

# Progress on the physics of the underdoped cuprates

International Institute of Physics  
Natal, Brazil  
April 11, 2013

Subir Sachdev





Max Metlitski

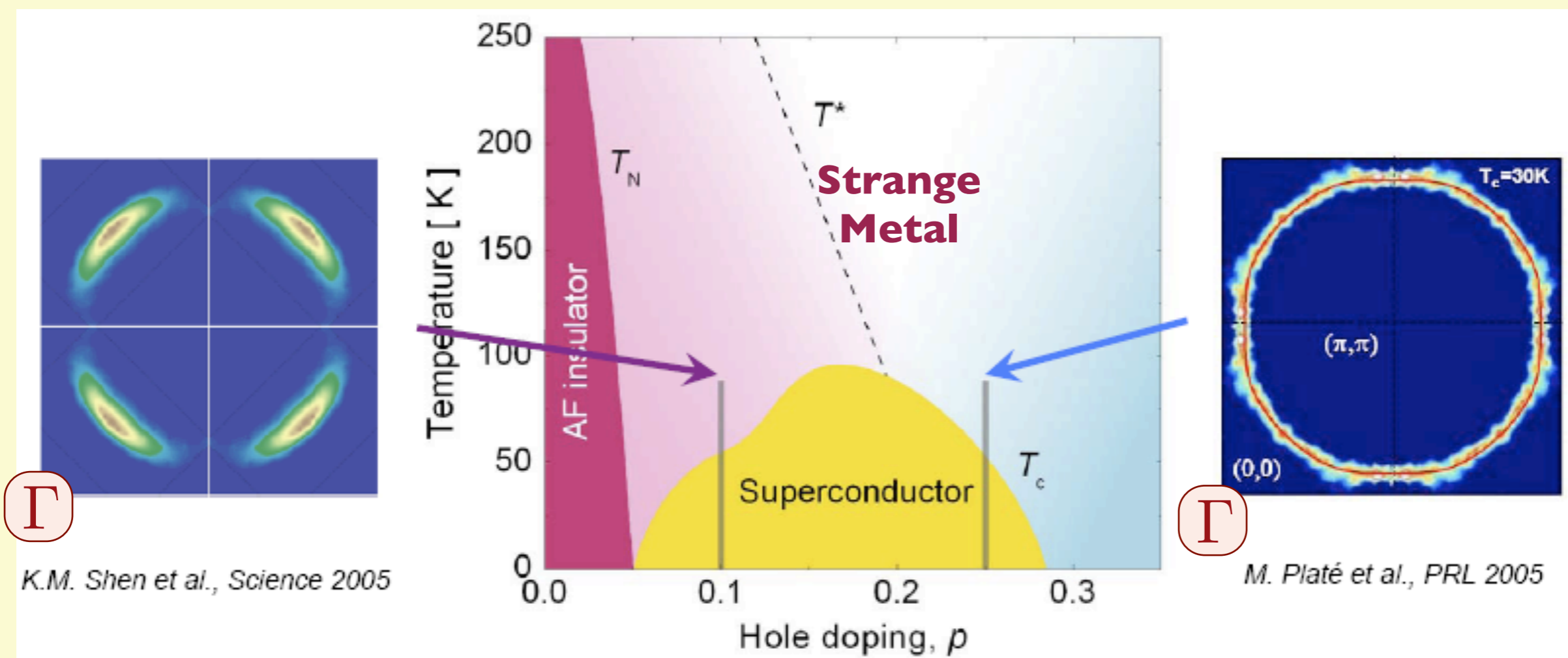
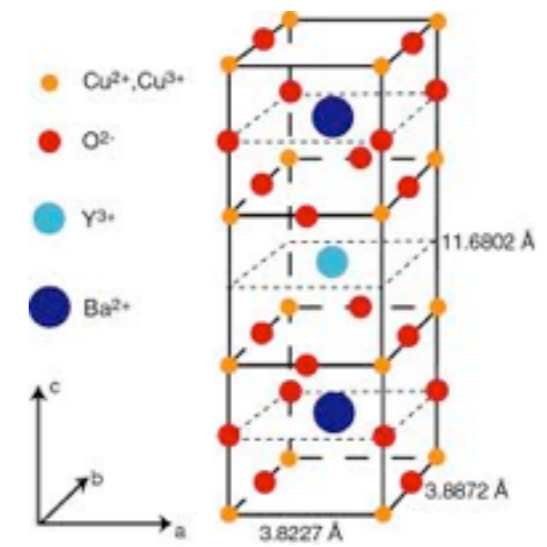


Erez Berg



Rolando La Placa





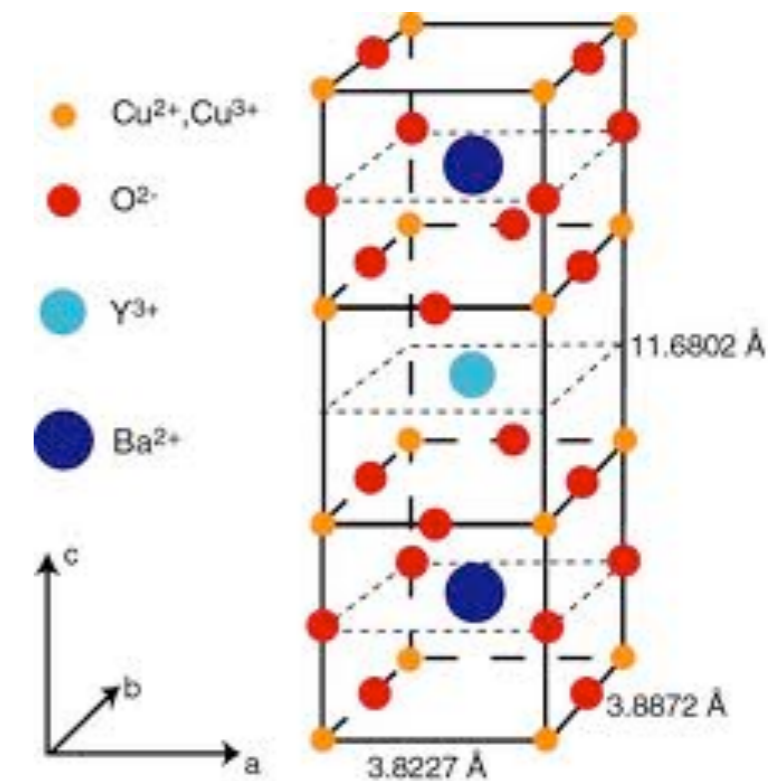
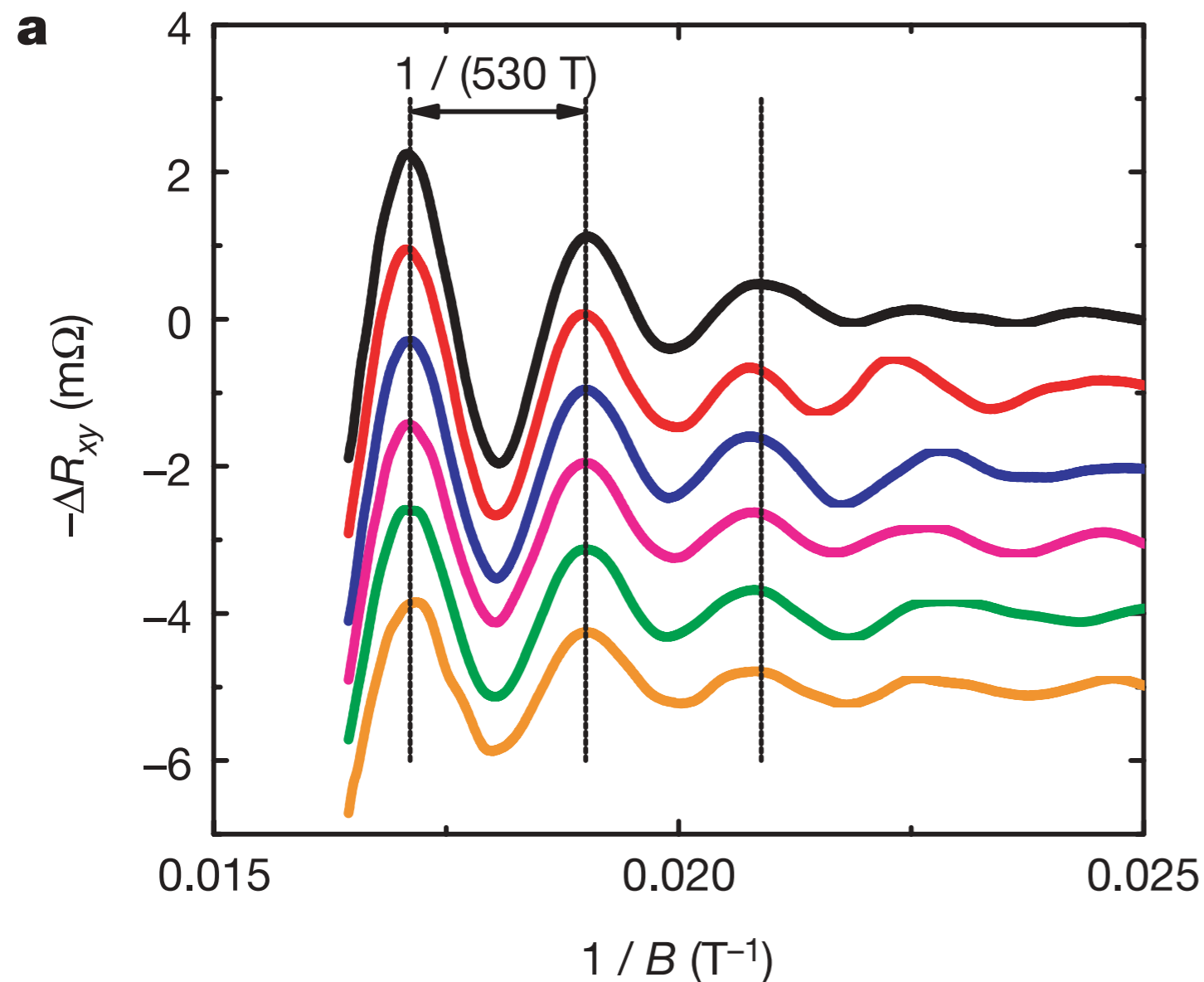
Smaller hole Fermi-pockets

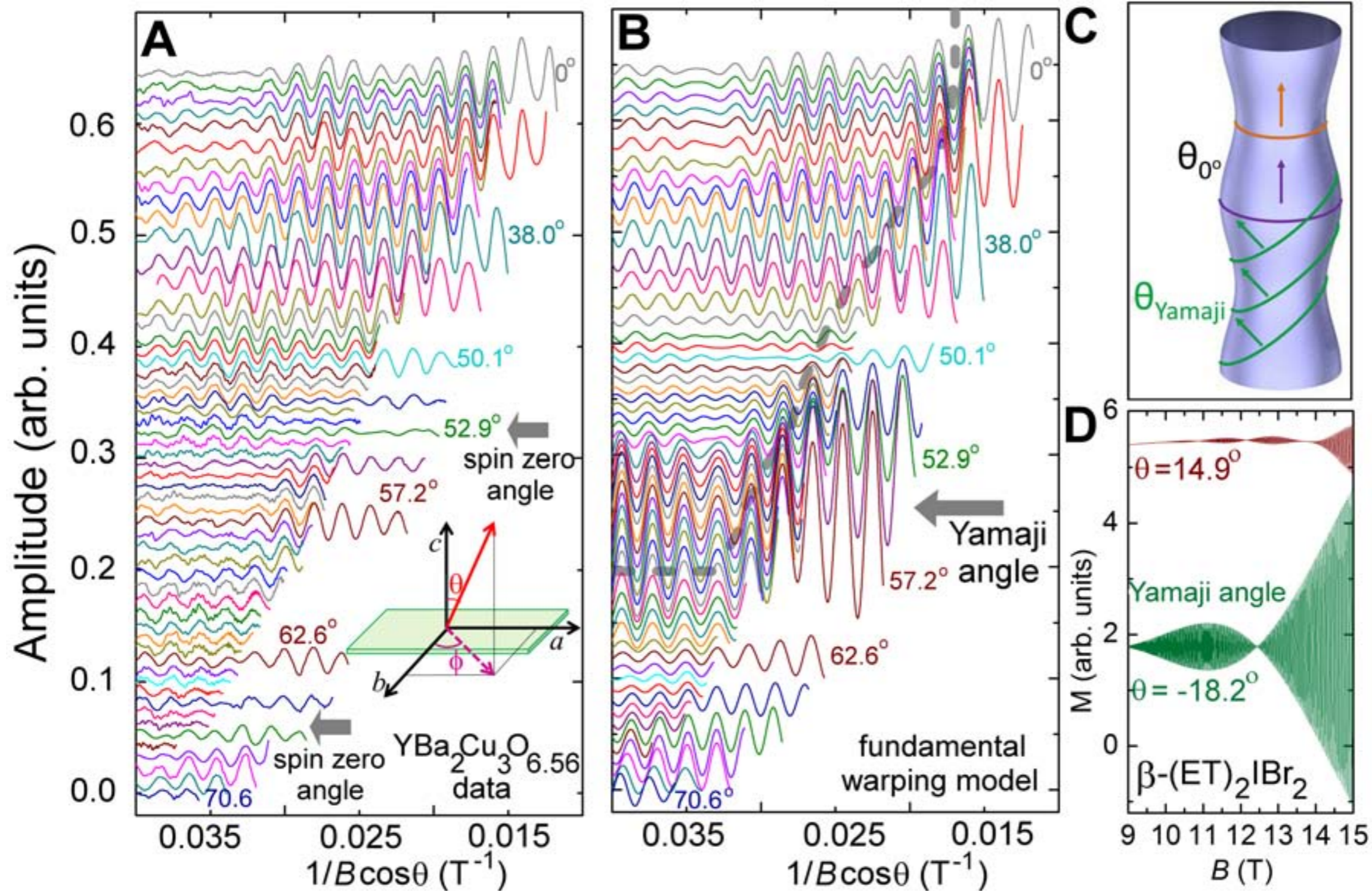
Large hole Fermi surface

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

Nicolas Doiron-Leyraud<sup>1</sup>, Cyril Proust<sup>2</sup>, David LeBoeuf<sup>1</sup>, Julien Levallois<sup>2</sup>, Jean-Baptiste Bonnemaïson<sup>1</sup>, Ruixing Liang<sup>3,4</sup>, D. A. Bonn<sup>3,4</sup>, W. N. Hardy<sup>3,4</sup> & Louis Taillefer<sup>1,4</sup>

Nature **447**, 565 (2007)





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

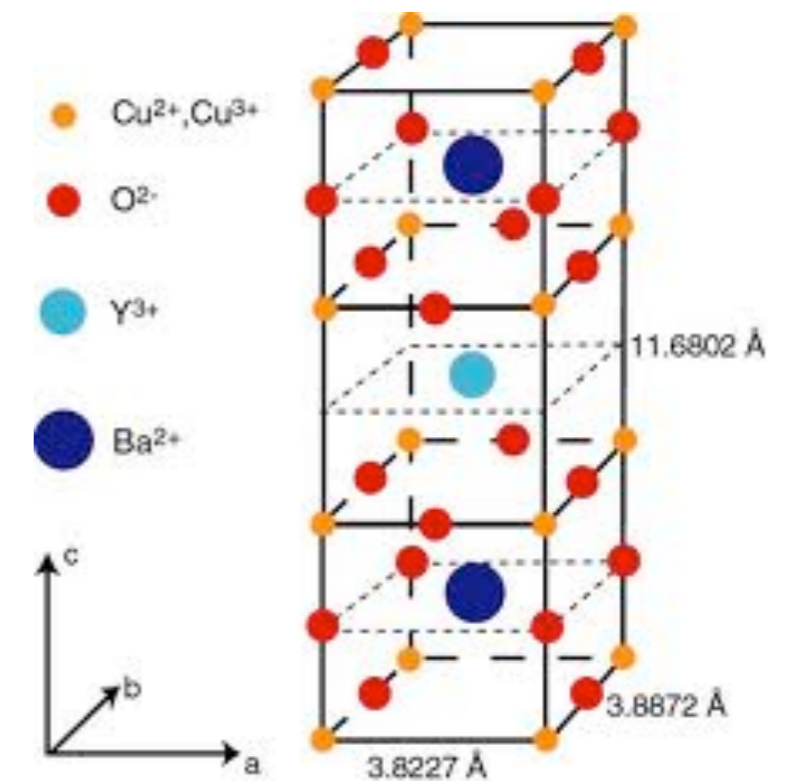
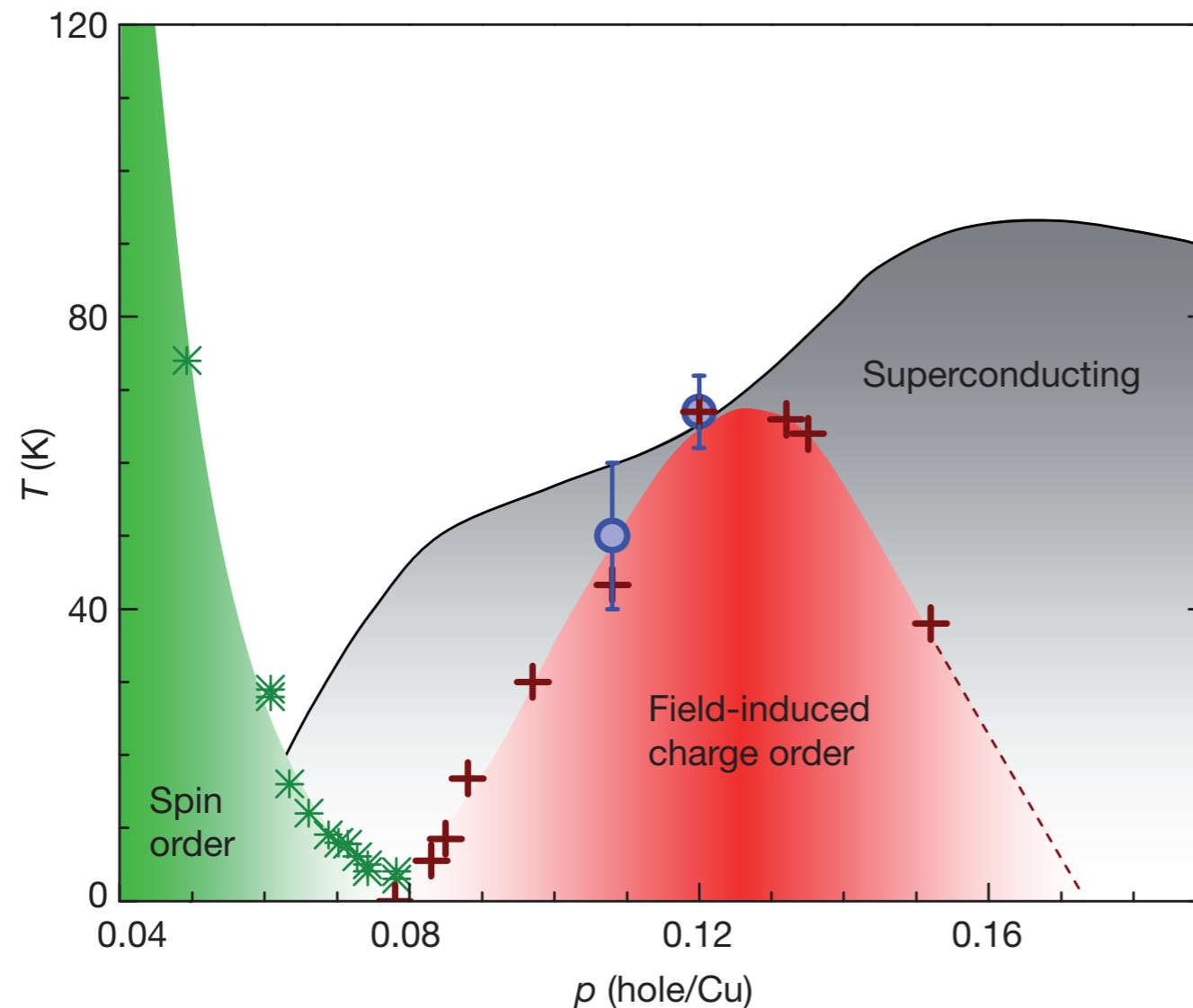
APS March meeting 2013  
B2.00004

Suchitra E. Sebastian,<sup>1\*</sup> N. Harrison,<sup>2</sup> F. F. Balakirev,<sup>2</sup> M. M. Altarawneh,<sup>2,3</sup>  
Ruixing Liang,<sup>4,5</sup> D. A. Bonn,<sup>4,5</sup> W. N. Hardy,<sup>4,5</sup> G. G. Lonzarich,<sup>1</sup>

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

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

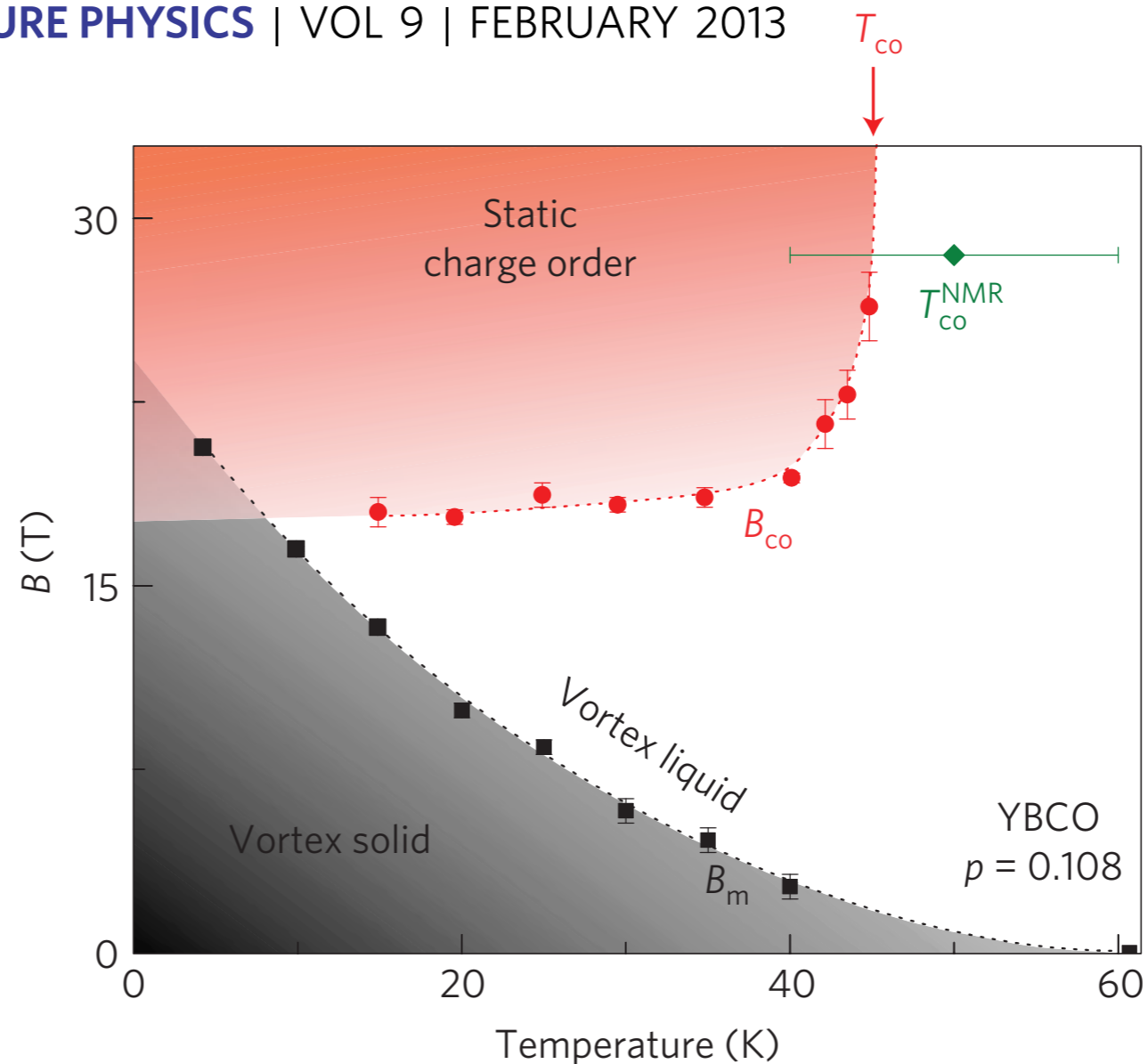
8 SEPTEMBER 2011 | VOL 477 | NATURE | 191



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

David LeBoeuf<sup>1\*</sup>, S. Krämer<sup>2</sup>, W. N. Hardy<sup>3,4</sup>, Ruixing Liang<sup>3,4</sup>, D. A. Bonn<sup>3,4</sup> and Cyril Proust<sup>1,4\*</sup>

