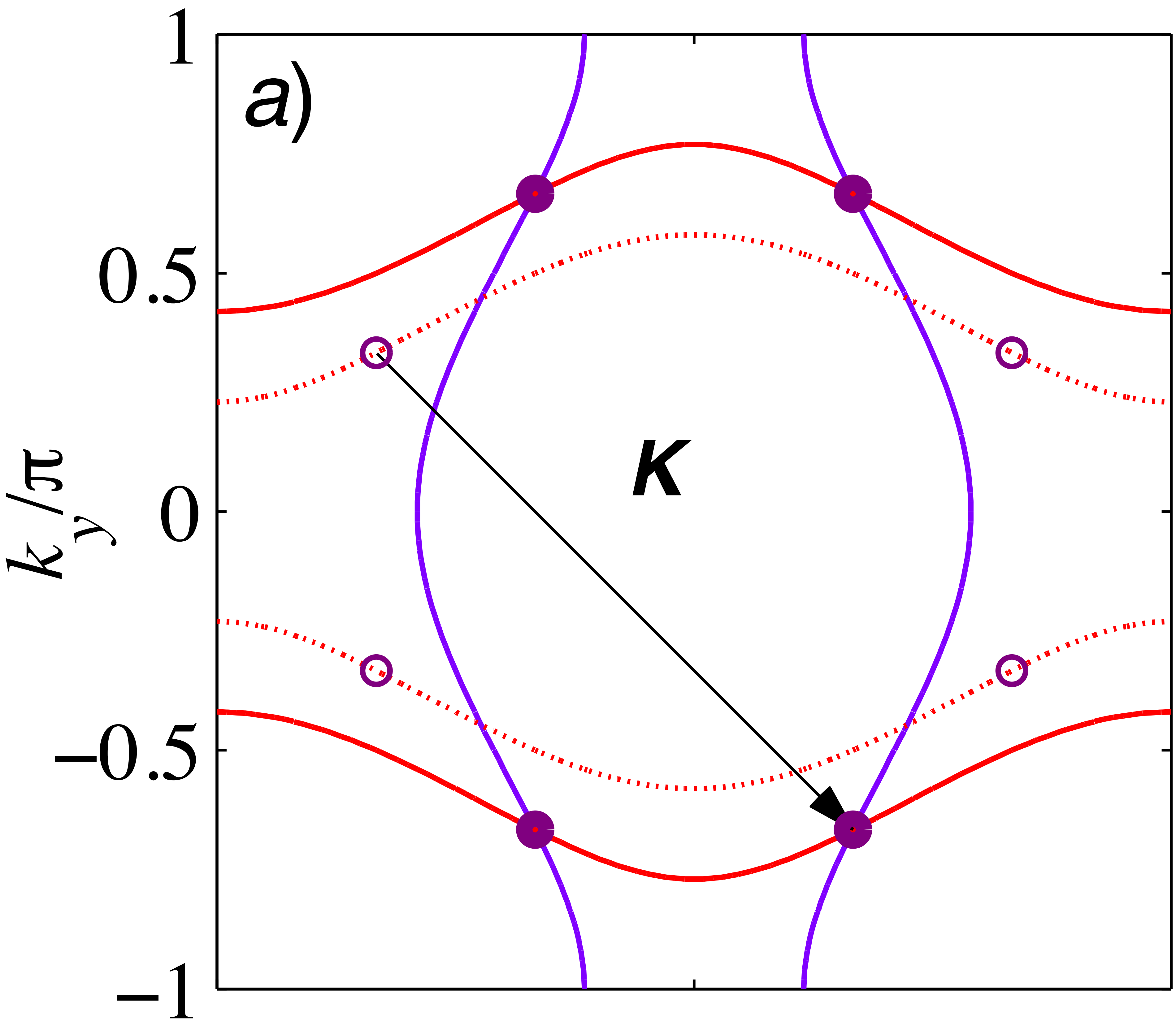

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Move one of the Fermi surface by $(\pi,\pi,)$