NATURE PHYSICS | VOL 9 | FEBRUARY 2013

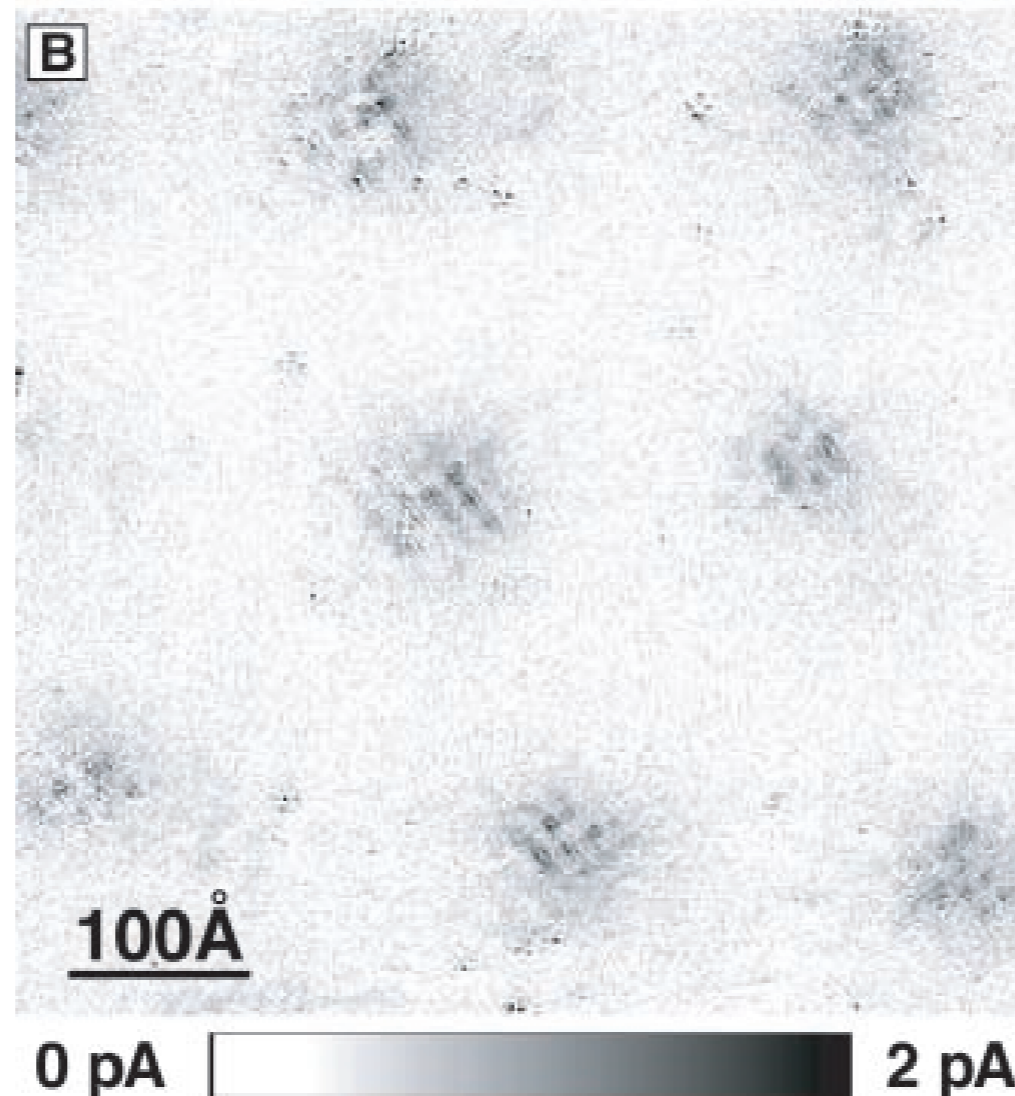


**The comparison of different acoustic modes indicates that the charge modulation is biaxial, which differs from a uniaxial stripe charge order.**

# A Four Unit Cell Periodic Pattern of Quasi-Particle States Surrounding Vortex Cores in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

J. E. Hoffman,<sup>1</sup> E. W. Hudson,<sup>1,2\*</sup> K. M. Lang,<sup>1</sup> V. Madhavan,<sup>1</sup>  
H. Eisaki,<sup>3†</sup> S. Uchida,<sup>3</sup> J. C. Davis<sup>1,2‡</sup>

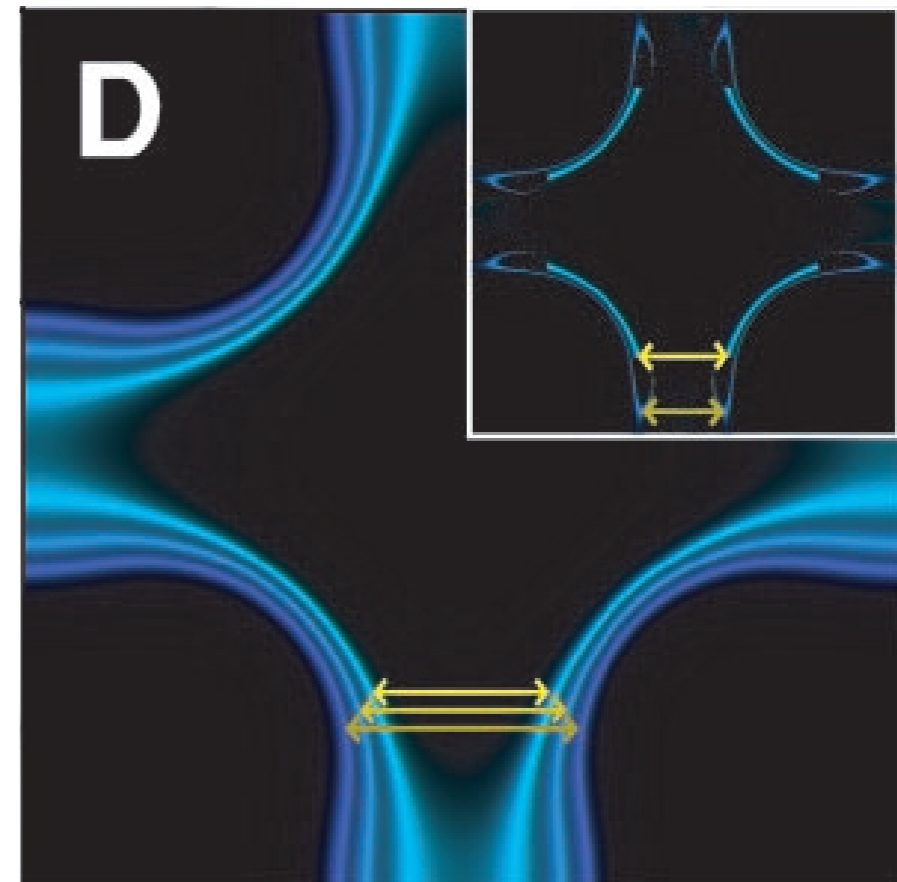
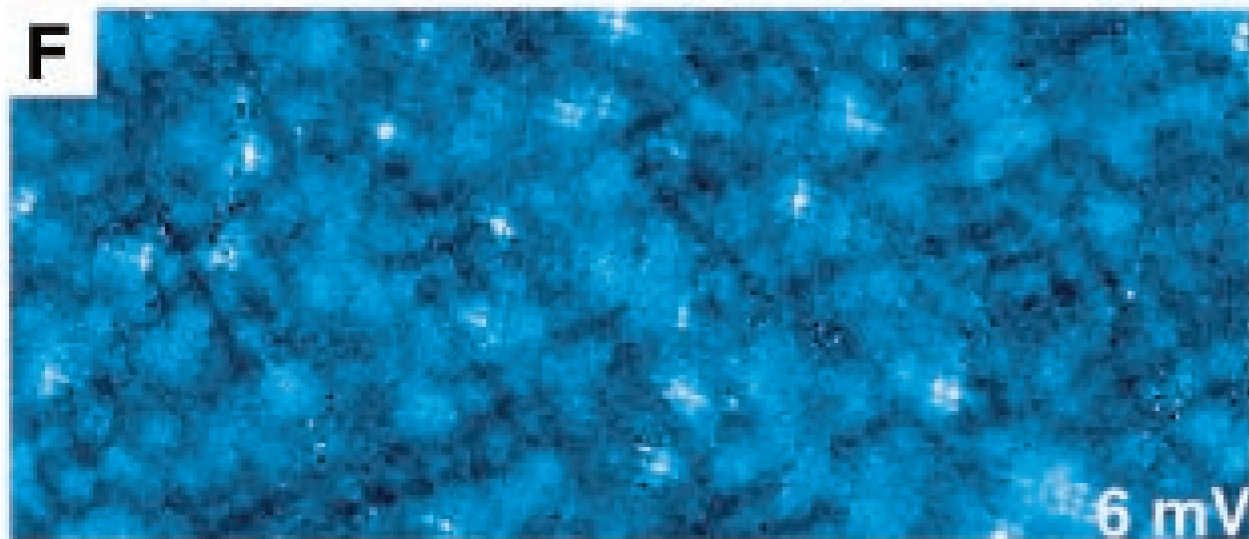
SCIENCE VOL 295 18 JANUARY 2002



# Local Ordering in the Pseudogap State of the High- $T_c$ Superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

Michael Vershinin,<sup>1\*</sup> Shashank Misra,<sup>1\*</sup> S. Ono,<sup>2</sup> Y. Abe,<sup>2†</sup>  
Yoichi Ando,<sup>2</sup> Ali Yazdani<sup>1‡§</sup>

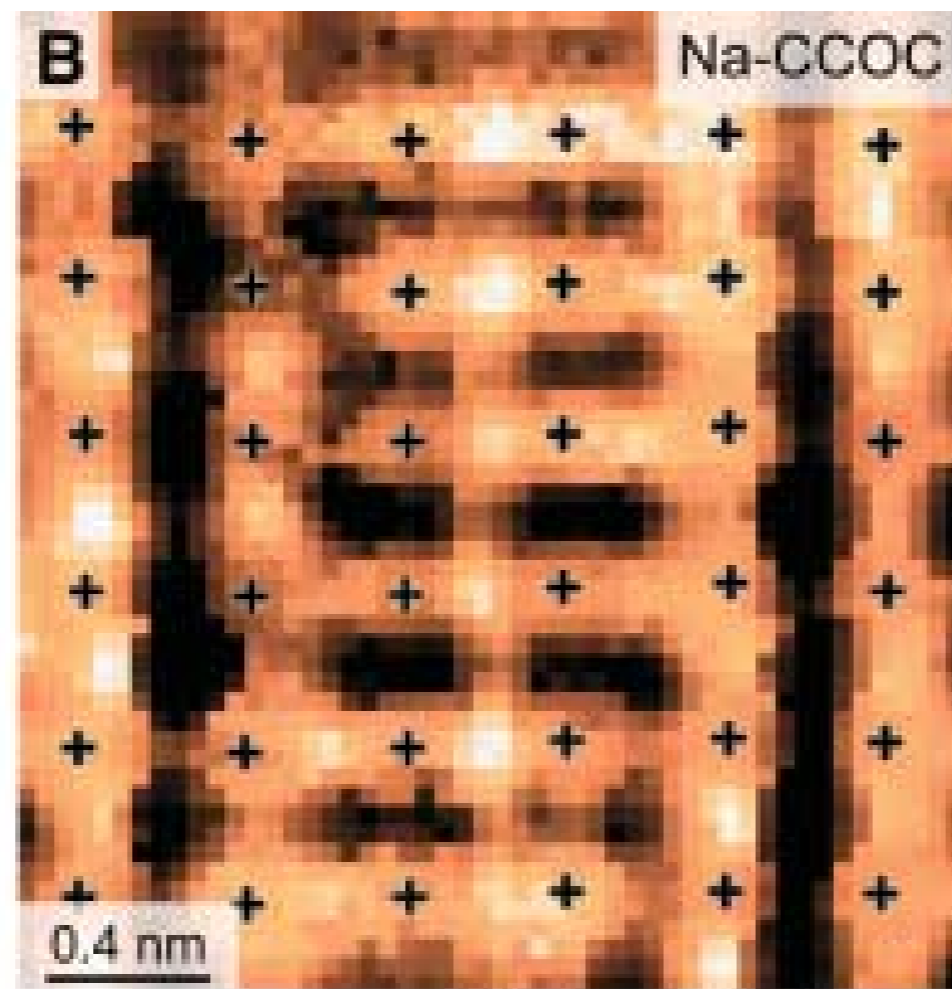
SCIENCE VOL 303 26 MARCH 2004



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

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

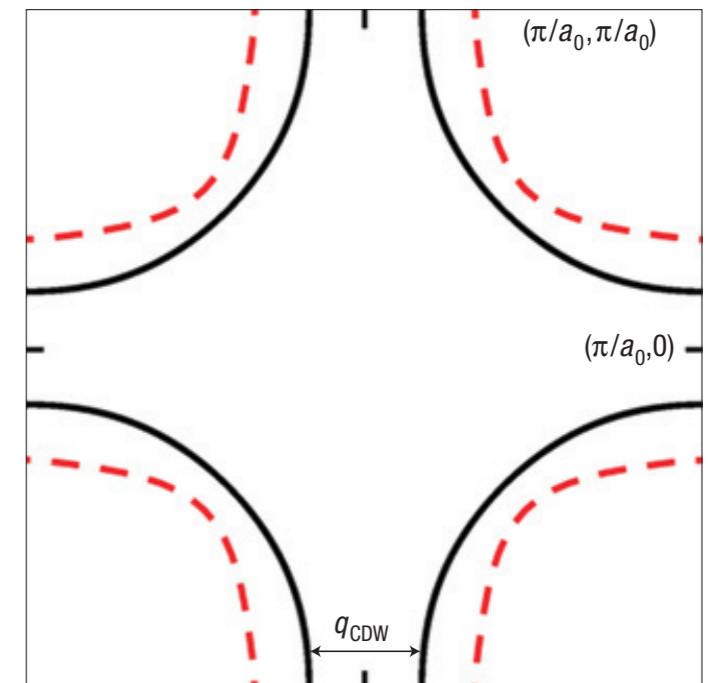
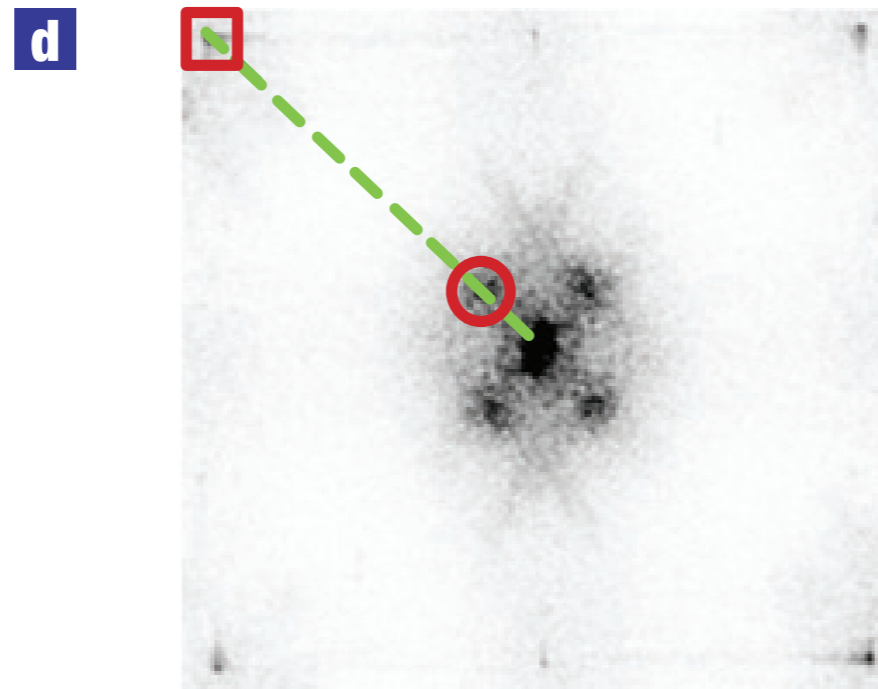
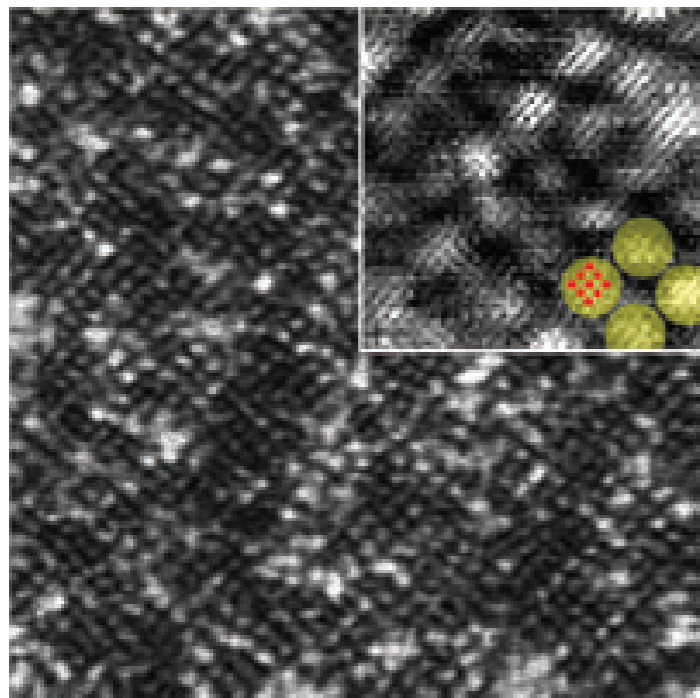
9 MARCH 2007 VOL 315 SCIENCE



# Charge-density-wave origin of cuprate checkerboard visualized by scanning tunnelling microscopy

W. D. WISE<sup>1</sup>, M. C. BOYER<sup>1</sup>, KAMALESH CHATTERJEE<sup>1</sup>, TAKESHI KONDO<sup>1,2\*</sup>, T. TAKEUCHI<sup>2,3</sup>, H. IKUTA<sup>2</sup>, YAYU WANG<sup>1\*</sup> AND E. W. HUDSON<sup>1†</sup>

nature physics | VOL 4 | SEPTEMBER 2008 |

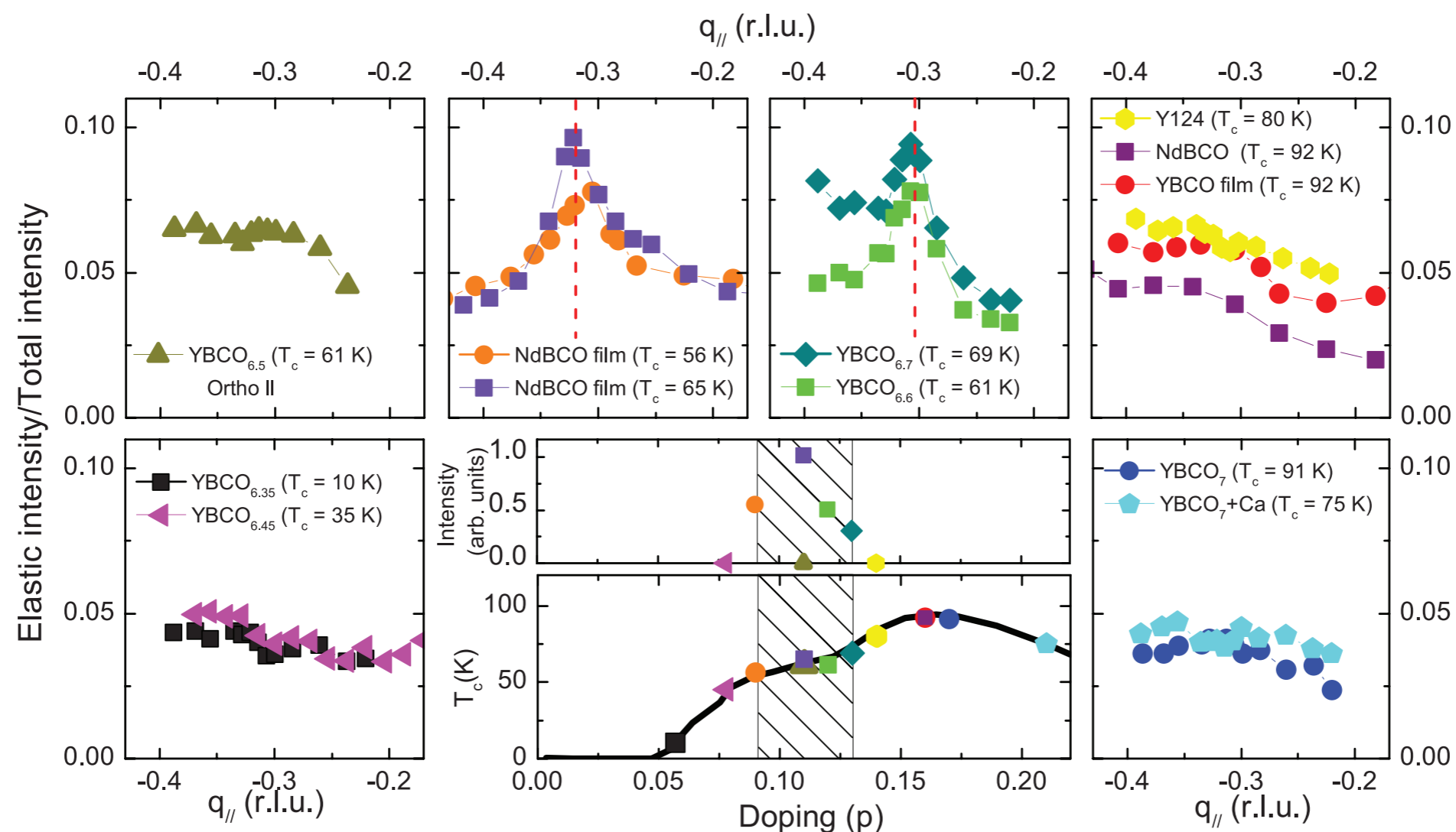


# Long-Range Incommensurate Charge Fluctuations in $(Y,Nd)Ba_2Cu_3O_{6+x}$

G. Ghiringhelli,<sup>1\*</sup> M. Le Tacon,<sup>2</sup> M. Minola,<sup>1</sup> S. Blanco-Canosa,<sup>2</sup> C. Mazzoli,<sup>1</sup>  
 N. B. Brookes,<sup>3</sup> G. M. De Luca,<sup>4</sup> A. Frano,<sup>2,5</sup> D. G. Hawthorn,<sup>6</sup> F. He,<sup>7</sup> T. Loew,<sup>2</sup>  
 M. Moretti Sala,<sup>3</sup> D. C. Peets,<sup>2</sup> M. Salluzzo,<sup>4</sup> E. Schierle,<sup>5</sup> R. Sutarto,<sup>7,8</sup> G. A. Sawatzky,<sup>8</sup>  
 E. Weschke,<sup>5</sup> B. Keimer,<sup>2\*</sup> L. Braicovich<sup>1</sup>