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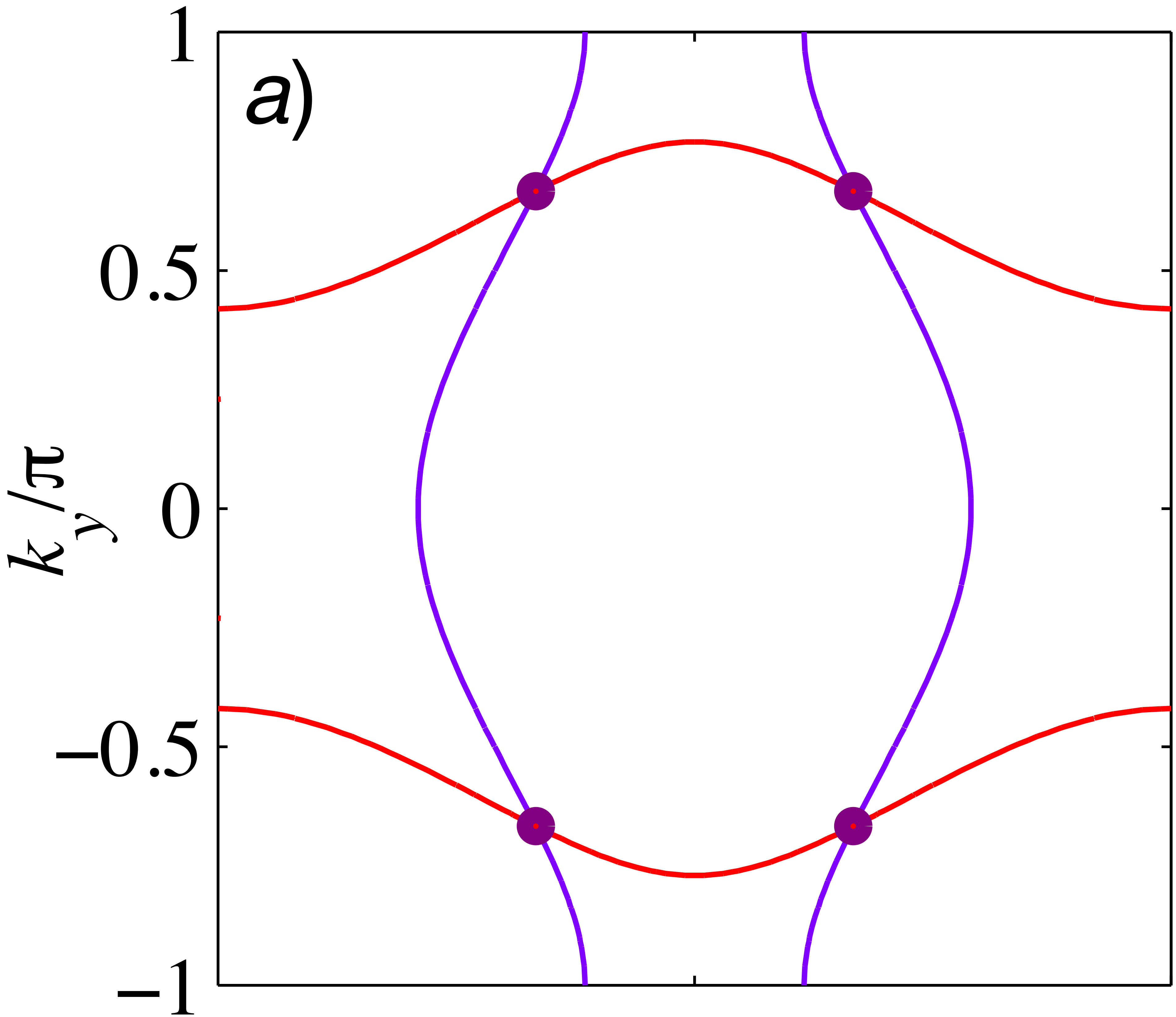

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Now hot spots are at Fermi surface intersections