SCIENCE VOL 337 17 AUGUST 2012

resonant soft x-ray scattering

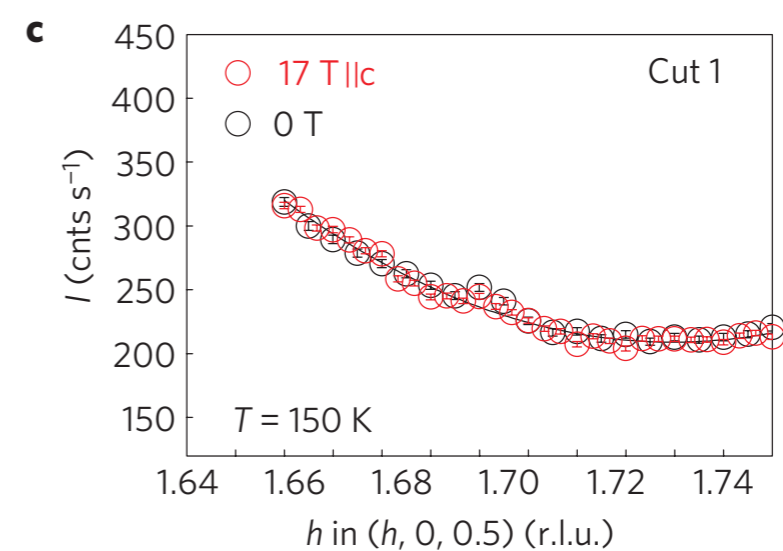
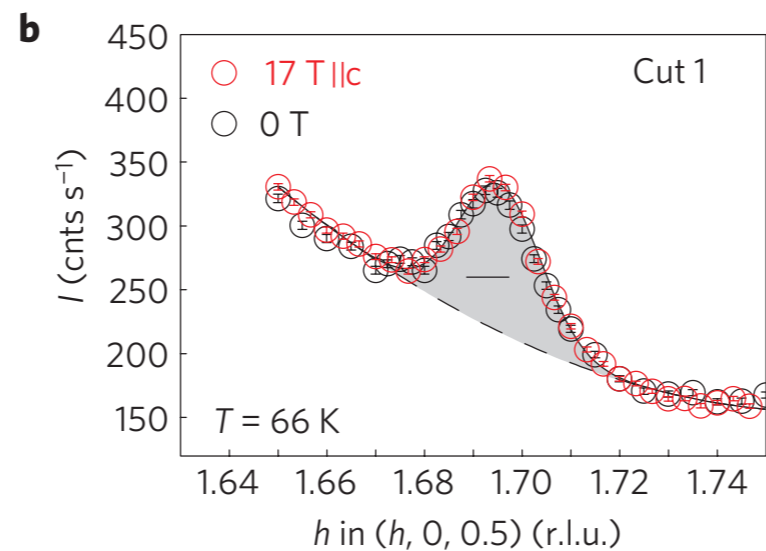
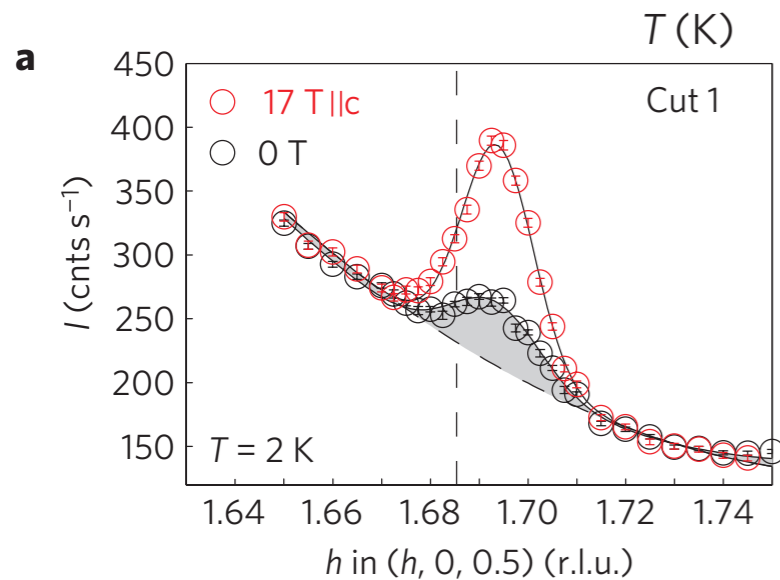
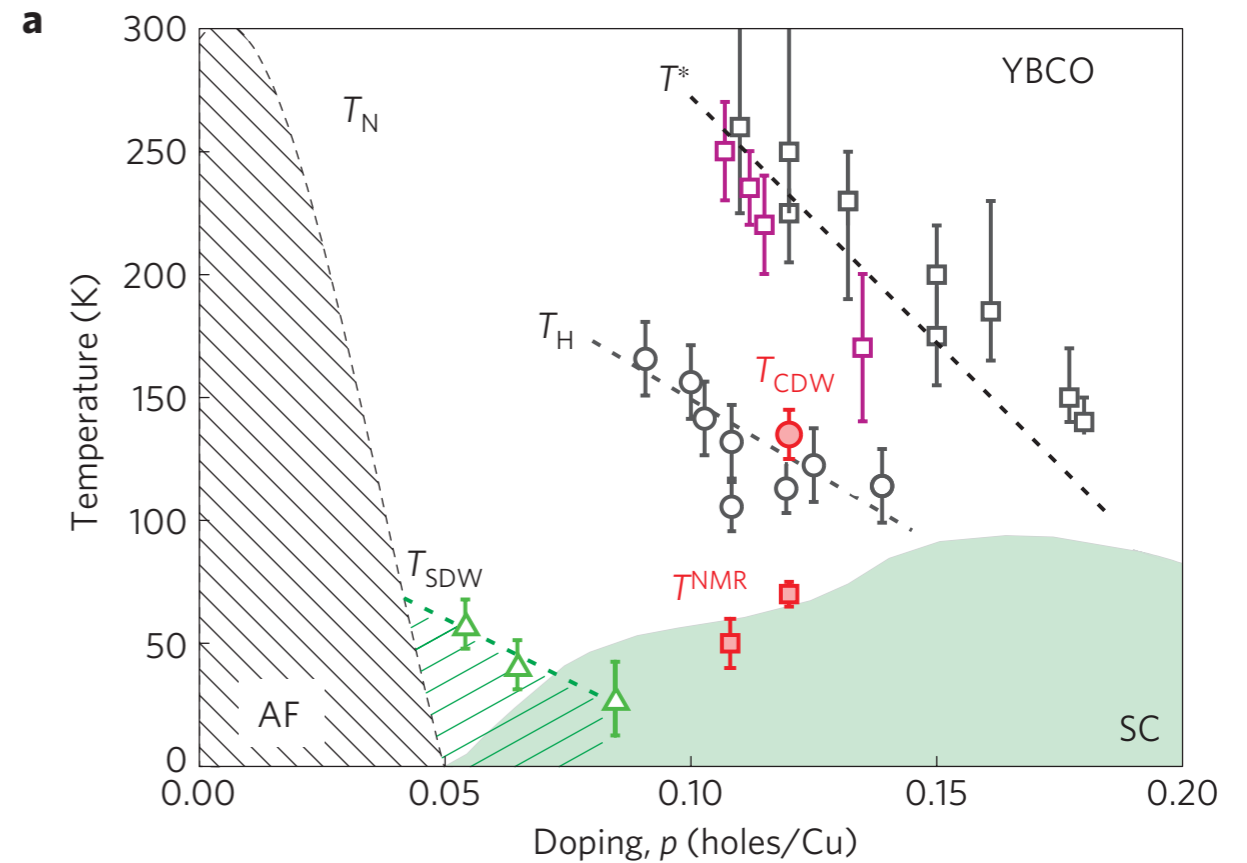
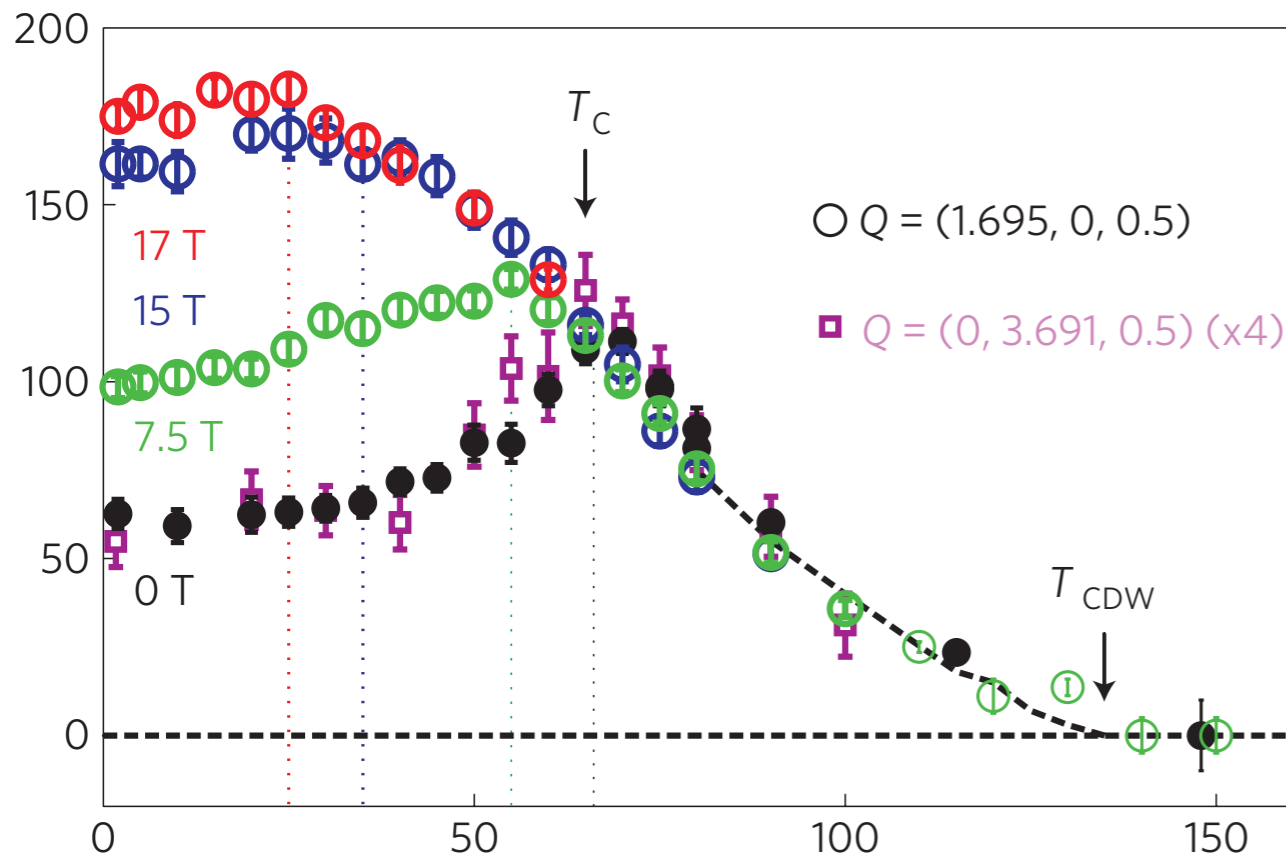


**Fig. 3.** Dependence of the CDW signal at 15 K on the hole doping level  $p$ . The CDW signal is present in several  $YBa_2Cu_3O_{6+x}$  and  $Nd_{1+y}Ba_{2-y}Cu_3O_7$  samples, but only for  $0.09 \leq p \leq 0.13$ . In this doping range (shaded in the

central panel), the  $T_c$ -versus- $p$  relation exhibits a plateau. The CDW peak position does not change with  $p$  outside of the experimental error, but its intensity is maximum at  $p \approx 0.11$ .

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

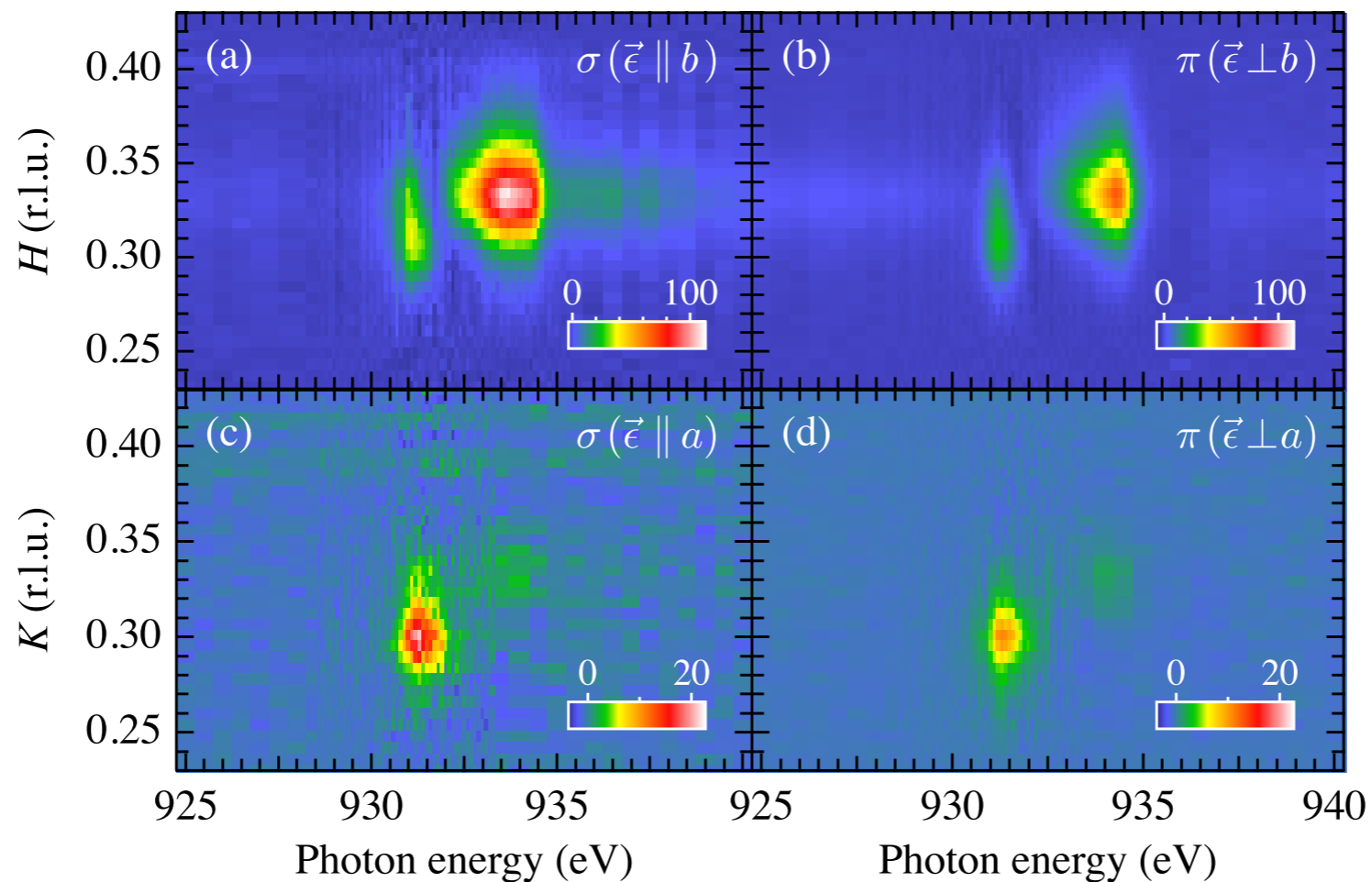
J. Chang<sup>1,2\*</sup>, E. Blackburn<sup>3</sup>, A. T. Holmes<sup>3</sup>, N. B. Christensen<sup>4</sup>, J. Larsen<sup>4,5</sup>, J. Mesot<sup>1,2</sup>, Ruixing Liang<sup>6,7</sup>, D. A. Bonn<sup>6,7</sup>, W. N. Hardy<sup>6,7</sup>, A. Watenphul<sup>8</sup>, M. v. Zimmermann<sup>8</sup>, E. M.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



# Distinct Charge Orders in the Planes and Chains of Ortho-III-Ordered $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ Superconductors Identified by Resonant Elastic X-ray Scattering

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

PRL **109**, 167001 (2012)

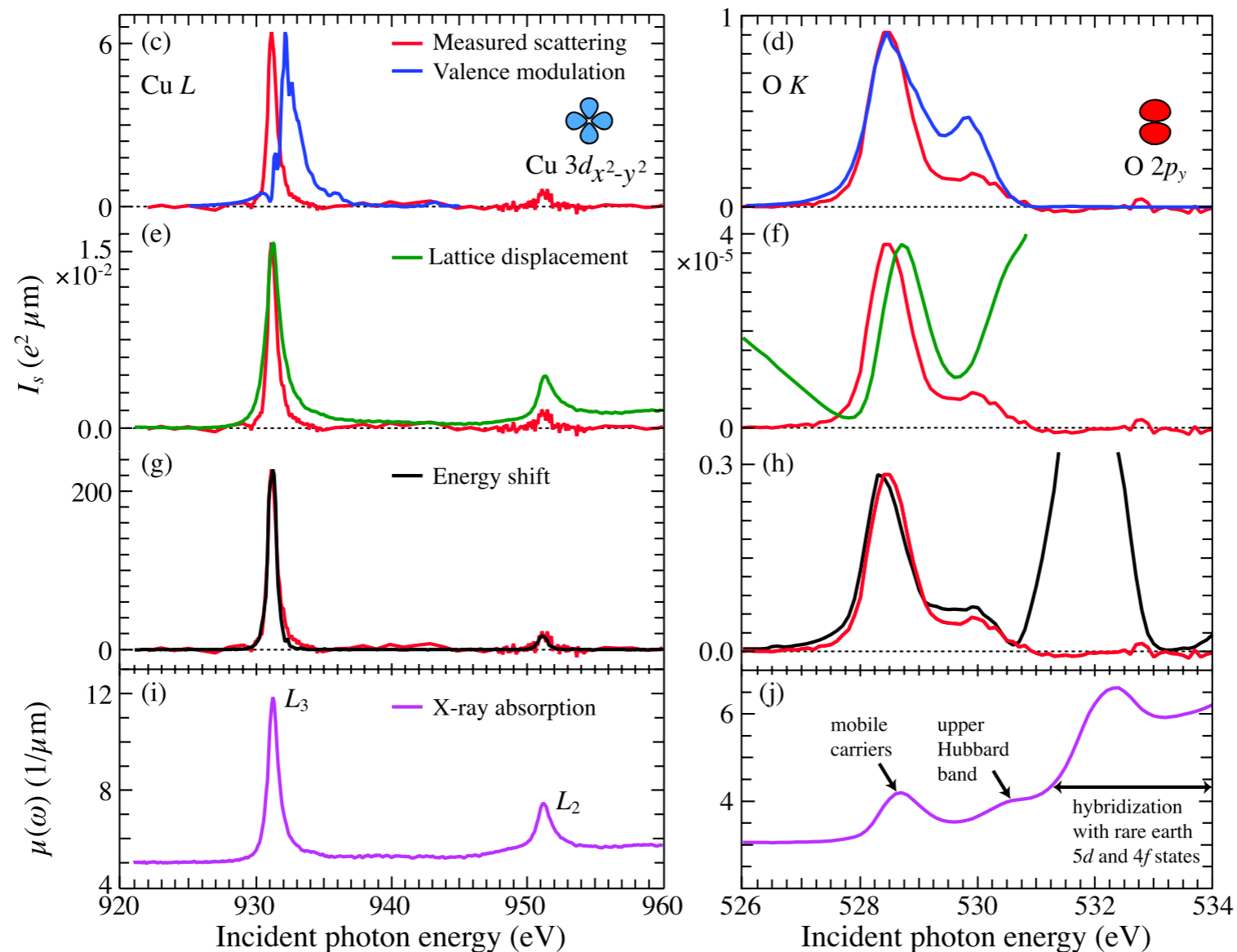


Moreover, the energy dependence of the CDW order in the planes is shown to result from a spatial modulation of energies of the Cu  $2p$  to  $3d_{x^2-y^2}$  transition, similar to stripe-ordered 214 cuprates.

# Resonant X-Ray Scattering Measurements of a Spatial Modulation of the Cu $3d$ and O $2p$ Energies in Stripe-Ordered Cuprate Superconductors

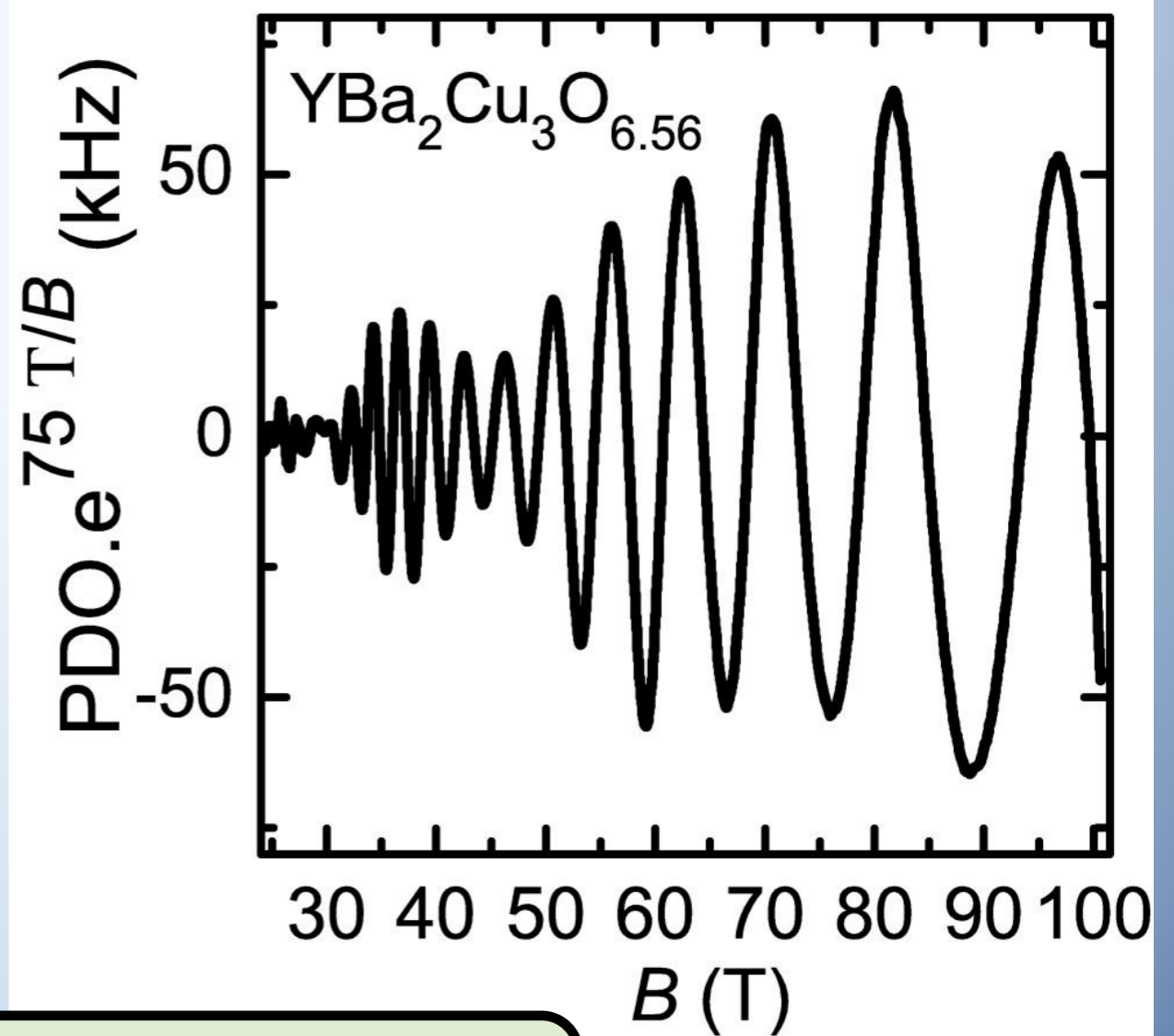
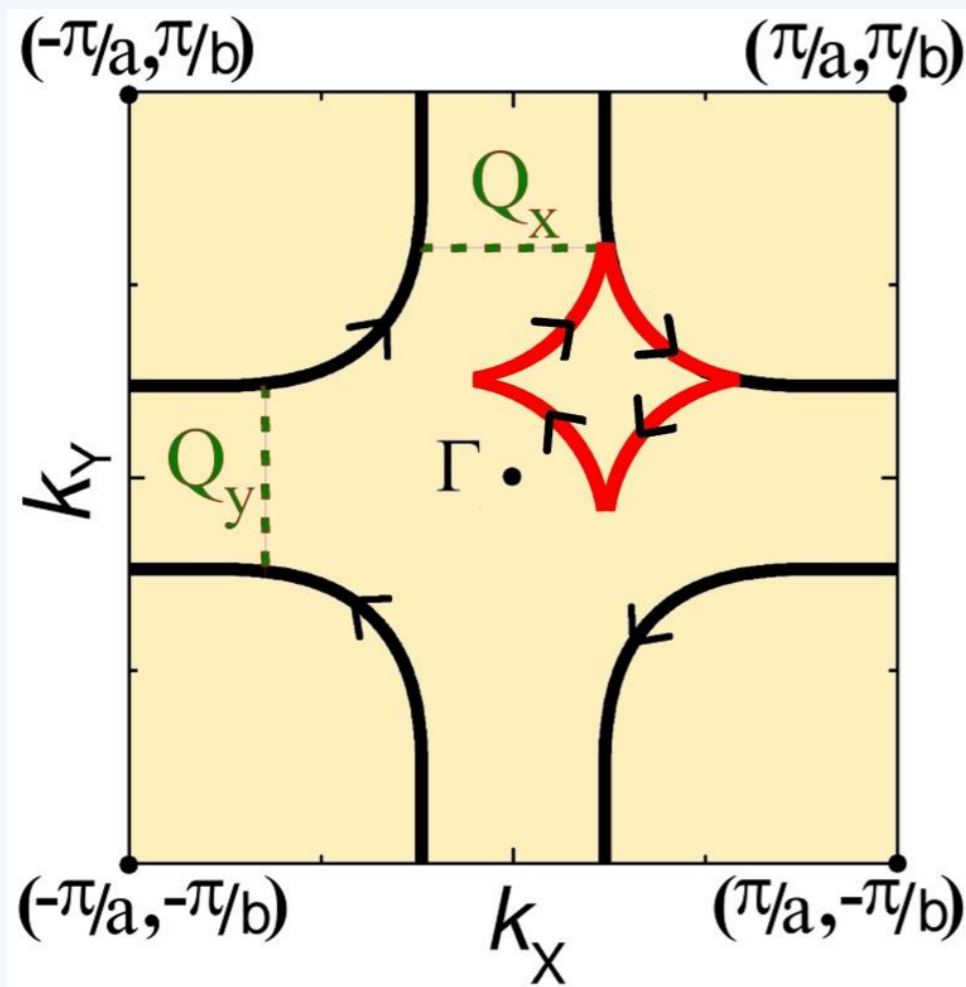
A. J. Achkar,<sup>1</sup> F. He,<sup>2</sup> R. Sutarto,<sup>3</sup> J. Geck,<sup>4</sup> H. Zhang,<sup>5</sup> Y.-J. Kim,<sup>5</sup> and D. G. Hawthorn<sup>1</sup>

PRL **110**, 017001 (2013)

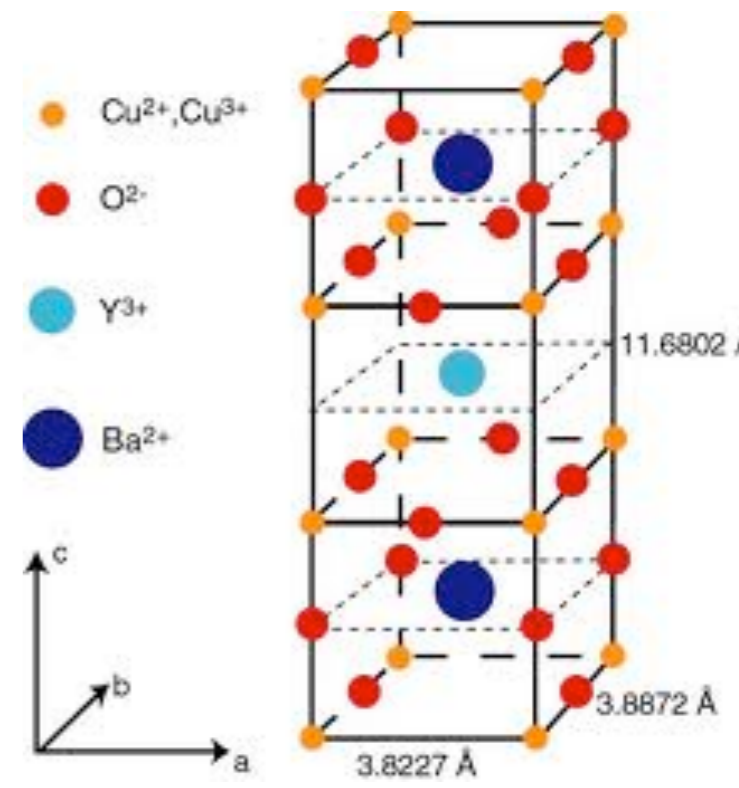
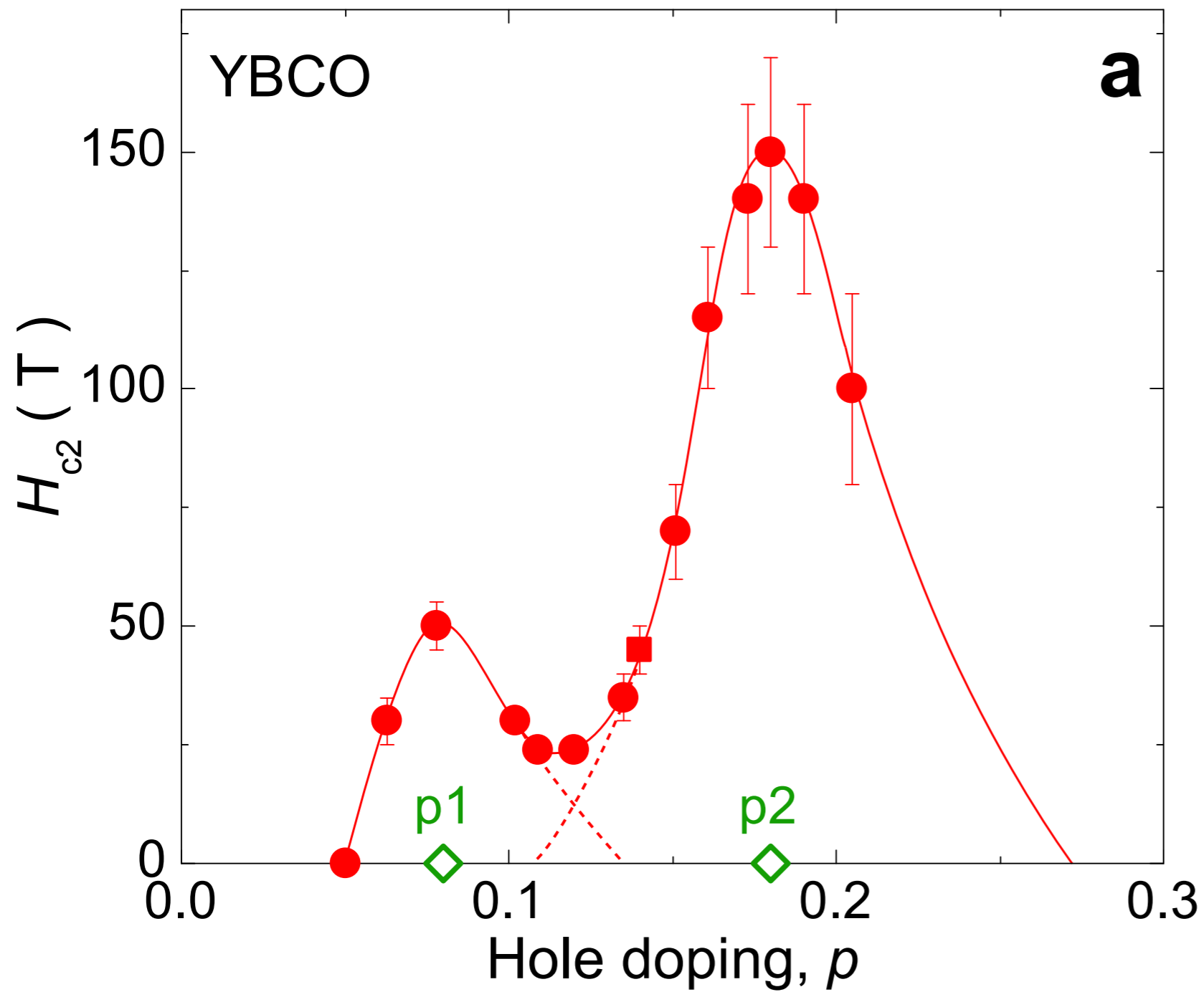


These energy shifts are interpreted as a spatial modulation of the electronic structure and may point to a valence-bond-solid interpretation of the stripe phase.