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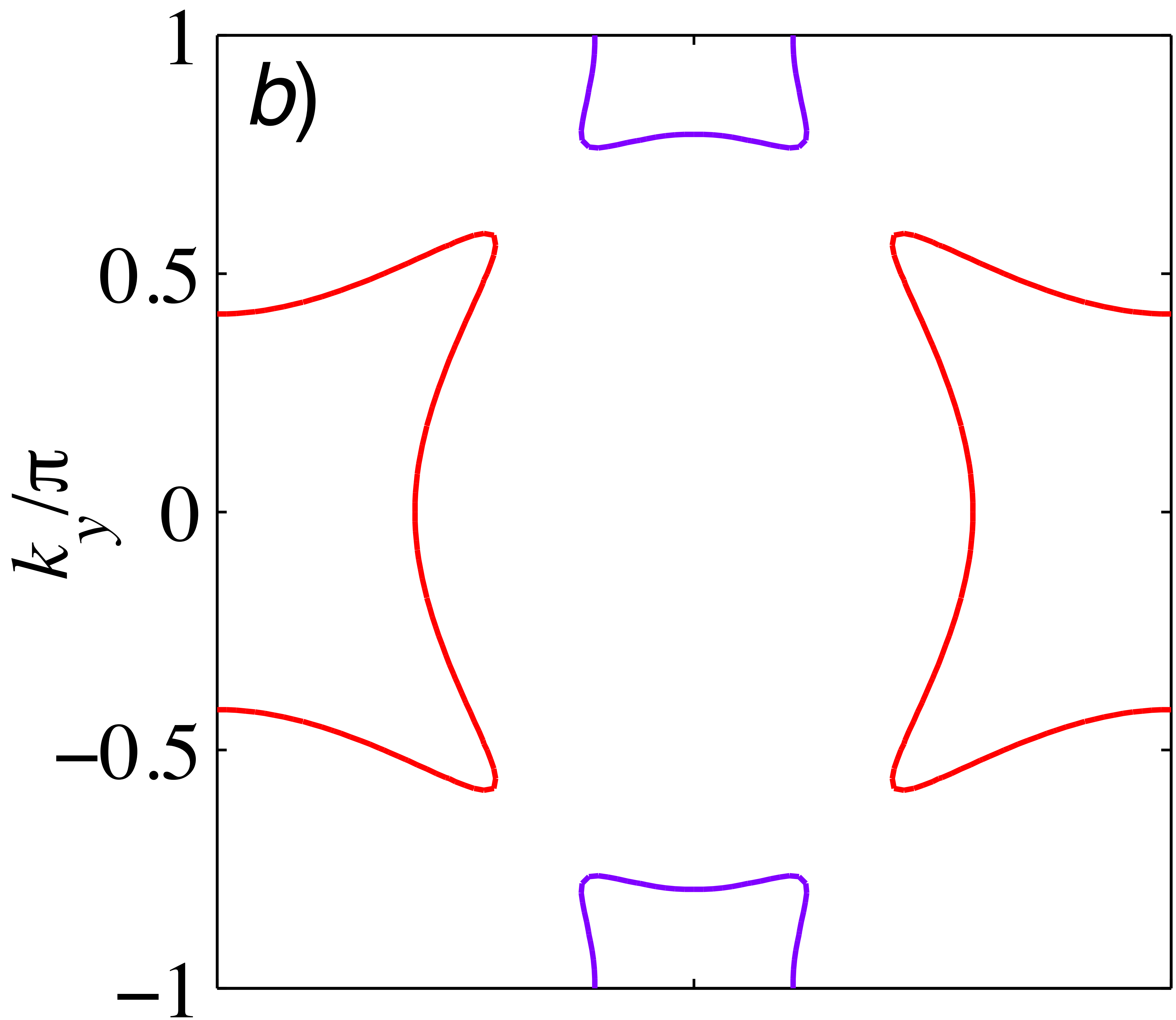

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Expected Fermi surfaces in the AFM ordered phase

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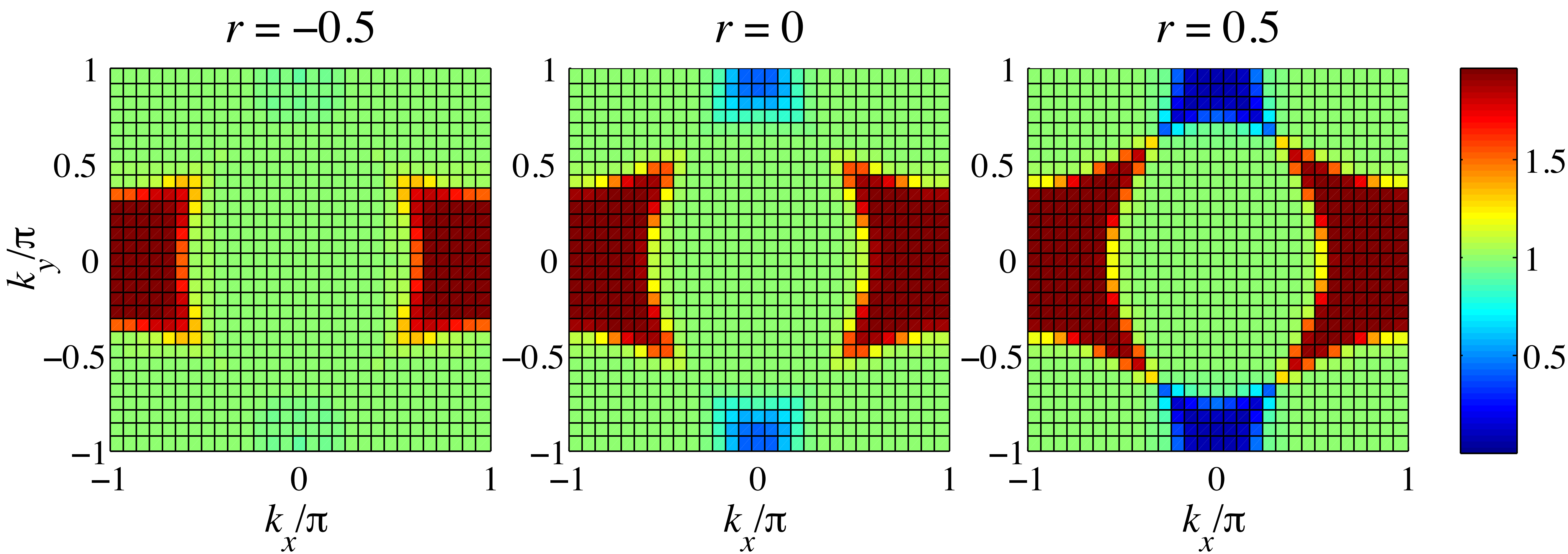

Electron occupation number $n_{\mathbf{k}}$
as a function of the tuning parameter r

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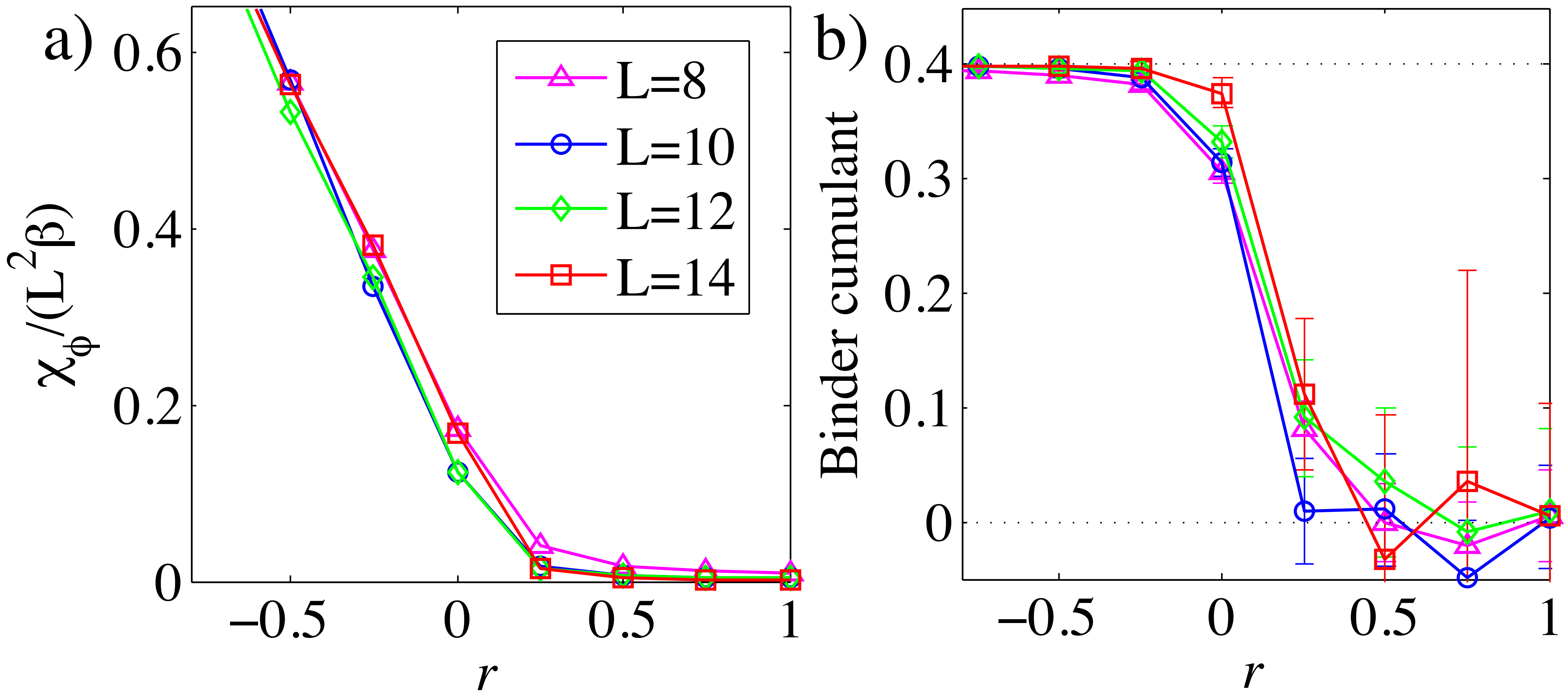
QMC for the onset of antiferromagnetism