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

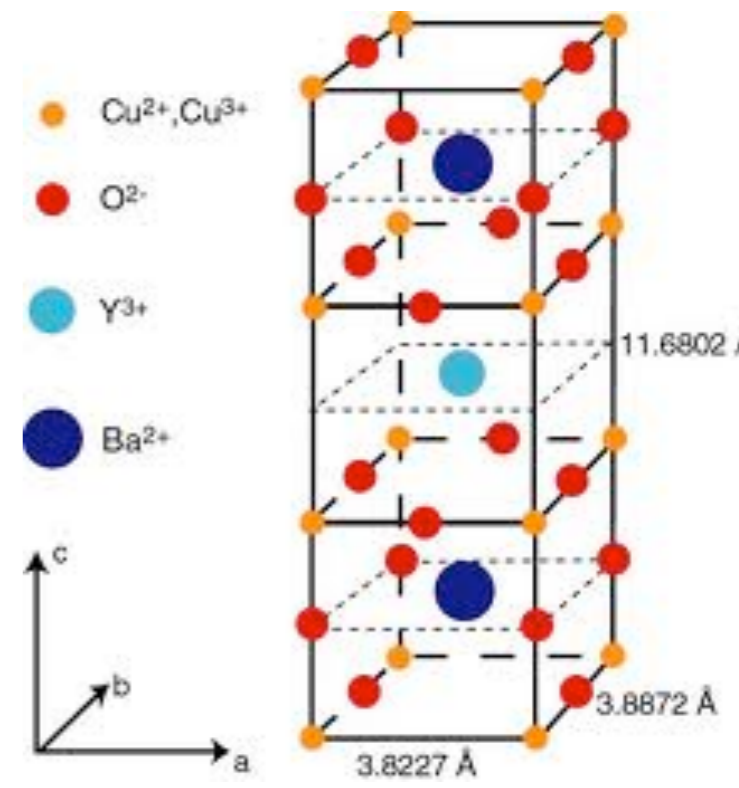
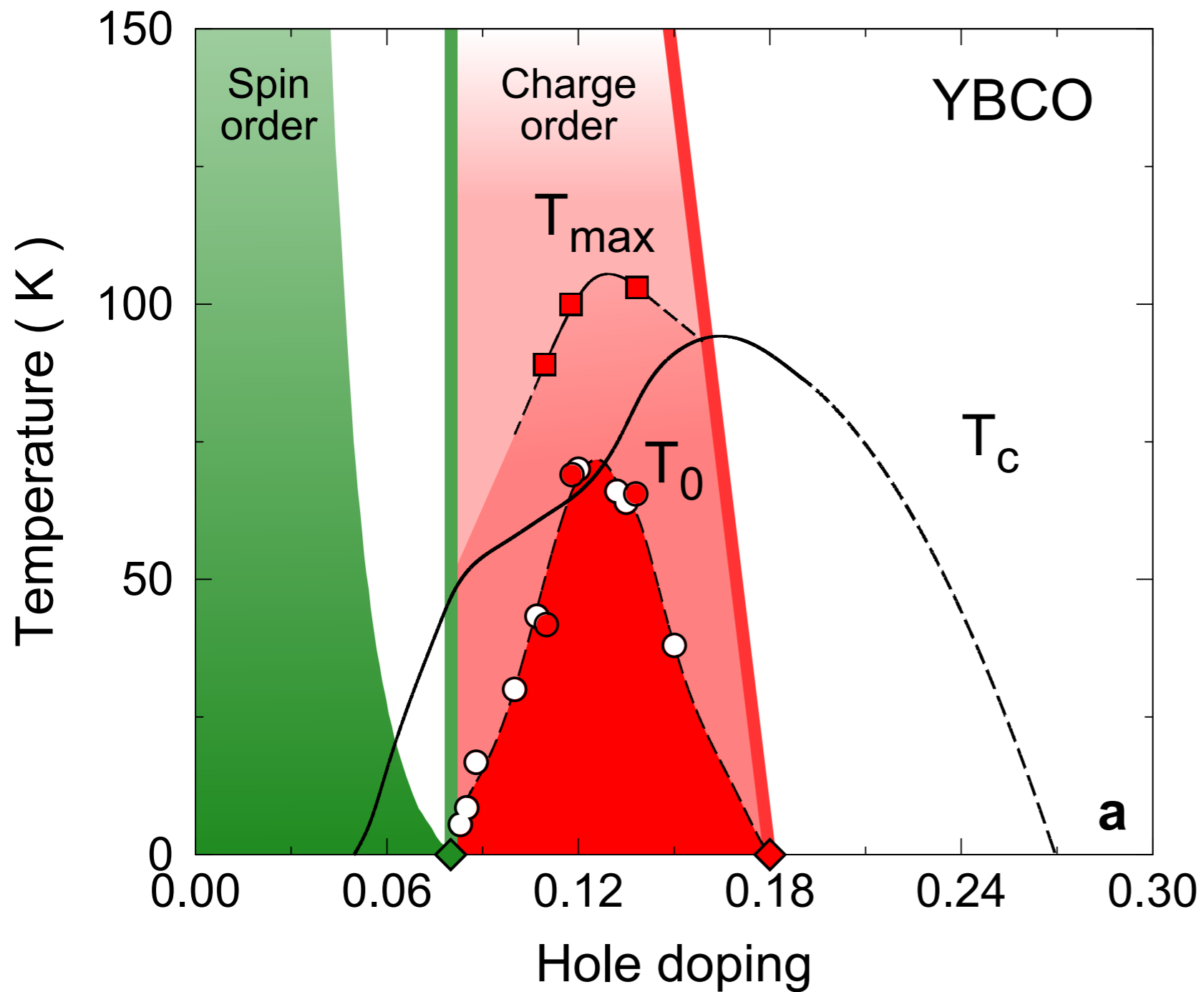


N. Harrison and S. E. Sebastian  
Phys. Rev. Lett. **106**, 226402 (2011)



APS March  
meeting 2013  
B36.00002

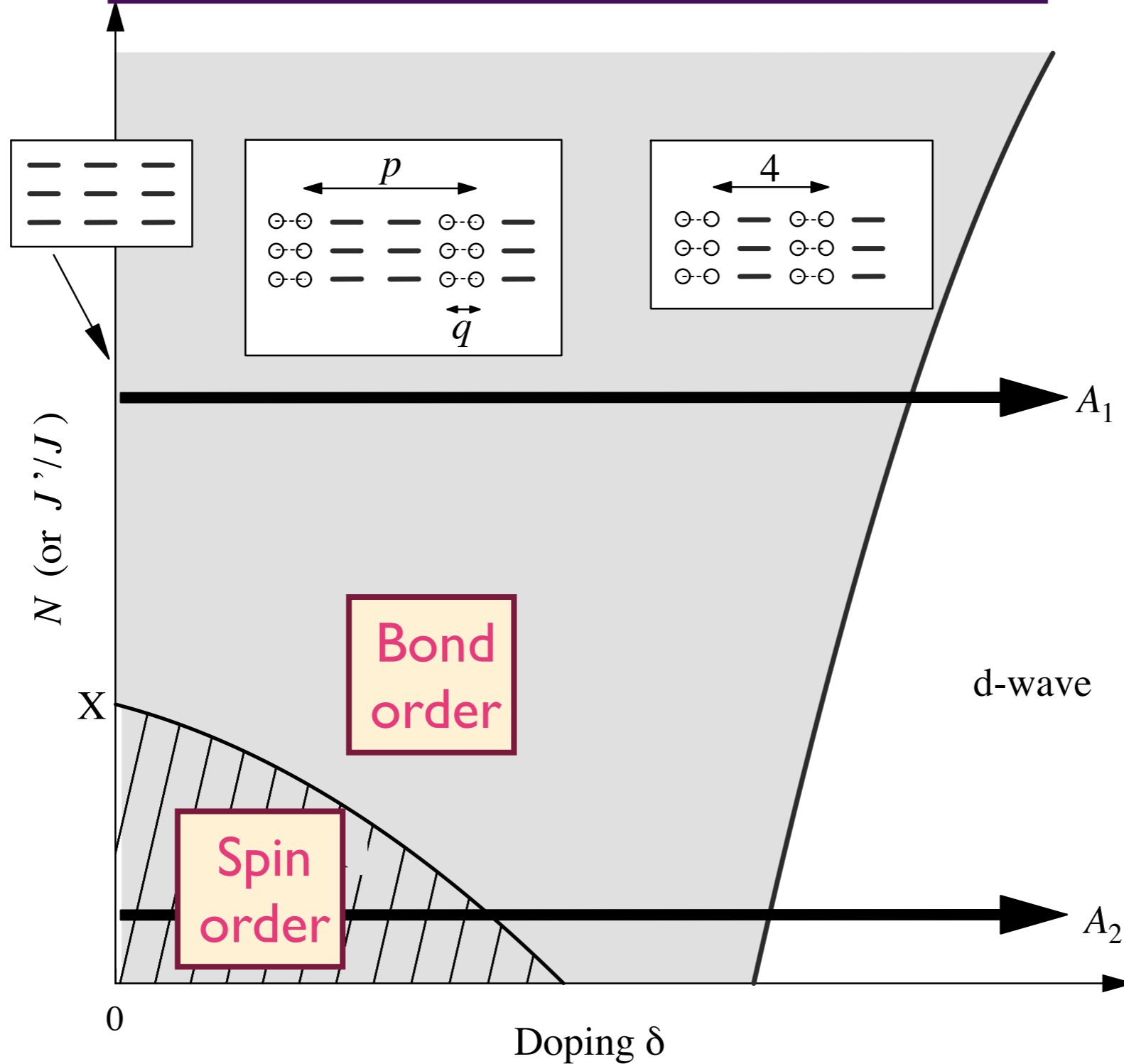
G. Grissonnanche, O. Cyr-Choinière, F. Laliberté, S. René de Cotret, A. Juneau-Fecteau, S. Dufour-Beauséjour, M.-È. Delage, D. LeBoeuf, J. Chang, B. J. Ramshaw, D.A. Bonn, W. N. Hardy, R. Liang, S. Adachi, N. E. Hussey, B. Vignolle, C. Proust, M. Sutherland, S. Krämer, J.-H. Park, D. Graf, N. Doiron-Leyraud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



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 D. Graf, N. Doiron-Leyraud & Louis Taillefer

# 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)

# Main results

- There is an approximate pseudospin symmetry in metals with antiferromagnetic spin correlations.
- The pseudospin partner of *d*-wave superconductivity is an incommensurate *d*-wave bond order

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

T. Holder and W. Metzner, Phys. Rev. B **85**, 165130 (2012)

C. Husemann and W. Metzner, Phys. Rev. B **86**, 085113 (2012)

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

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

# Outline

1. Stability of metal in Hartree-Fock-BCS theory
2. Emergent pseudospin symmetry in low energy theory of metal with antiferromagnetic interactions
3. Quantum Monte Carlo without the sign problem

# Outline

1. Stability of metal in Hartree-Fock-BCS theory

2. Emergent pseudospin symmetry in low energy theory of metal with antiferromagnetic interactions

3. Quantum Monte Carlo without the sign problem

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

Optimize the free energy w.r.t. a mean field Hamiltonian which allows for spin-singlet superconductivity (pairing order  $\Delta_S(\mathbf{k})$ ) and spin-singlet “charge” order ( $\Delta_Q(\mathbf{k})$ ):

$$H_{MF} = - \sum_{i,j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \sum_{\mathbf{k}} \Delta_S(\mathbf{k}) \epsilon_{\alpha\beta} c_{\mathbf{k},\alpha} c_{-\mathbf{k},\beta} + \text{H.c.} \\ + \sum_{\mathbf{k},\mathbf{Q}} \Delta_Q(\mathbf{k}) c_{\mathbf{k}+\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}-\mathbf{Q}/2,\alpha}$$

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

Optimize the free energy w.r.t. a mean field Hamiltonian which allows for spin-singlet superconductivity (pairing order  $\Delta_S(\mathbf{k})$ ) and spin-singlet “charge” order ( $\Delta_Q(\mathbf{k})$ ):

$$H_{MF} = - \sum_{i,j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} + \sum_{\mathbf{k}} \Delta_S(\mathbf{k}) \epsilon_{\alpha\beta} c_{\mathbf{k},\alpha} c_{-\mathbf{k},\beta} + \text{H.c.} \\ + \sum_{\mathbf{k},\mathbf{Q}} \Delta_Q(\mathbf{k}) c_{\mathbf{k}+\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}-\mathbf{Q}/2,\alpha}$$

In real space, the “charge” order  $\Delta_Q(\mathbf{k})$  corresponds to a modulation in local and non-local “density” variables:

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

We obtain purely “bond” order with no modulation in the site density,  $\langle c_{i\alpha}^\dagger c_{i\alpha} \rangle$ , if  $\sum_{\mathbf{k}} \Delta_Q(\mathbf{k}) = 0$ .

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

Optimize the free energy w.r.t. a mean field Hamiltonian which allows for spin-singlet superconductivity (pairing order  $\Delta_S(\mathbf{k})$ ) and spin-singlet “charge” order ( $\Delta_Q(\mathbf{k})$ ):

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

$$F = F_0 + \sum_{\mathbf{k}} \Delta_S^*(\mathbf{k}) \mathcal{M}_S(\mathbf{k}, \mathbf{k}') \Delta_S(\mathbf{k}') \\ + \sum_{\mathbf{k},\mathbf{Q}} \Delta_Q^*(\mathbf{k}) \mathcal{M}_Q(\mathbf{k}, \mathbf{k}') \Delta_Q(\mathbf{k}')$$

Due to pseudospin symmetry, the kernels have identical forms:

$$\mathcal{M}_S(\mathbf{k}, \mathbf{k}') = \Pi_S(\mathbf{k}) \left[ \delta_{\mathbf{k}, \mathbf{k}'} - \frac{3}{V} J(\mathbf{k} - \mathbf{k}') \Pi_S(\mathbf{k}') \right]$$

$$\mathcal{M}_Q(\mathbf{k}, \mathbf{k}') = \Pi_Q(\mathbf{k}) \left[ \delta_{\mathbf{k}, \mathbf{k}'} - \frac{3}{V} J(\mathbf{k} - \mathbf{k}') \Pi_Q(\mathbf{k}') \right]$$

The pseudospin symmetry is broken only by the differing forms of the polarizabilities of fermions with dispersion  $\varepsilon(\mathbf{k})$ .

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

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

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$$\mathcal{M}_Q(\mathbf{k}, \mathbf{k}') = \Pi_Q(\mathbf{k}) \left[ \delta_{\mathbf{k}, \mathbf{k}'} - \frac{3}{V} J(\mathbf{k} - \mathbf{k}') \Pi_Q(\mathbf{k}') \right]$$

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We diagonalized  $J(\mathbf{k} - \mathbf{k}')\Pi_S(\mathbf{k}')$  and  $J(\mathbf{k} - \mathbf{k}')\Pi_Q(\mathbf{k}')$  and obtained the lowest eigenvalues  $\lambda_S$  and  $\lambda_Q$  and the corresponding right eigenvectors  $\Delta_S(\mathbf{k})$  and  $\Delta_Q(\mathbf{k})$ .

Due to pseudospin symmetry, the kernels have identical forms:

$$\mathcal{M}_S(\mathbf{k}, \mathbf{k}') = \Pi_S(\mathbf{k}) \left[ \delta_{\mathbf{k}, \mathbf{k}'} - \frac{3}{V} J(\mathbf{k} - \mathbf{k}') \Pi_S(\mathbf{k}') \right]$$

$$\mathcal{M}_Q(\mathbf{k}, \mathbf{k}') = \Pi_Q(\mathbf{k}) \left[ \delta_{\mathbf{k}, \mathbf{k}'} - \frac{3}{V} J(\mathbf{k} - \mathbf{k}') \Pi_Q(\mathbf{k}') \right]$$

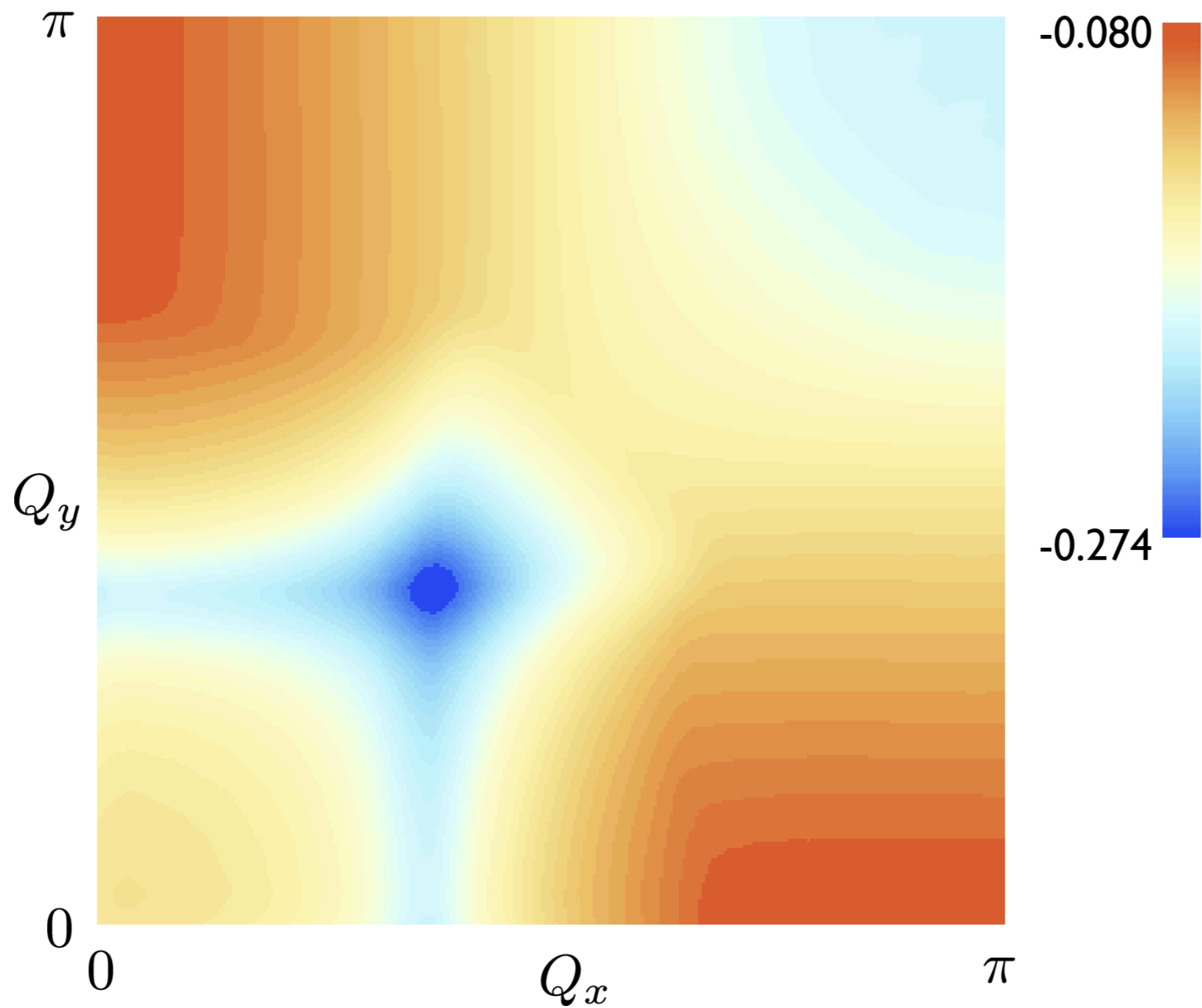
The pseudospin symmetry is broken only by the differing forms of the polarizabilities of fermions with dispersion  $\varepsilon(\mathbf{k})$ .

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

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

We diagonalized  $J(\mathbf{k} - \mathbf{k}')\Pi_S(\mathbf{k}')$  and  $J(\mathbf{k} - \mathbf{k}')\Pi_Q(\mathbf{k}')$  and obtained the lowest eigenvalues  $\lambda_S$  and  $\lambda_Q$  and the corresponding right eigenvectors  $\Delta_S(\mathbf{k})$  and  $\Delta_Q(\mathbf{k})$ .