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

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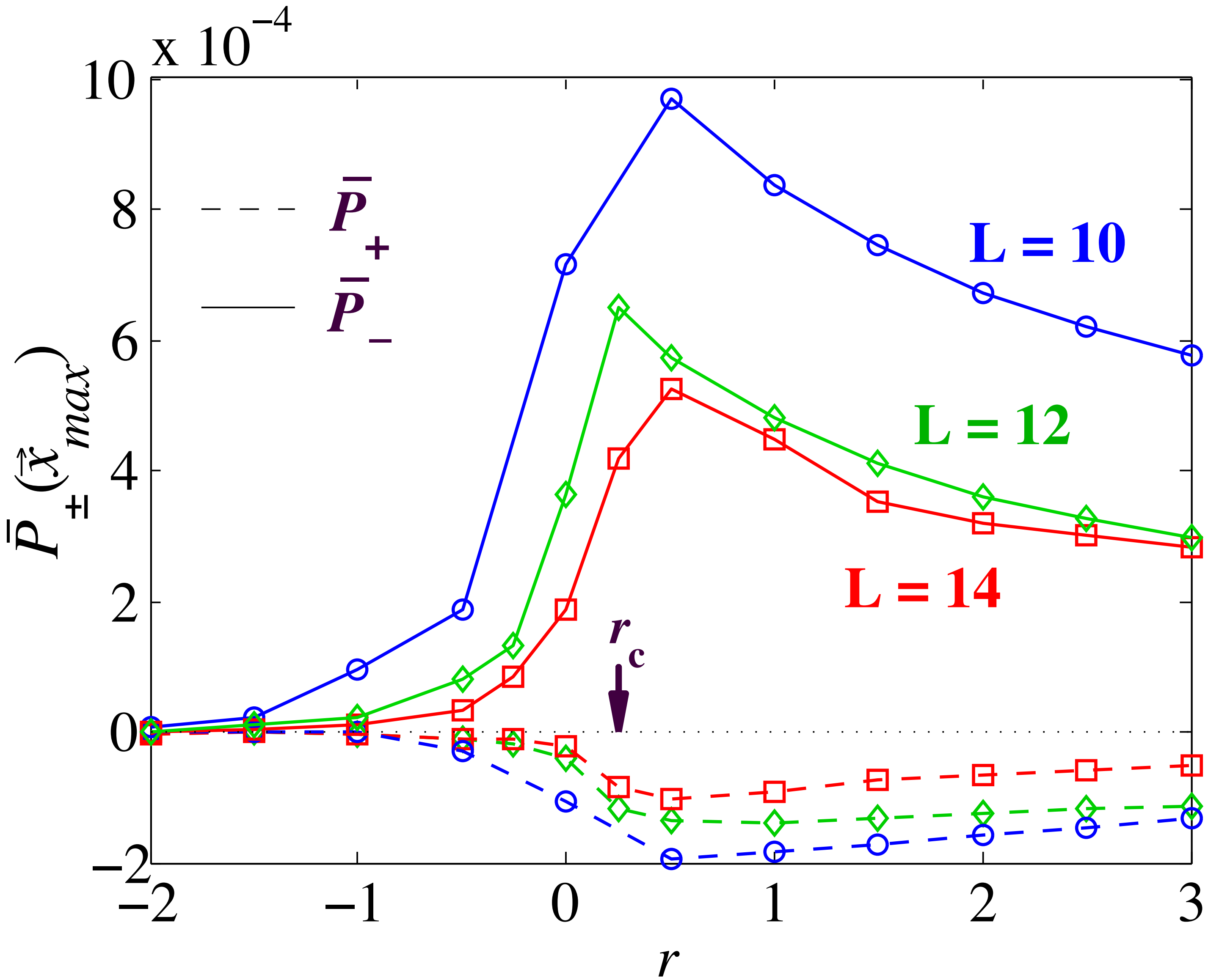
QMC for the onset of antiferromagnetism



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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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.