The smallest eigenvalue was always  $\lambda_S$  with with eigenvector  $\Delta_S(k) = \Delta_0(\cos k_x - \cos k_y) + \dots$



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

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

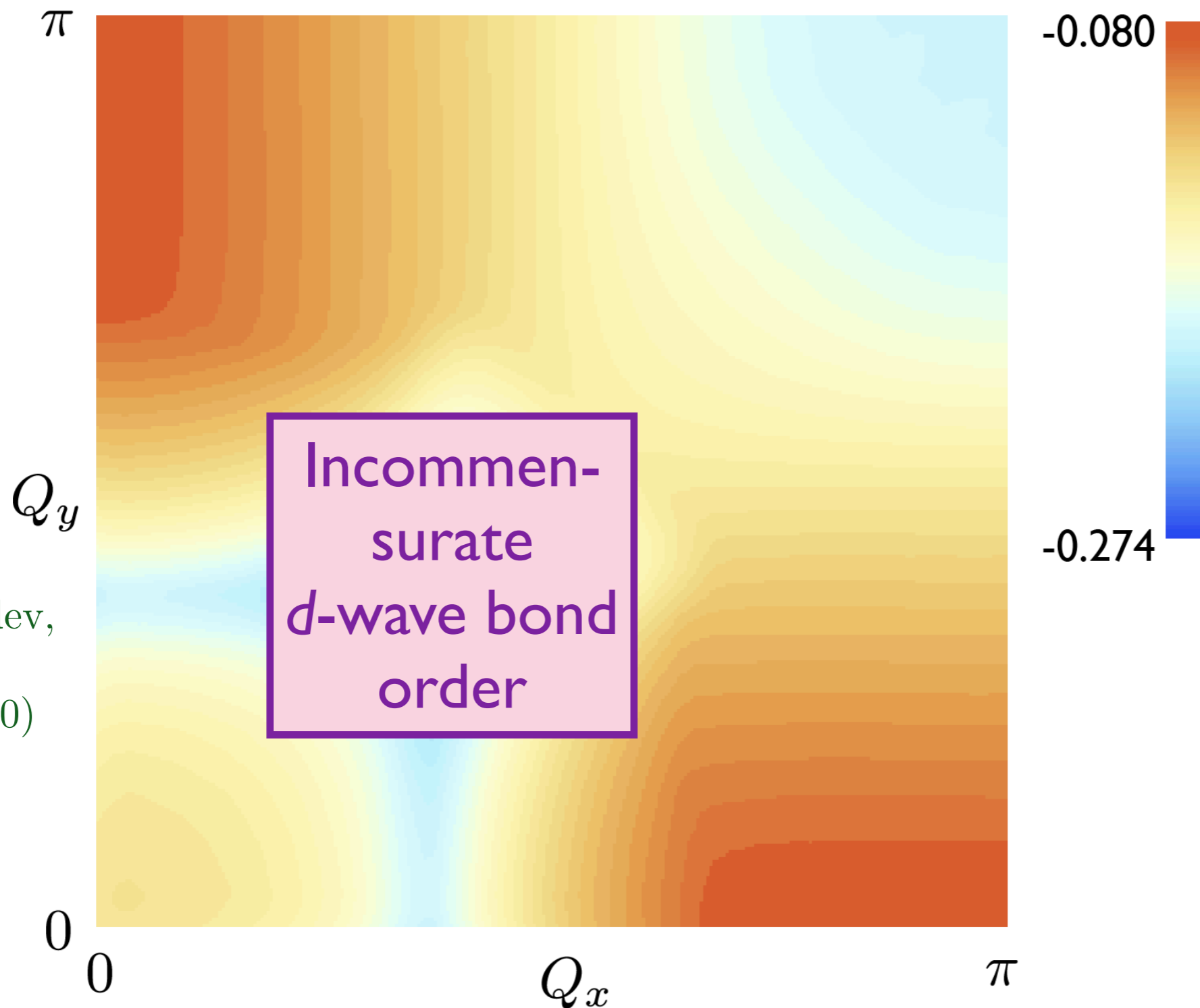
$\gamma$	$\psi_{\gamma}(\mathbf{k})$	$Q =$ (1.15, 1.15)	$Q =$ (1.15, 0)	$Q =$ (0, 0)	$Q =$ ( $\pi, \pi$ )	$\Delta_S(\mathbf{k})$
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$s'$	$\cos k_x + \cos k_y$	0	0.044	0	0	0
$s''$	$\cos(2k_x) + \cos(2k_y)$	0	-0.046	0	0	0
$d$	$\cos k_x - \cos k_y$	0.993	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

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

$\gamma$	$\psi_{\gamma}(\mathbf{k})$	$Q =$ (1.15, 1.15)	$Q =$ (1.15, 0)	$Q =$ (0, 0)	$Q =$ ( $\pi, \pi$ )	$\Delta_S(\mathbf{k})$
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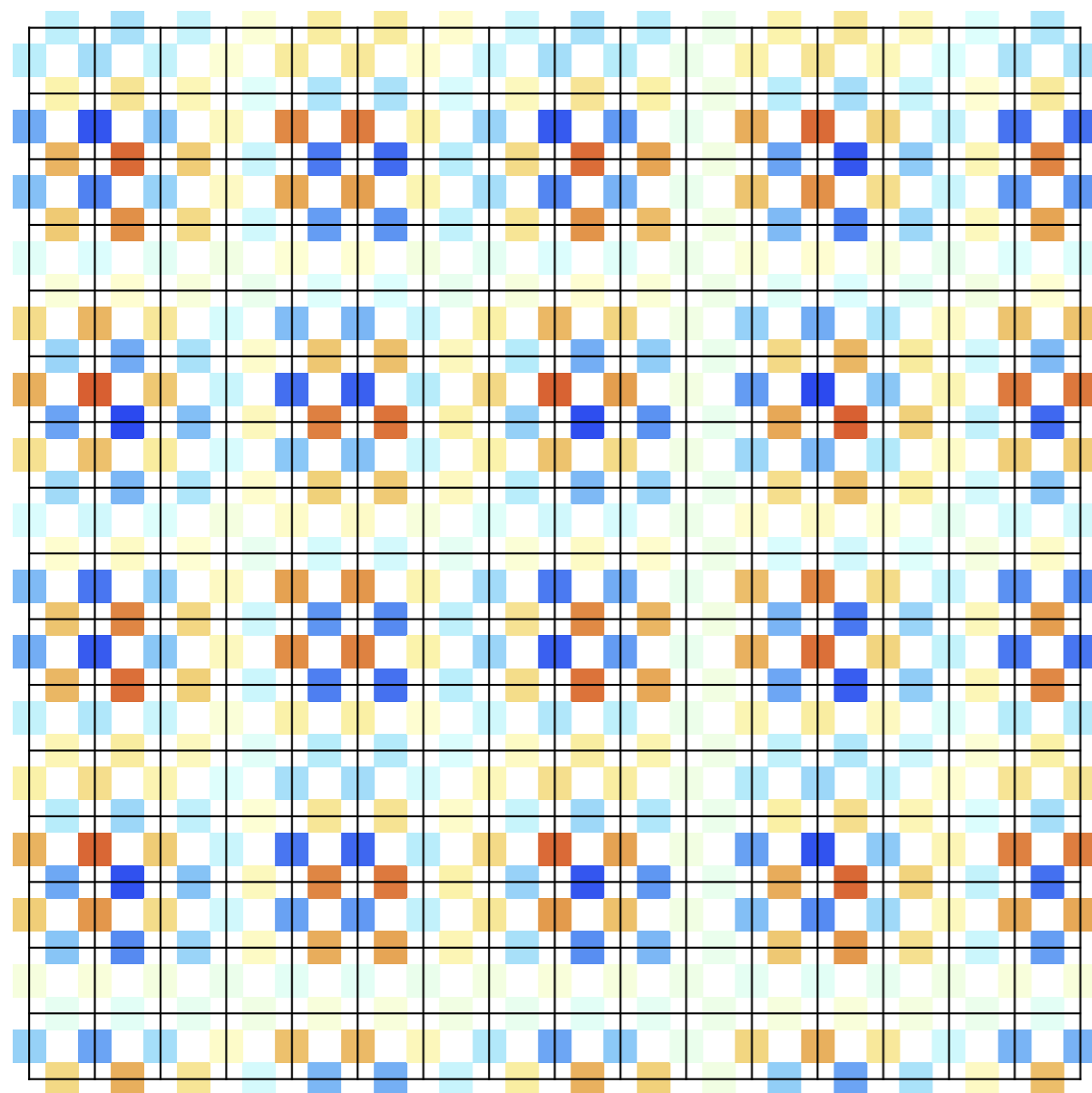
## Charge-ordering eigenvector



M. A. Metlitski and S. Sachdev,  
 Phys. Rev. B  
**82**, 075128 (2010)

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

# 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)

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

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

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

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

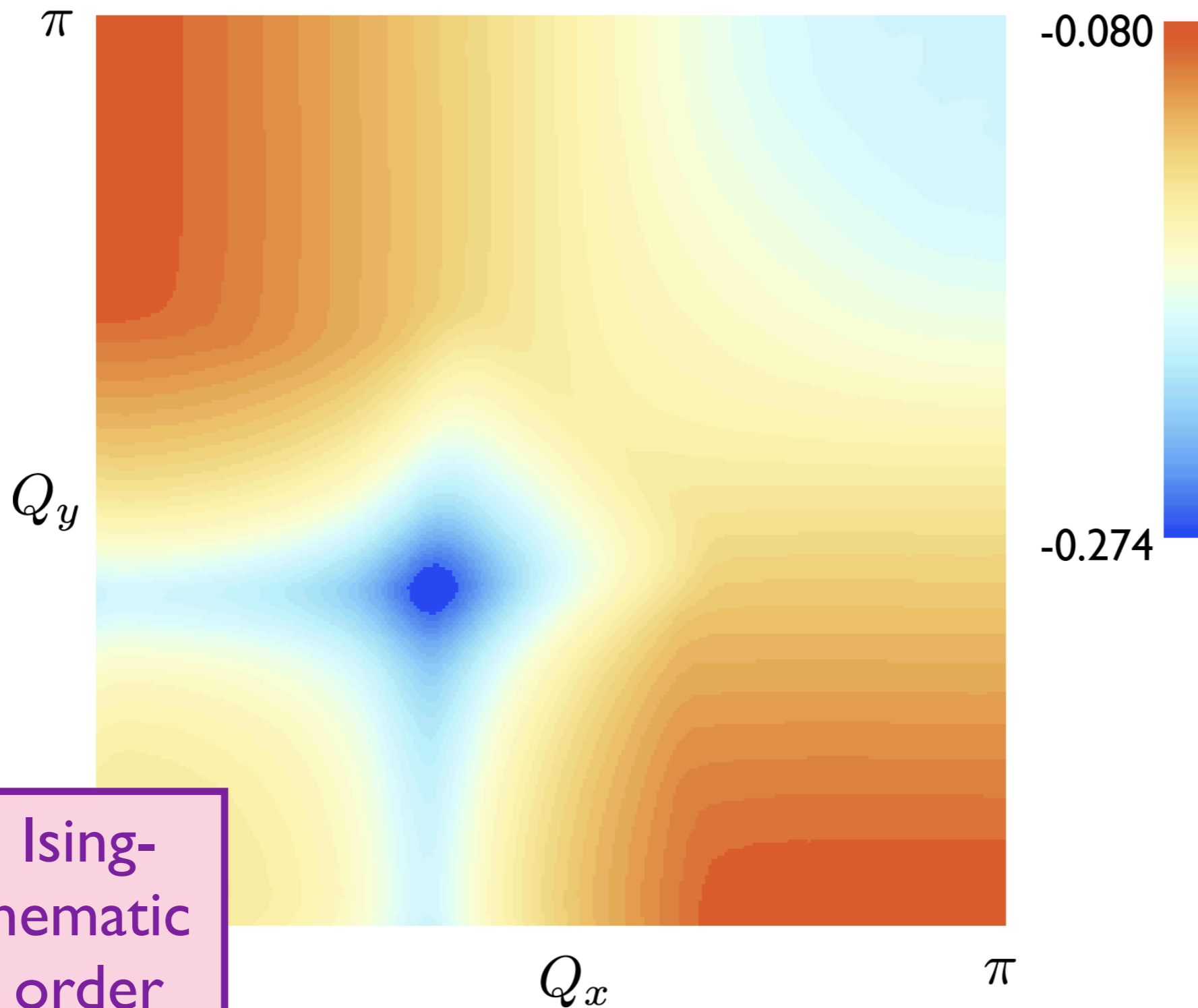
$$\Delta_Q(\mathbf{k}) = \sum_{\gamma} c_{Q,\gamma} \psi_{\gamma}(\mathbf{k})$$

$\gamma$	$\psi_{\gamma}(\mathbf{k})$	$Q =$ (1.15, 1.15)	$Q =$ (1.15, 0)	$Q =$ (0, 0)	$Q =$ ( $\pi, \pi$ )	$\Delta_S(\mathbf{k})$
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## Charge-ordering eigenvector

S. A. Kivelson,  
E. Fradkin, and  
V. J. Emery,  
Nature **393**, 550  
(1998).  
H. Yamase and  
H. Kohno, J.  
Phys. Soc. Jpn.  
**69**, 2151 (2000).  
C. J. Halboth  
and W. Metz-  
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Lett. **85**, 5162  
(2000).

Ising-  
nematic  
order

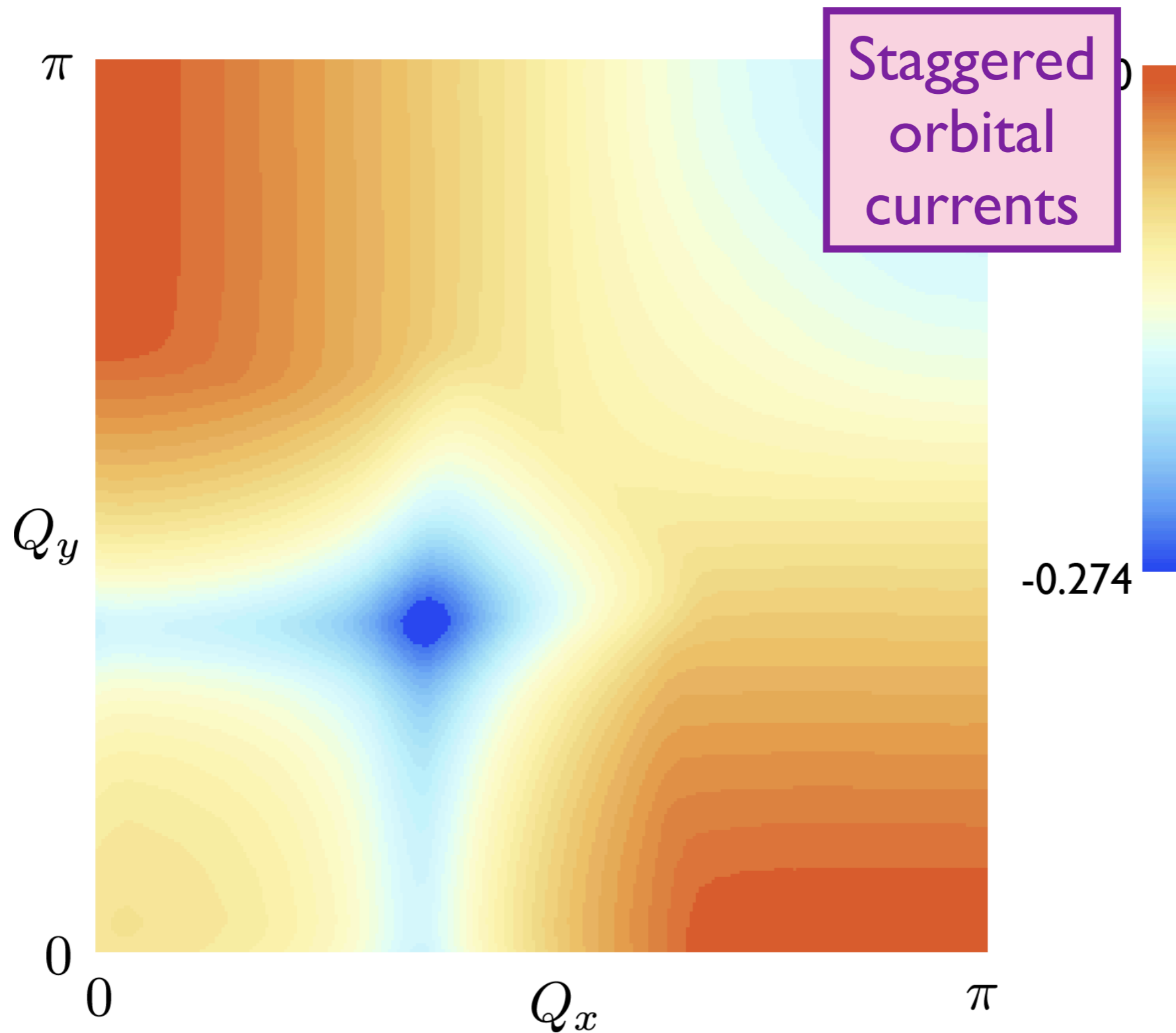


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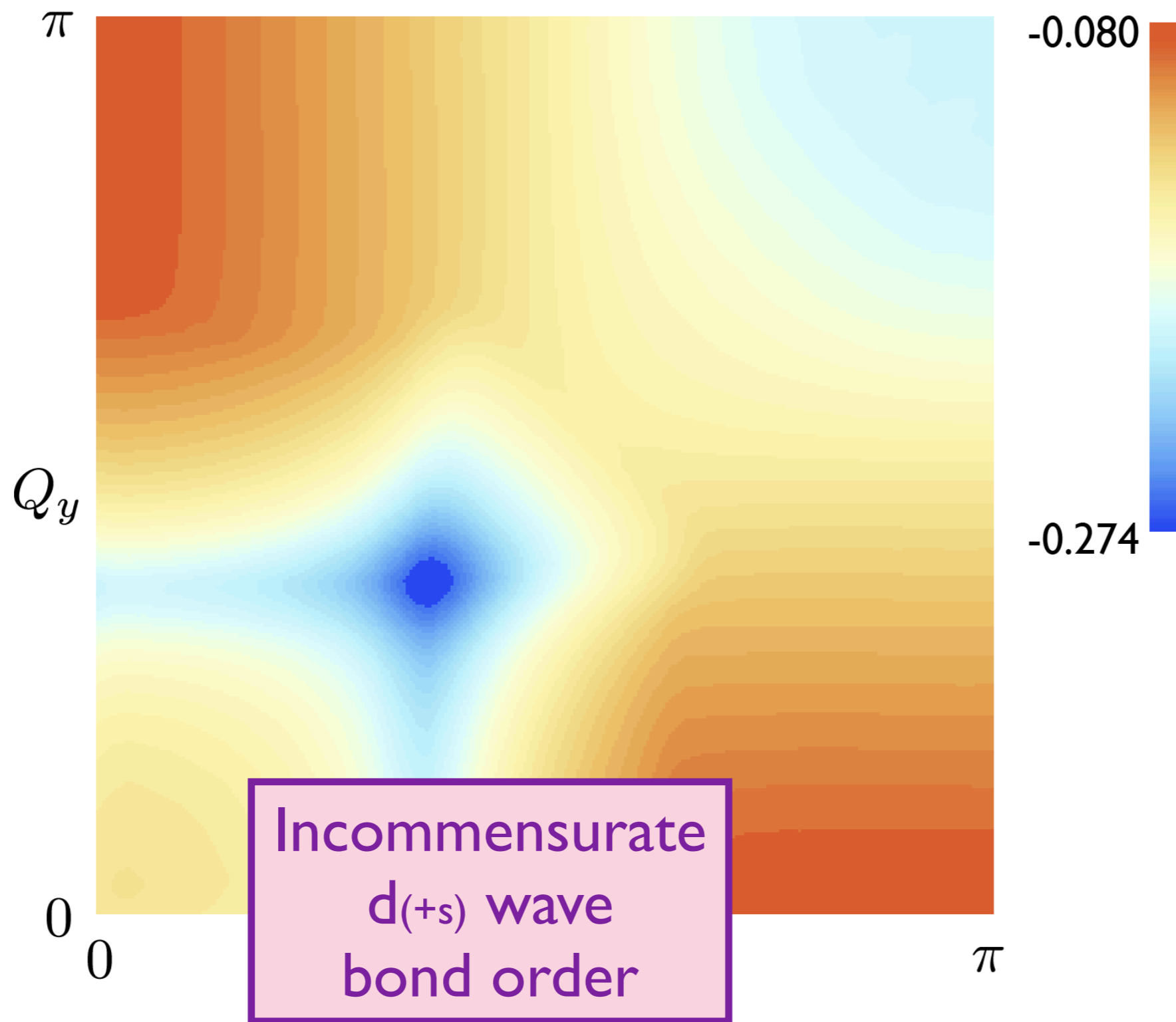
S. Chakravarty,  
R. B. Laughlin, D. K. Morr,  
and C. Nayak,  
*Phys. Rev. B* **63**, 094503 (2001).  
Also the related  
staggered-flux  
liquid of X.-G. Wen  
and P. A. Lee,  
*Phys. Rev. Lett.* **76**, 503 (1996).

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

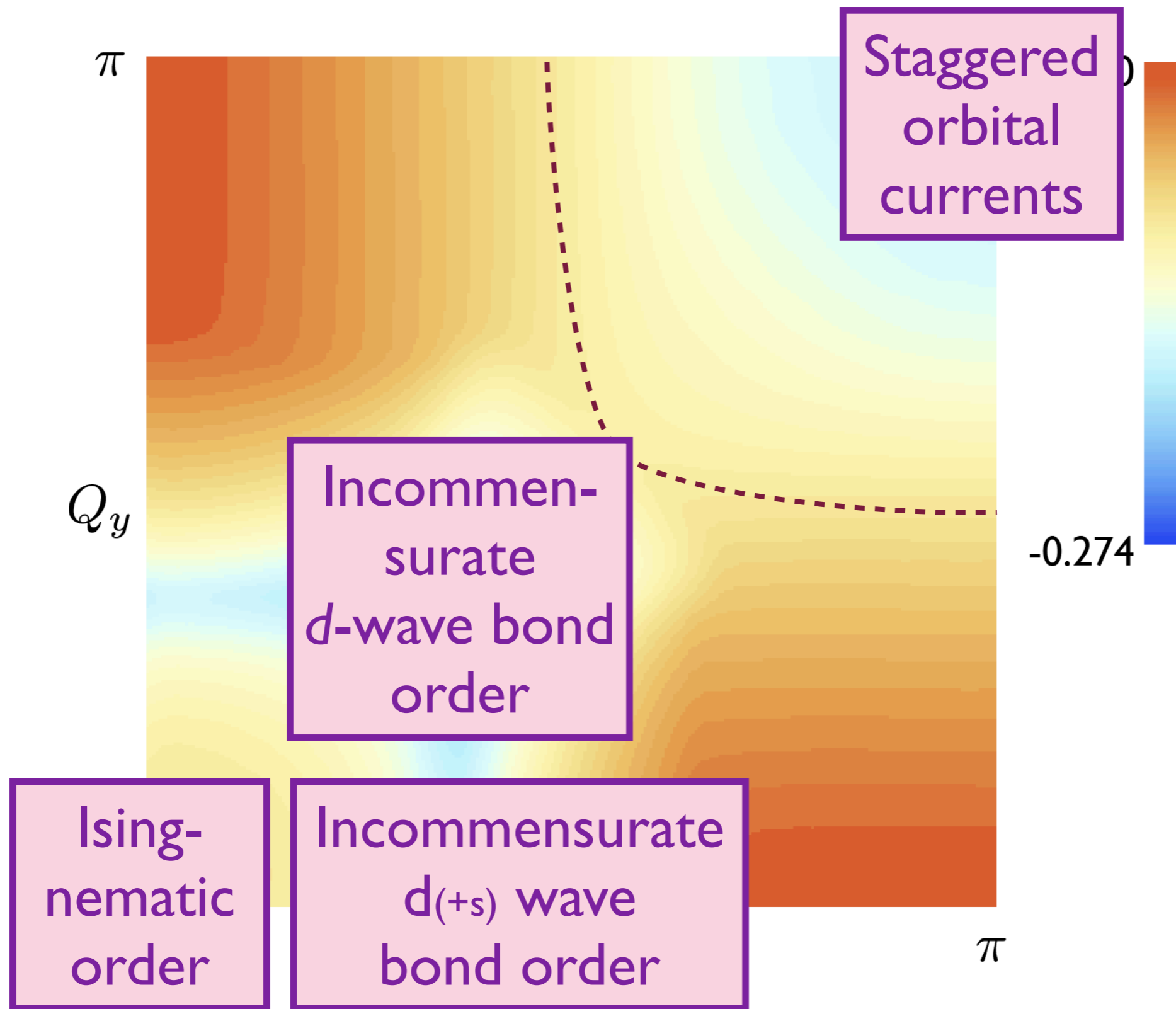
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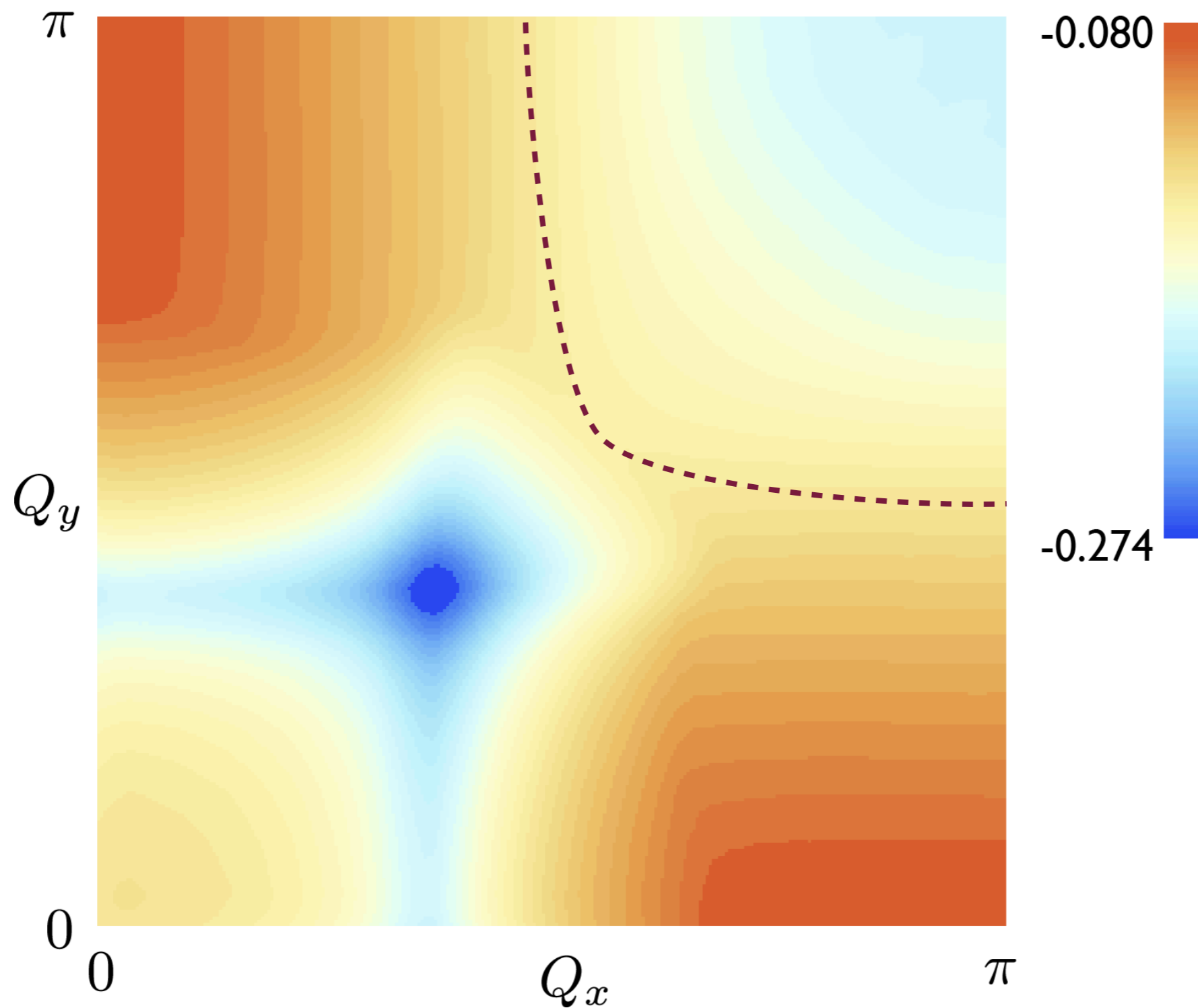
## Charge-ordering eigenvector



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



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



What determines the  $\mathbf{Q}$  at which  $\lambda_{\mathbf{Q}}$  is a minimum ?

# Outline

1. Stability of metal in Hartree-Fock-BCS theory
2. Emergent pseudospin symmetry in low energy theory of metal with antiferromagnetic interactions
3. Quantum Monte Carlo without the sign problem

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1. Stability of metal in Hartree-Fock-BCS theory

2. Emergent pseudospin symmetry in low energy theory of metal with antiferromagnetic interactions

3. Quantum Monte Carlo without the sign problem

## Pseudospin symmetry of the exchange interaction

$$H_J = \sum_{i<j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

with  $\vec{S}_i = \frac{1}{2} c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\beta}$  is the antiferromagnetic exchange interaction. Introduce the Nambu spinor

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

Then we can write

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

which is invariant under the SU(2) pseudospin transformations

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

This pseudospin symmetry is important in classifying spin liquid ground states of  $H_J$ .

- I. Affleck, Z. Zou, T. Hsu, and P. W. Anderson, Phys. Rev. B **38**, 745 (1988)
- E. Dagotto, E. Fradkin, and A. Moreo, Phys. Rev. B **38**, 2926 (1988)
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## Pseudospin symmetry of the exchange interaction

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

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- E. Dagotto, E. Fradkin, and A. Moreo, Phys. Rev. B **38**, 2926 (1988)
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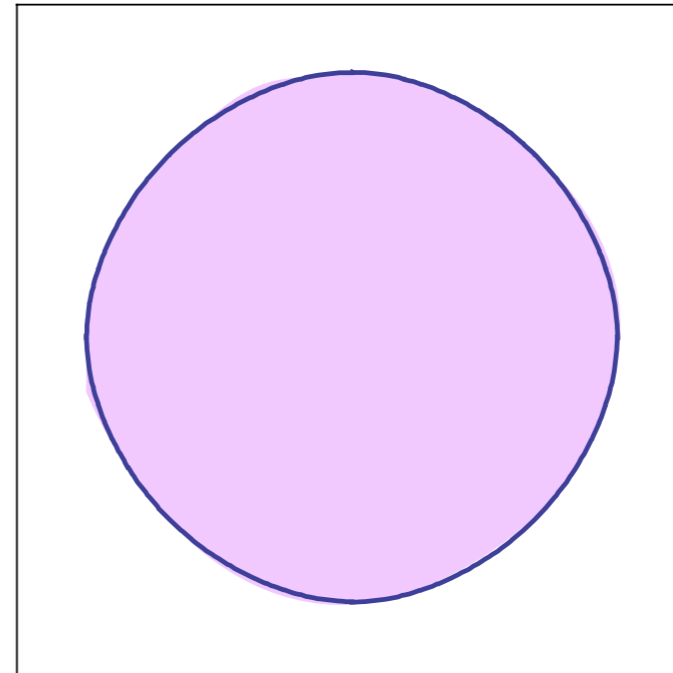
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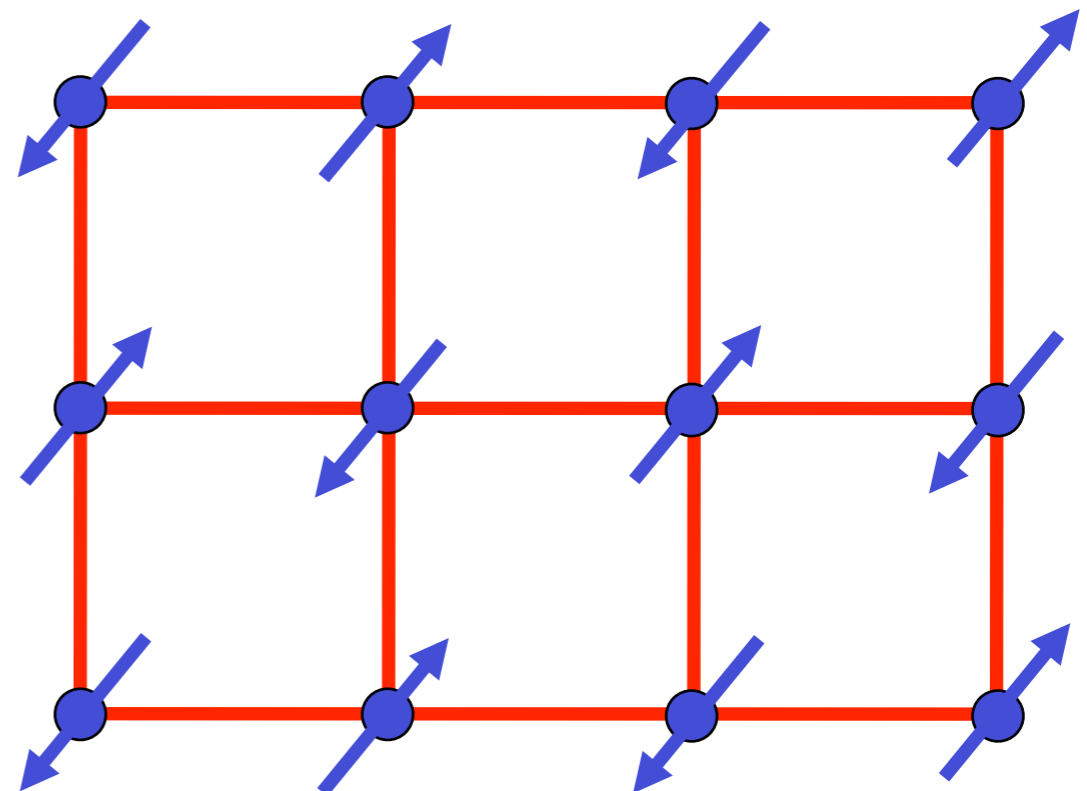
We will start with the Néel state, and find important consequences of the pseudospin symmetry in metals with antiferromagnetic correlations.

# Fermi surface+antiferromagnetism

Metal with “large”  
Fermi surface



+

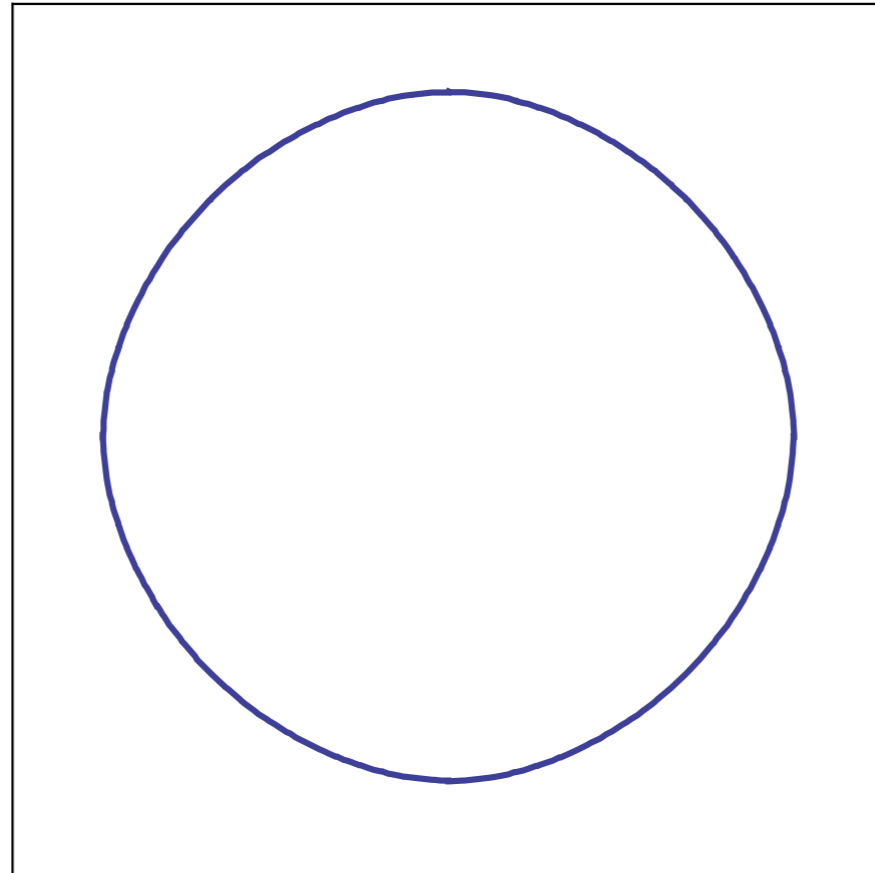


The electron spin polarization obeys

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

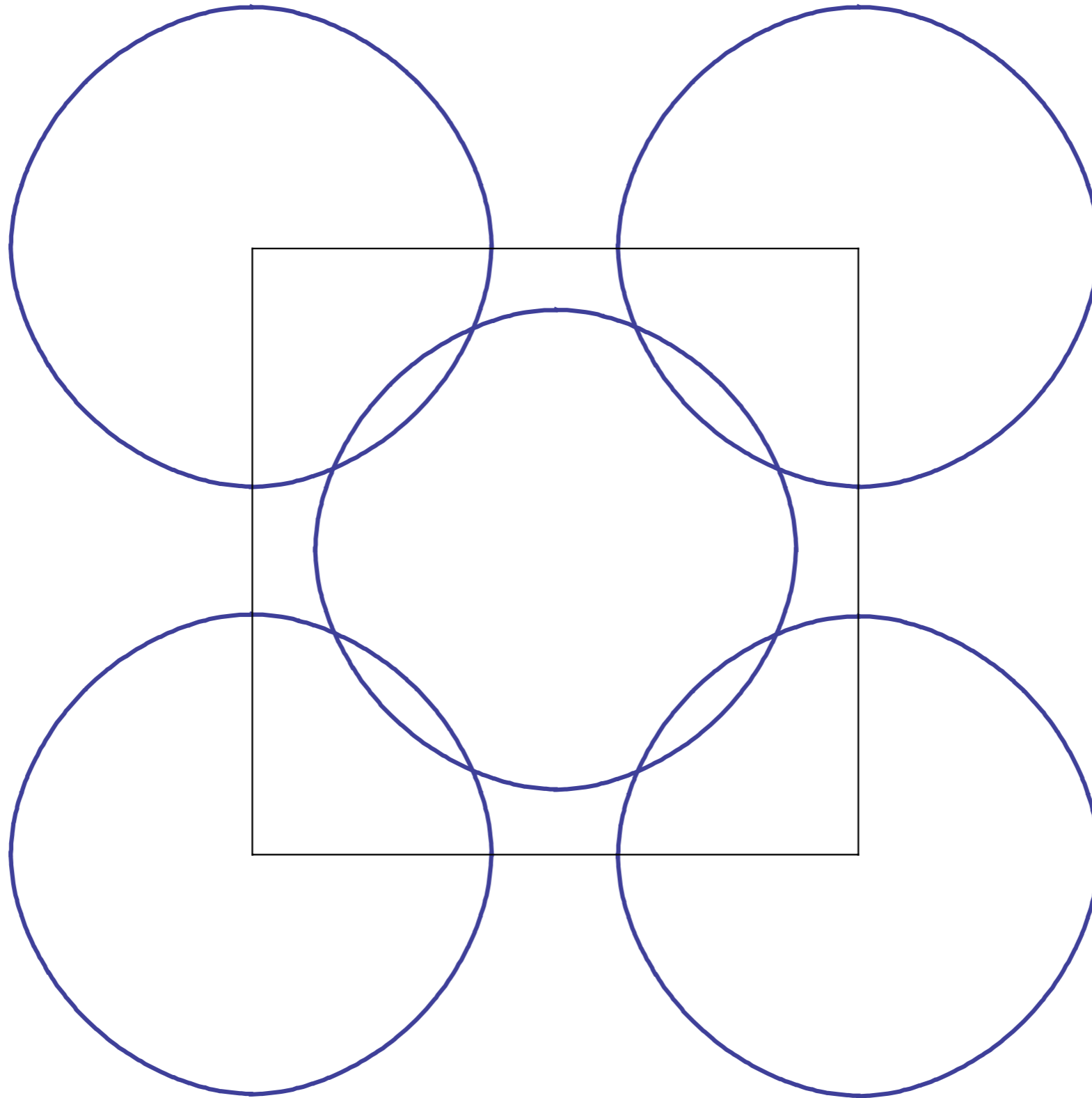
where  $\mathbf{K}$  is the ordering wavevector.

# Fermi surface+antiferromagnetism



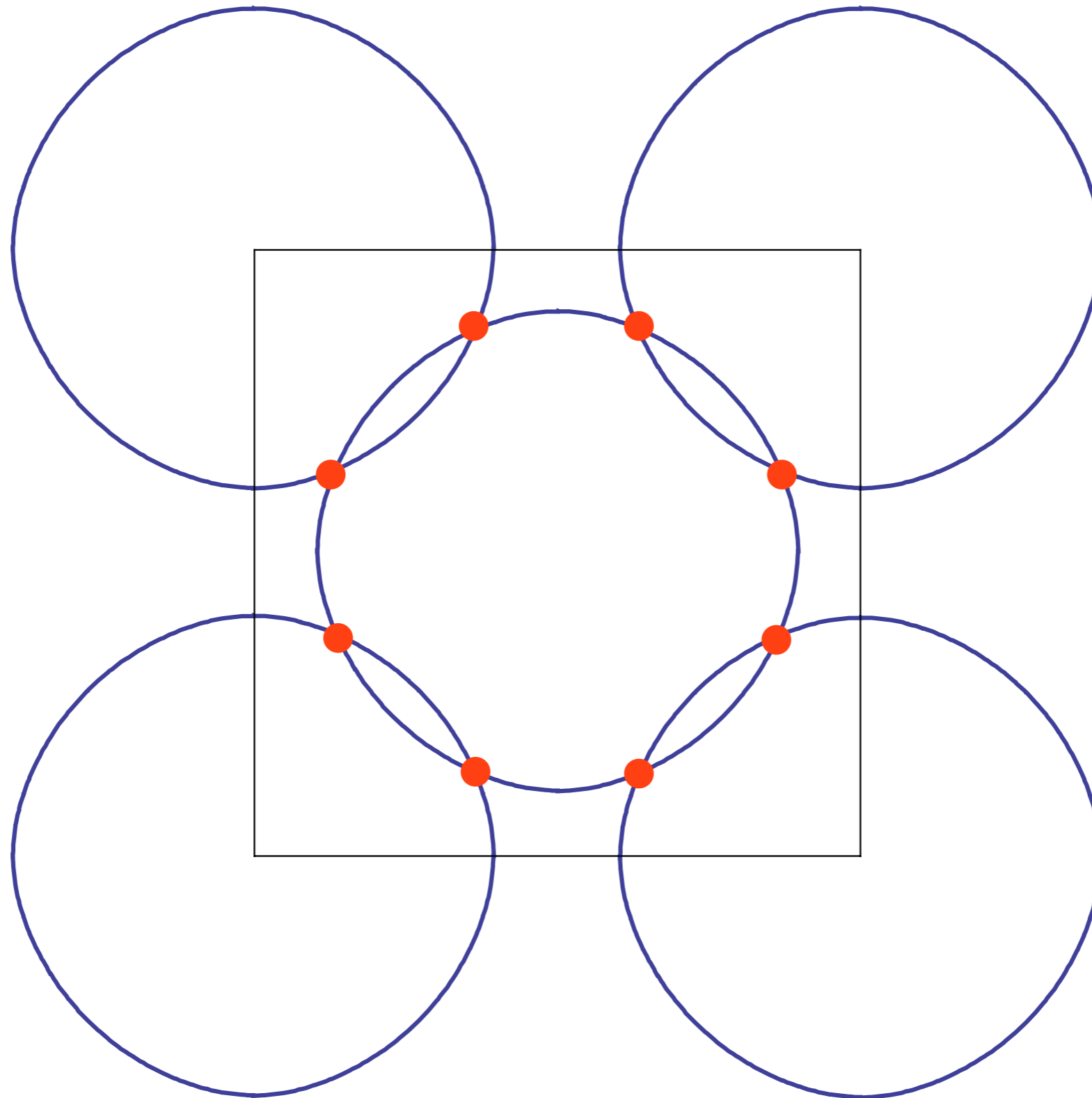
**Metal with “large” Fermi surface**

# Fermi surface+antiferromagnetism



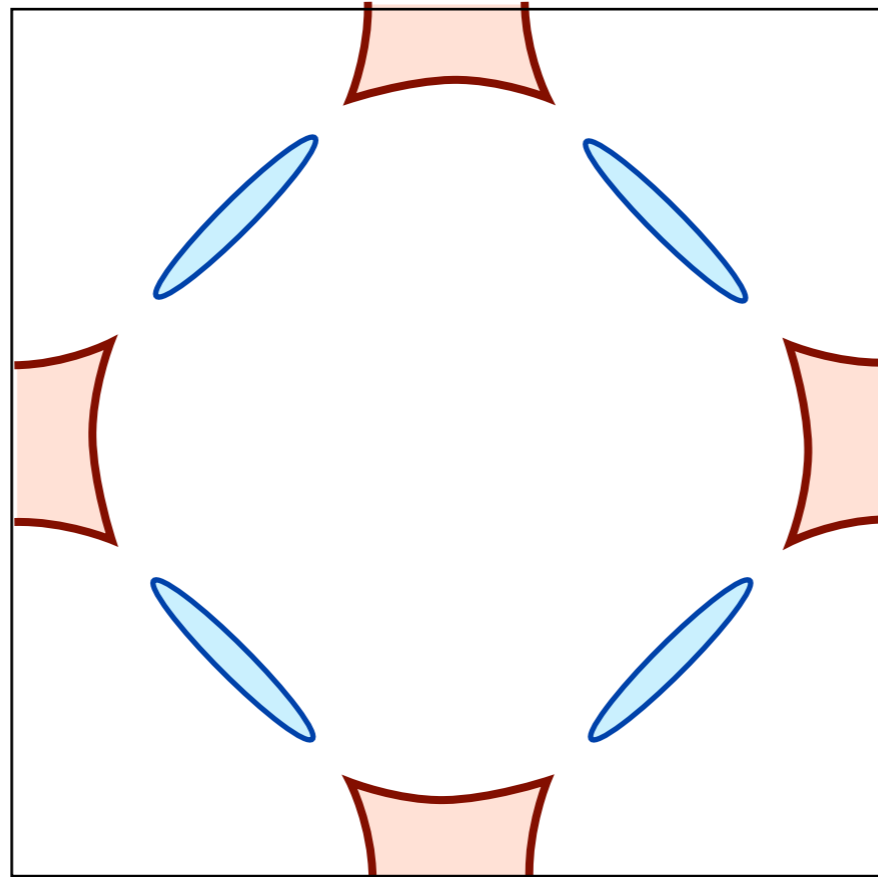
Fermi surfaces translated by  $\mathbf{K} = (\pi, \pi)$ .

# Fermi surface+antiferromagnetism



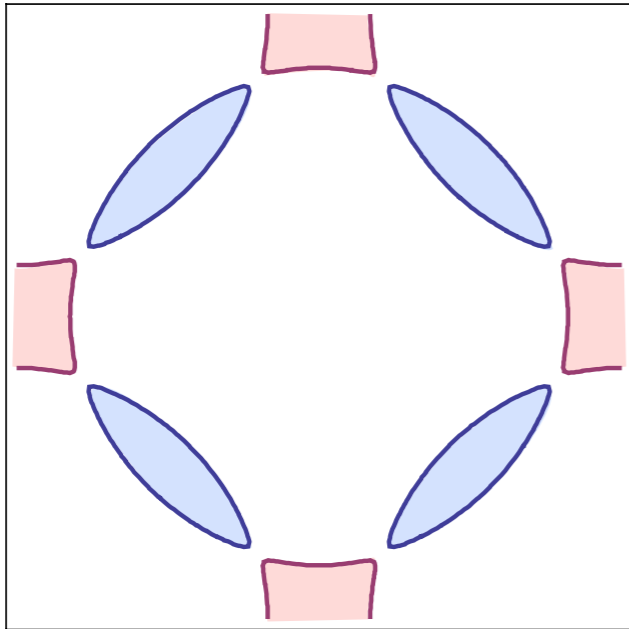
**“Hot” spots**

# Fermi surface+antiferromagnetism



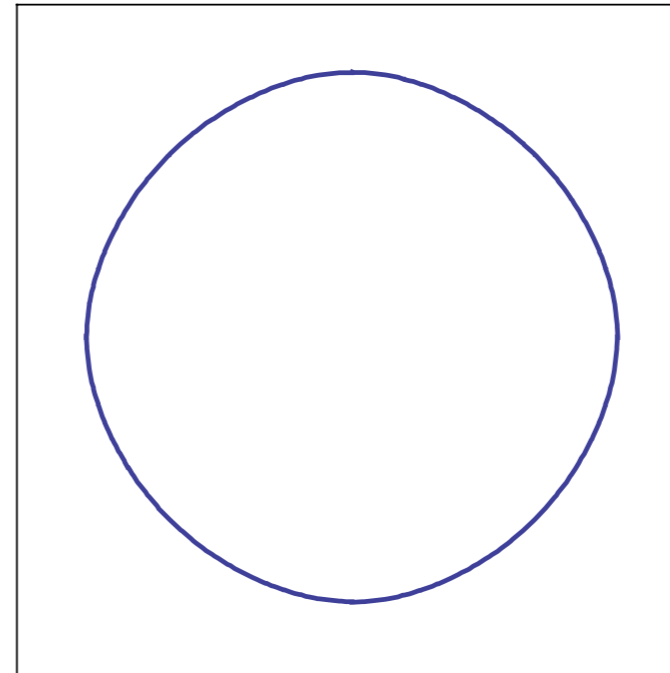
Electron and hole pockets in  
antiferromagnetic phase  
with antiferromagnetic order parameter  $\langle \vec{\varphi} \rangle \neq 0$

# Fermi surface+antiferromagnetism



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

Metal with electron  
and hole pockets

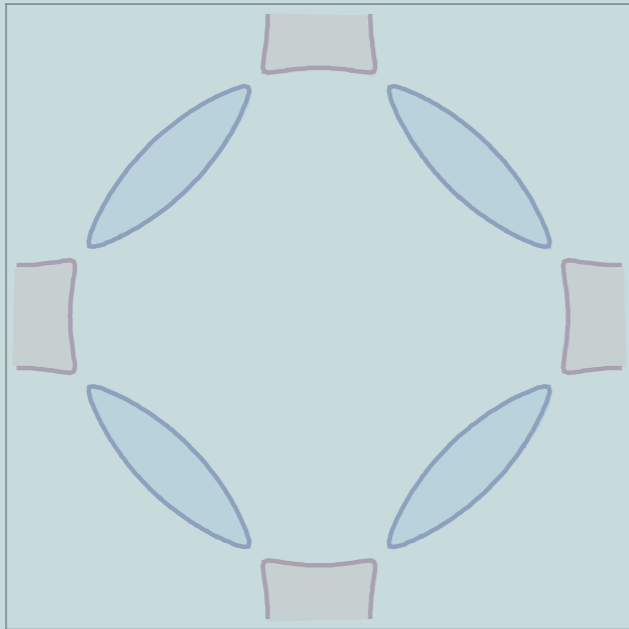


$$\langle \vec{\varphi} \rangle = 0$$

Metal with “large”  
Fermi surface

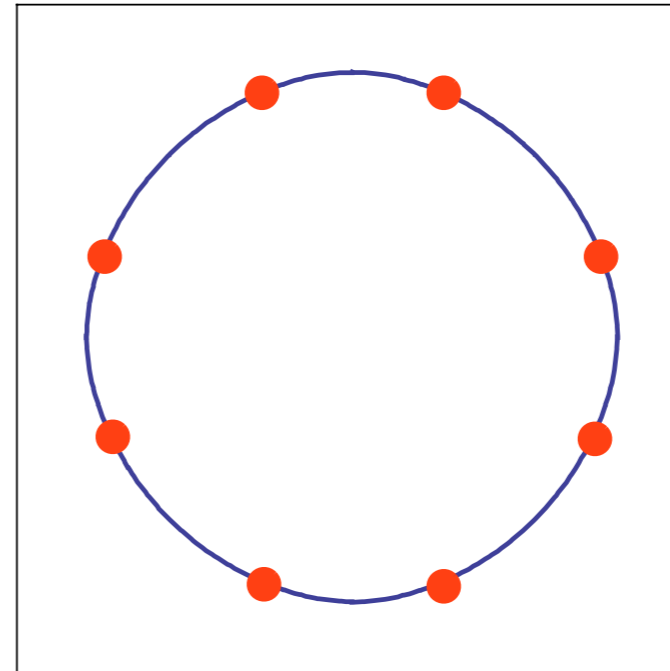
$r$

# Fermi surface+antiferromagnetism



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

Metal with electron  
and hole pockets



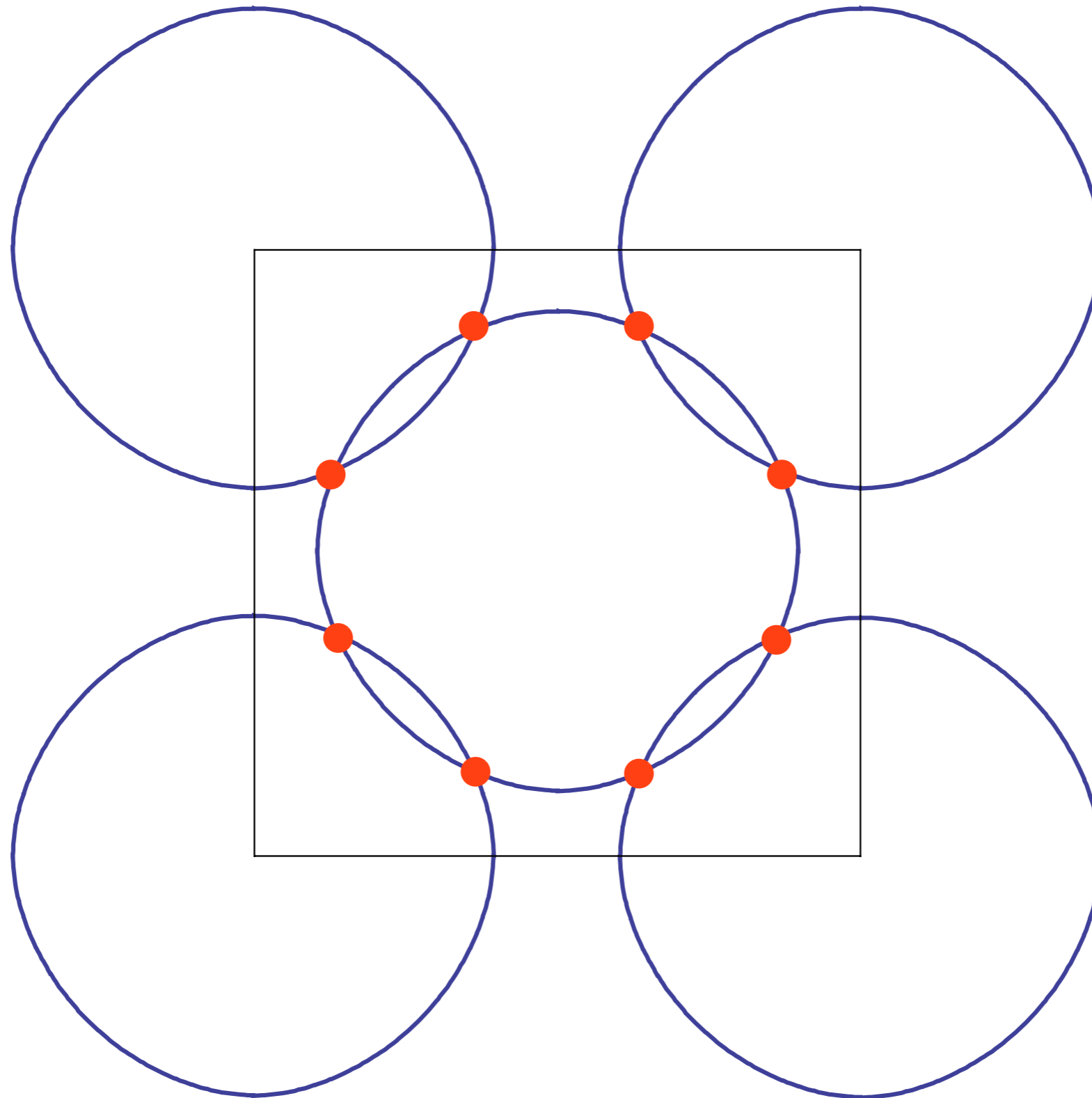
$$\langle \vec{\varphi} \rangle = 0$$

Metal with “large”  
Fermi surface

Focus of  
this talk

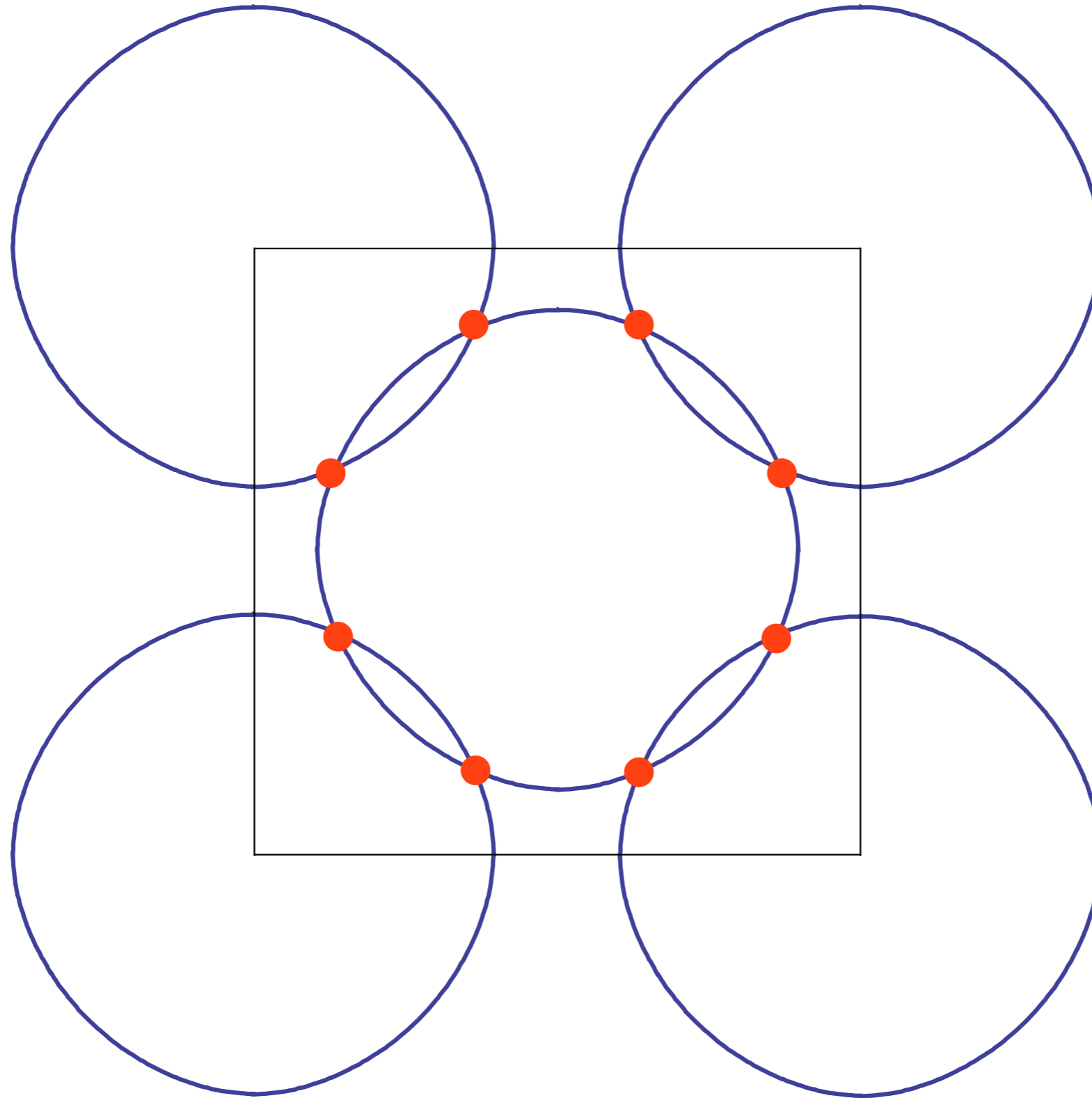
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# Fermi surface+antiferromagnetism



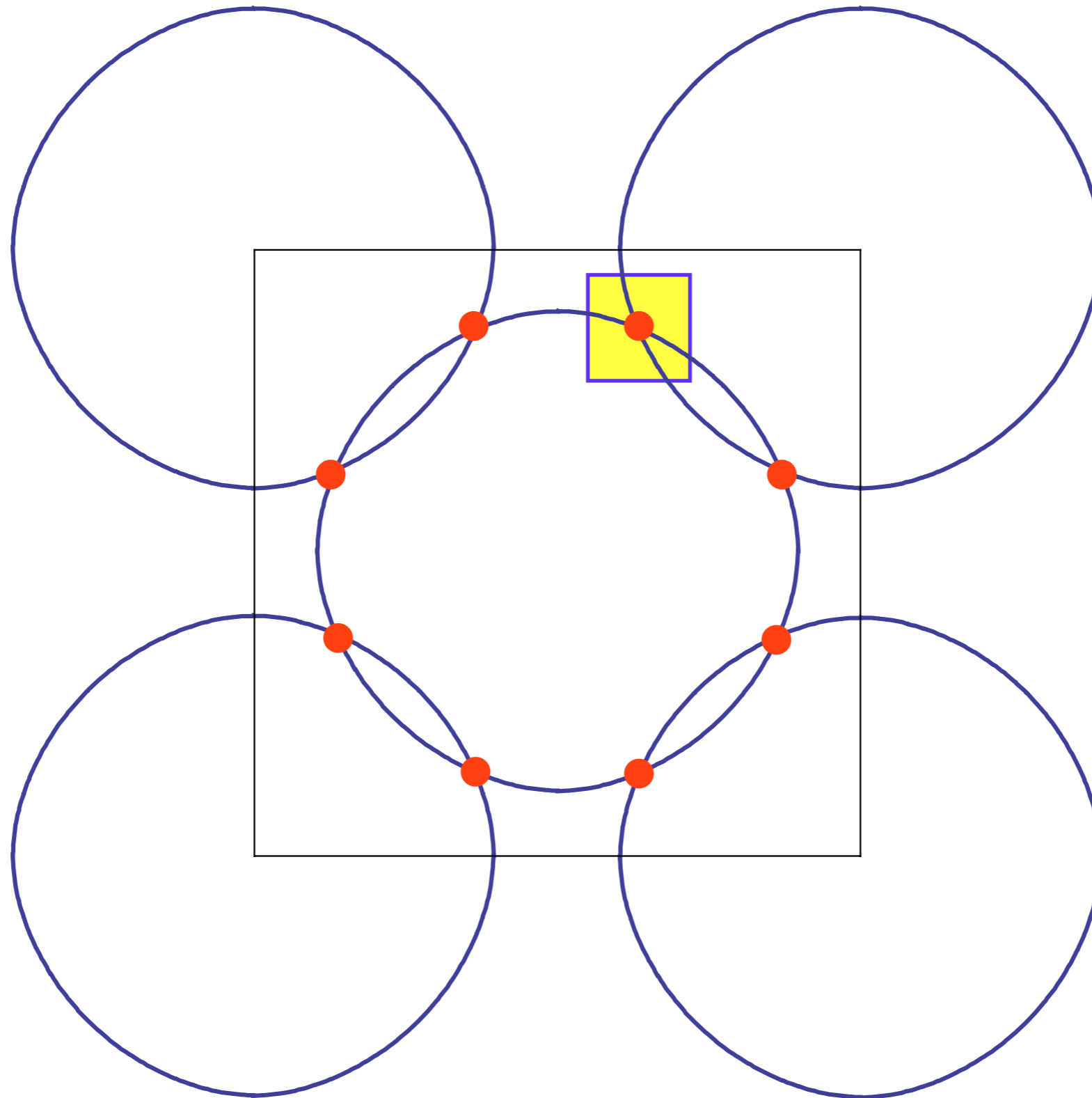
**“Hot” spots**

# Fermi surface+antiferromagnetism



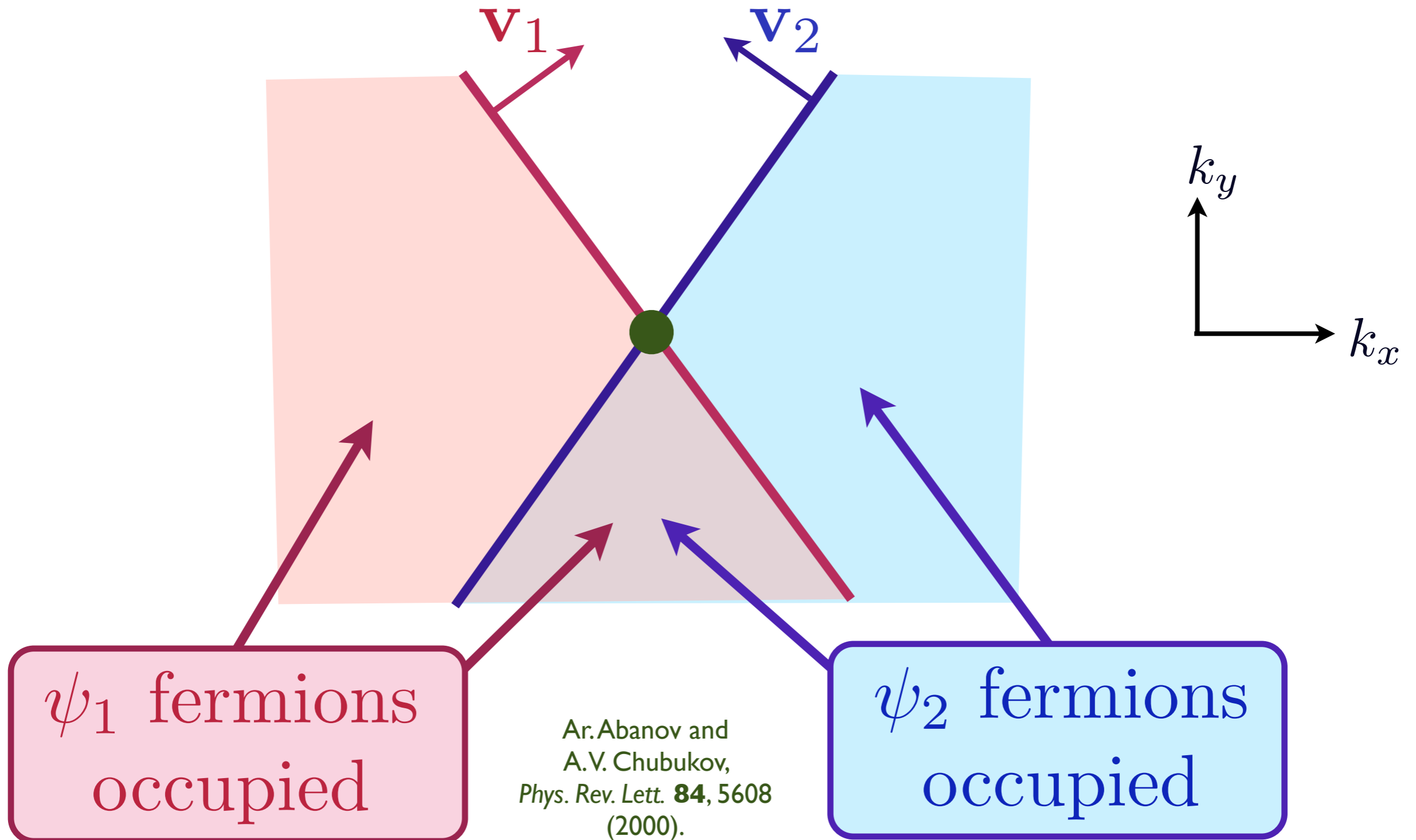
**Low energy theory for critical point near hot spots**

# Fermi surface+antiferromagnetism

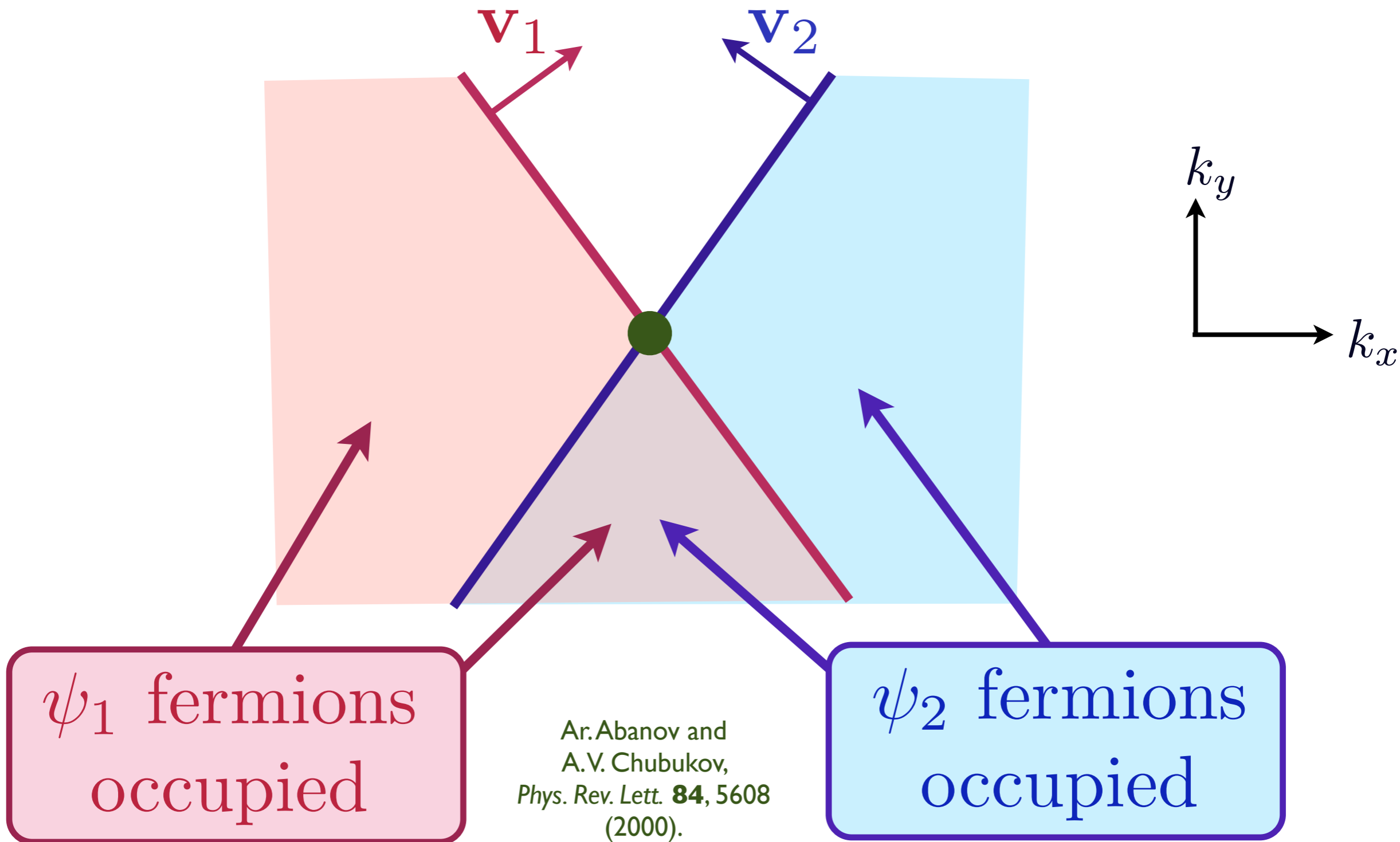


**Low energy theory for critical point near hot spots**

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



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



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This low-energy theory is invariant under independent SU(2) pseudospin rotations on each pair of hot-spots: there is a global SU(2)<sup>4</sup> symmetry, and  $\Pi_S(\mathbf{k}) = \Pi_Q(\mathbf{k})$  near the hot spots.

$\psi_1$  fermions occupied

$\psi_2$  fermions occupied

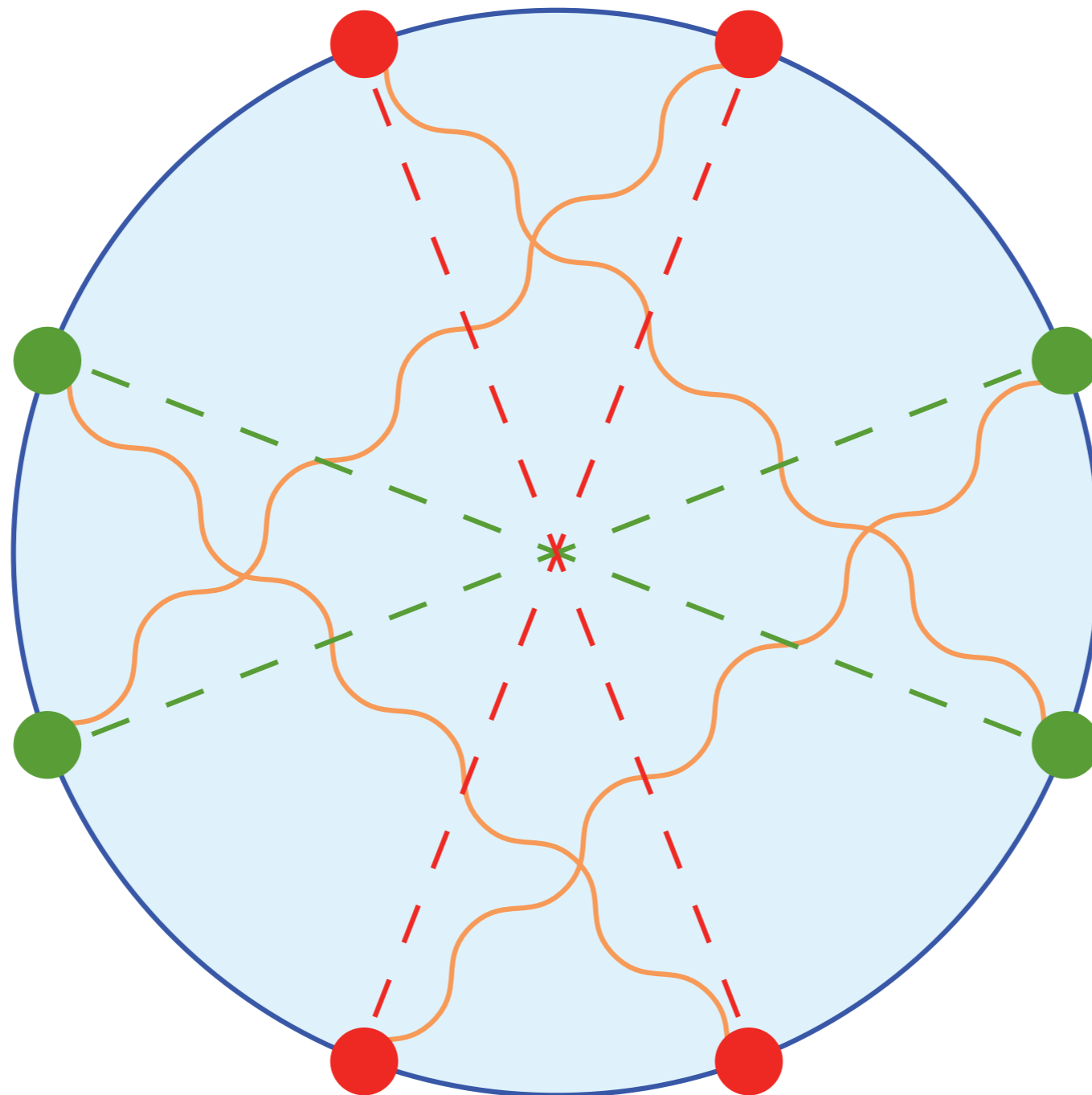
M.A. Metlitski and S. Sachdev, Phys. Rev. B **85**, 075127 (2010)

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)



Unconventional pairing at and near hot spots

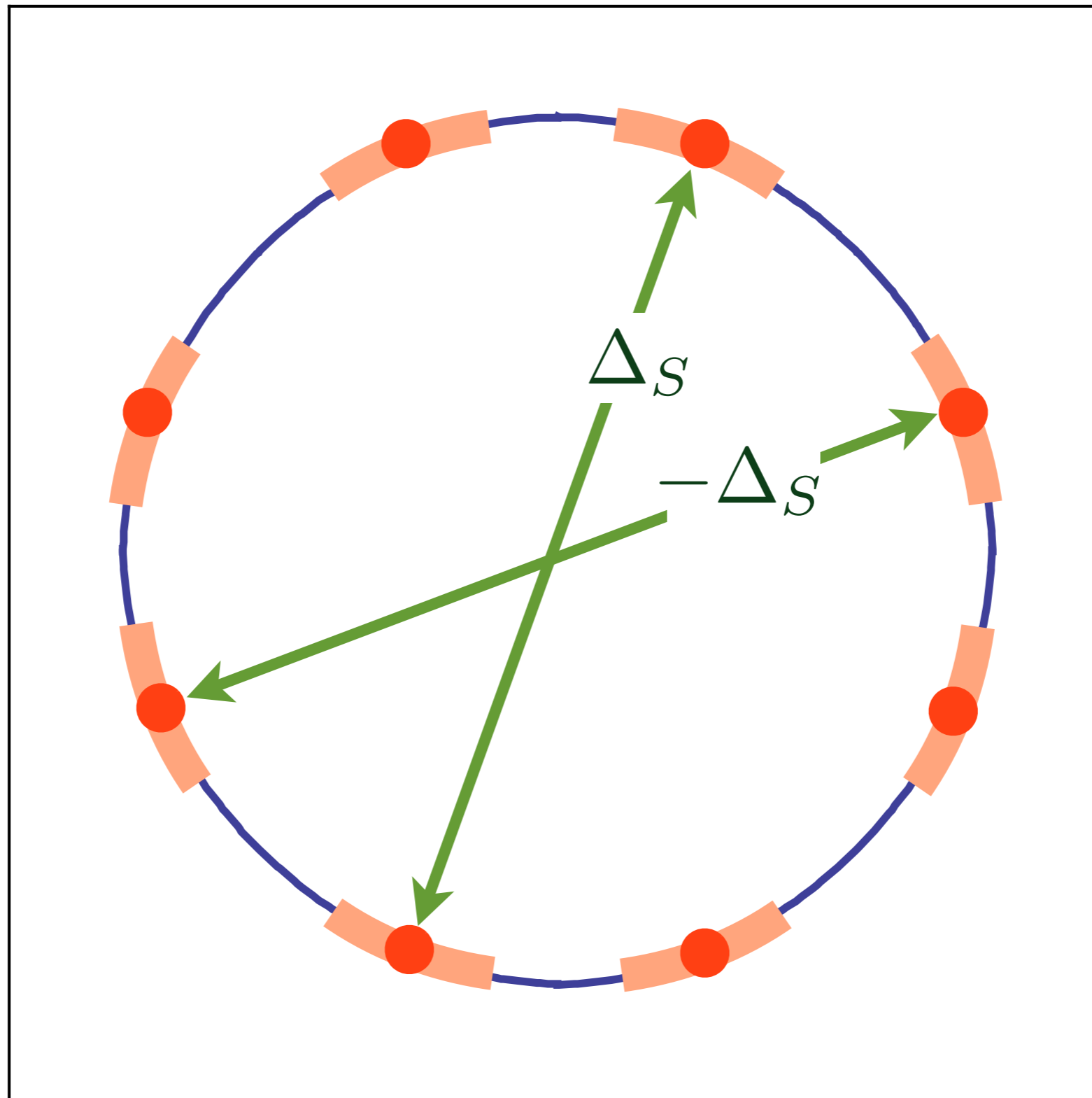
$$\langle c_{\mathbf{k}\alpha}^\dagger c_{-\mathbf{k}\beta}^\dagger \rangle = \varepsilon_{\alpha\beta} \Delta_S (\cos k_x - \cos k_y)$$

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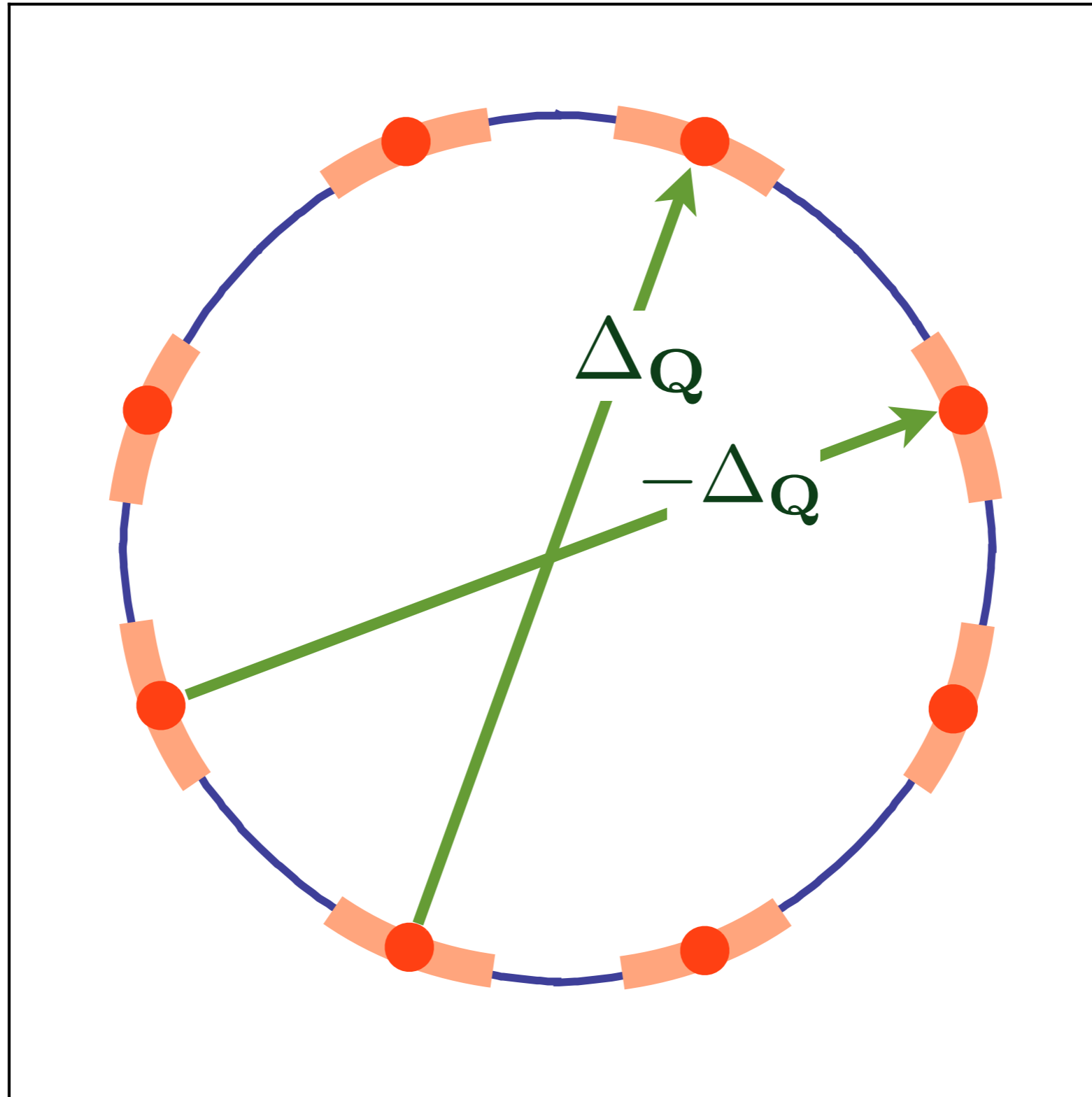
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Unconventional pairing at and near hot spots

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

After  
pseudospin  
rotation on  
*half* the  
hot-spots



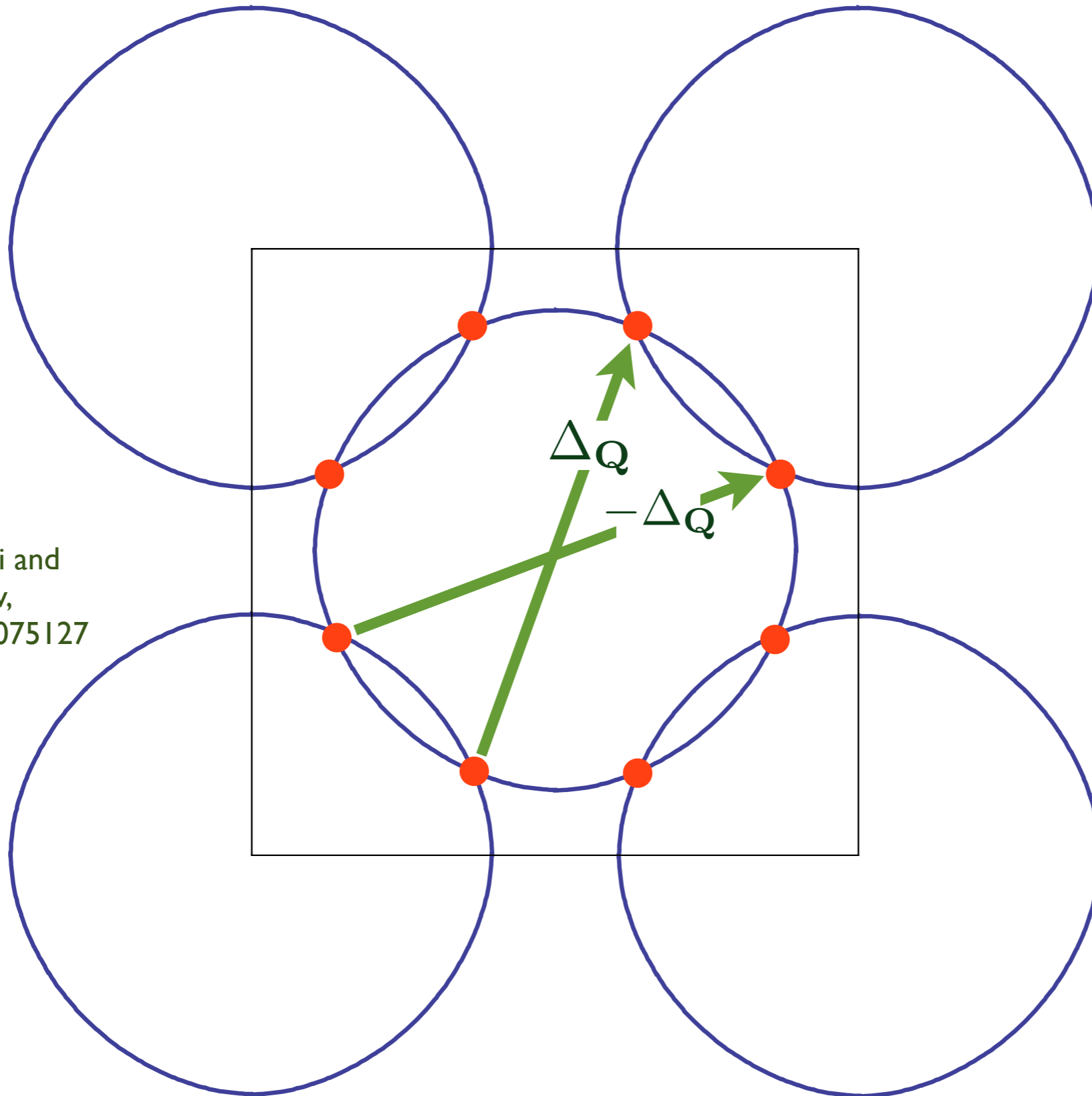
$\mathbf{Q}$  is ' $2k_F$ '  
wavevector

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

Unconventional particle-hole pairing at and near hot spots

# Incommensurate $d$ -wave bond order

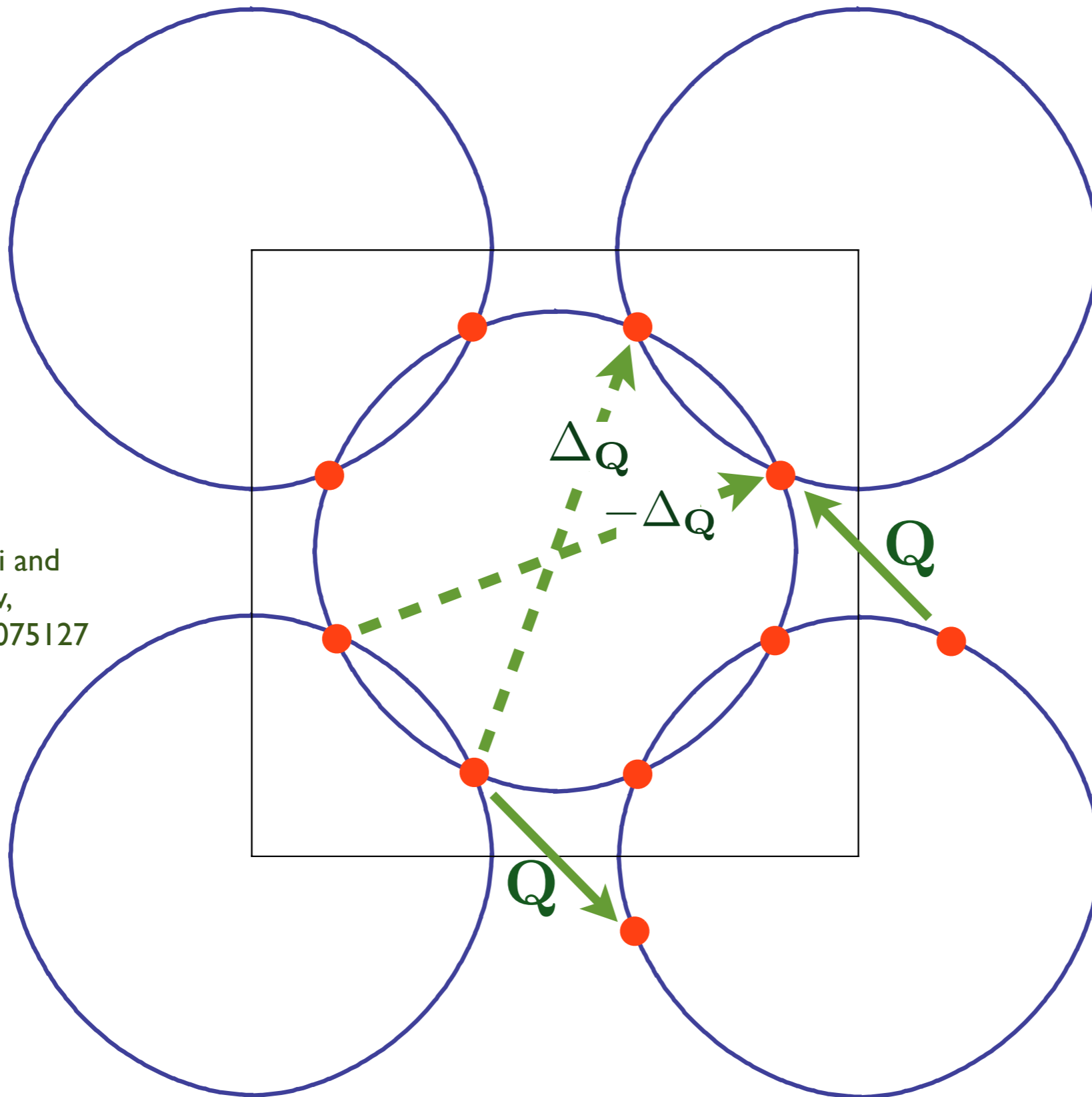
M.A. Metlitski and  
S. Sachdev,  
*Phys. Rev. B* **85**, 075127  
(2010)



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

# Incommensurate $d$ -wave bond order

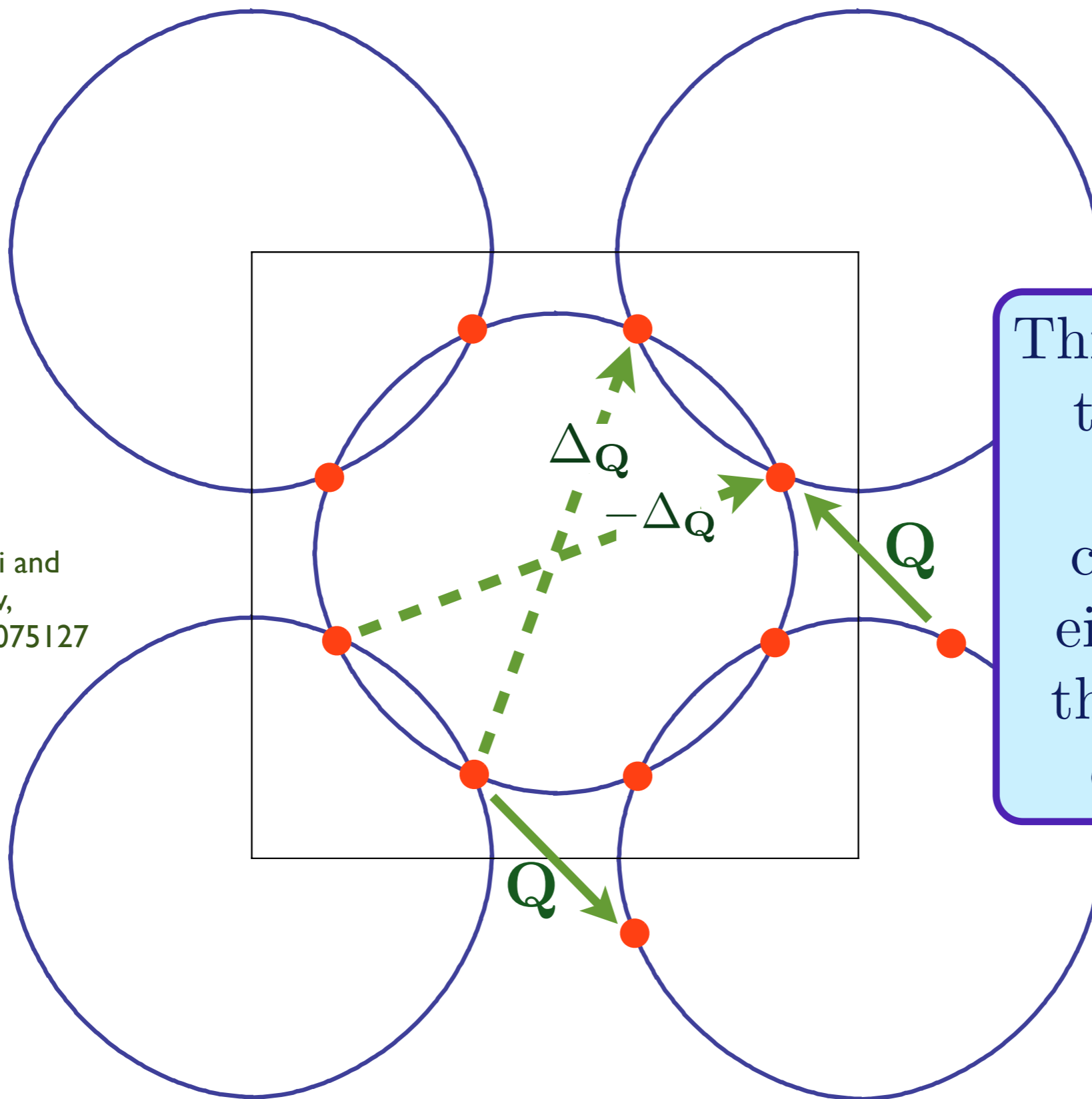
M.A. Metlitski and  
S. Sachdev,  
*Phys. Rev. B* **85**, 075127  
(2010)



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

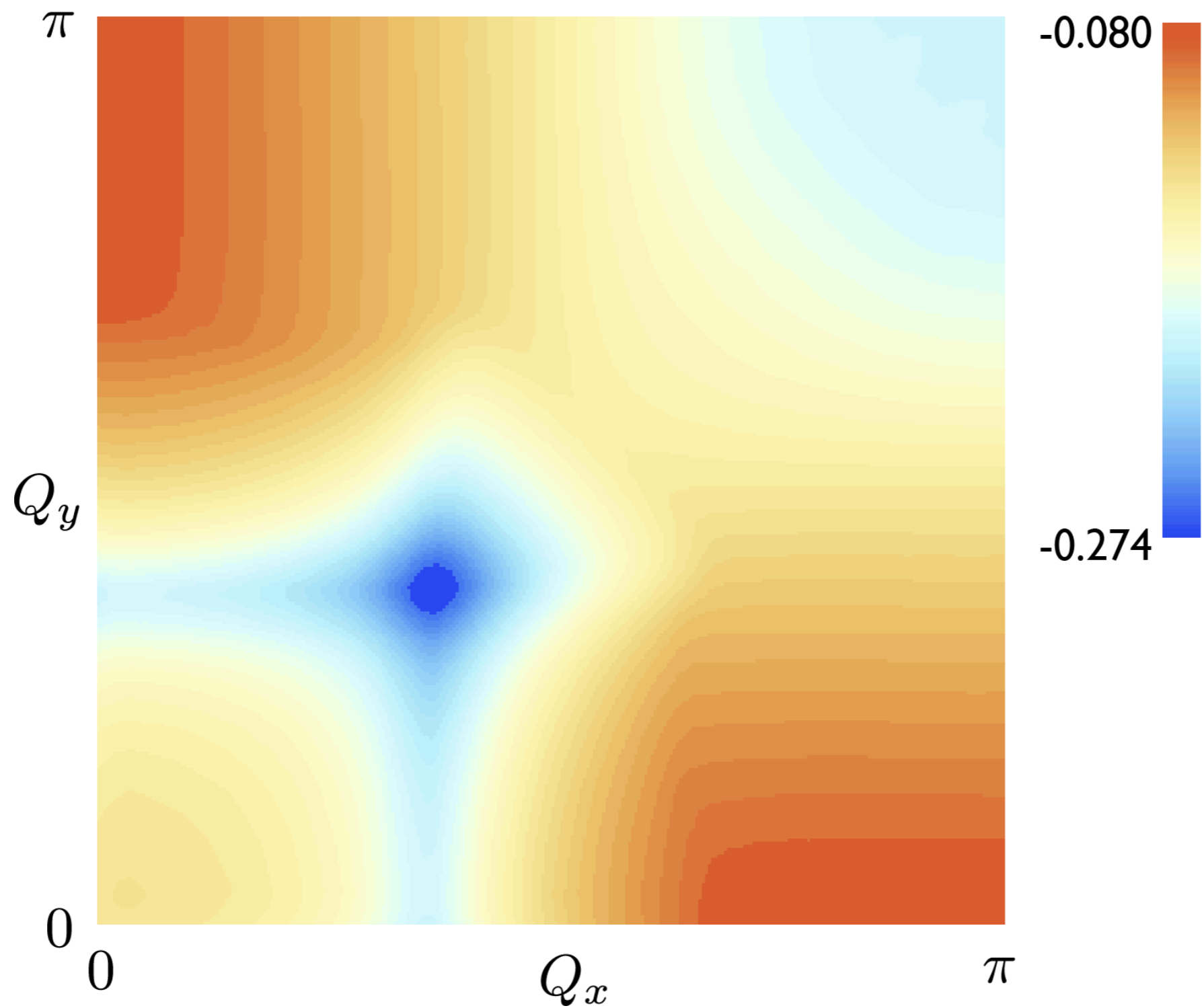
# Incommensurate $d$ -wave bond order

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



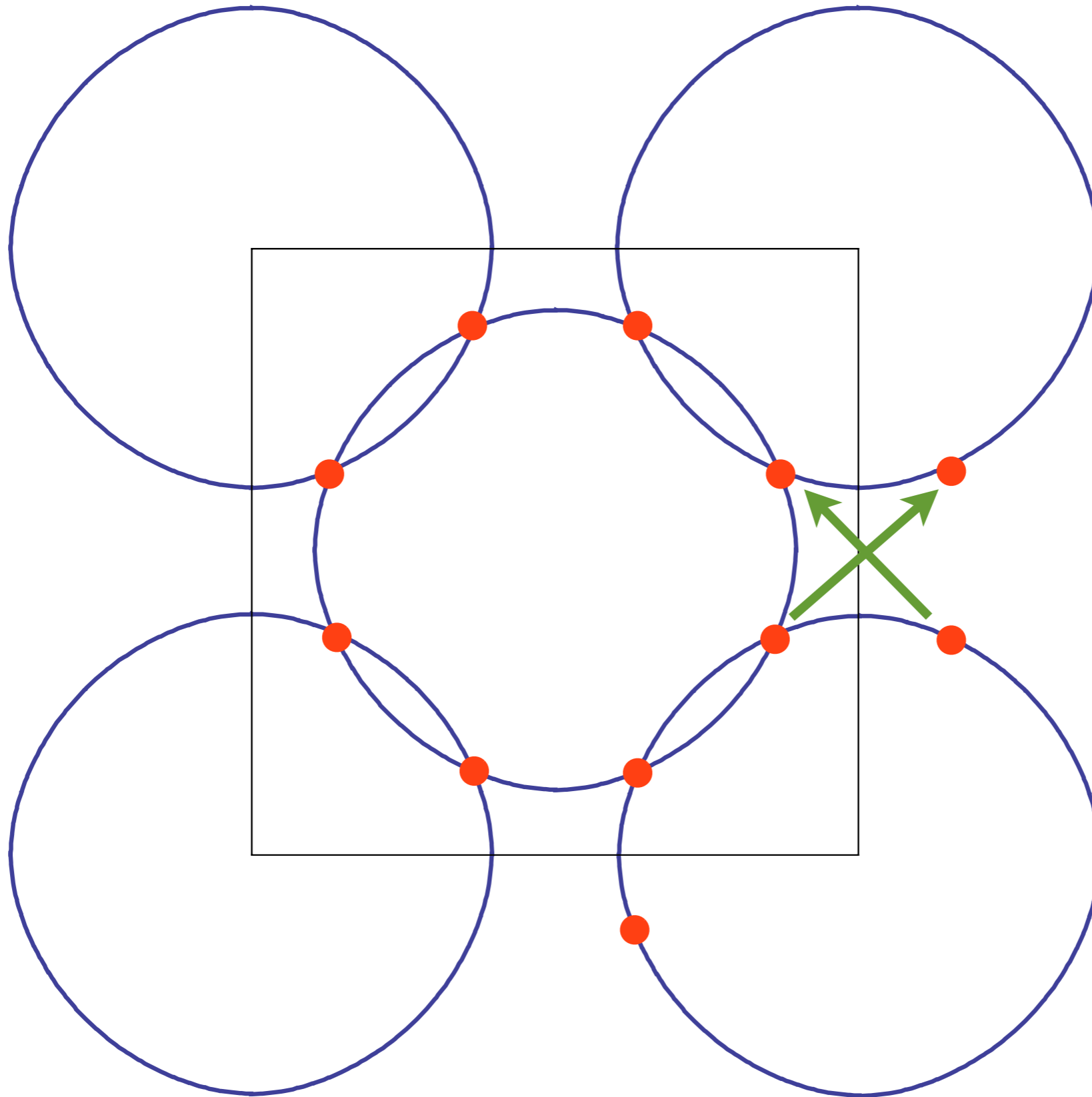
This  $\mathbf{Q}$  is very close to the  $\mathbf{Q}$  which minimizes the charge-ordering eigenvalue  $\lambda_{\mathbf{Q}}$  in the Hartree-Fock computation !

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



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

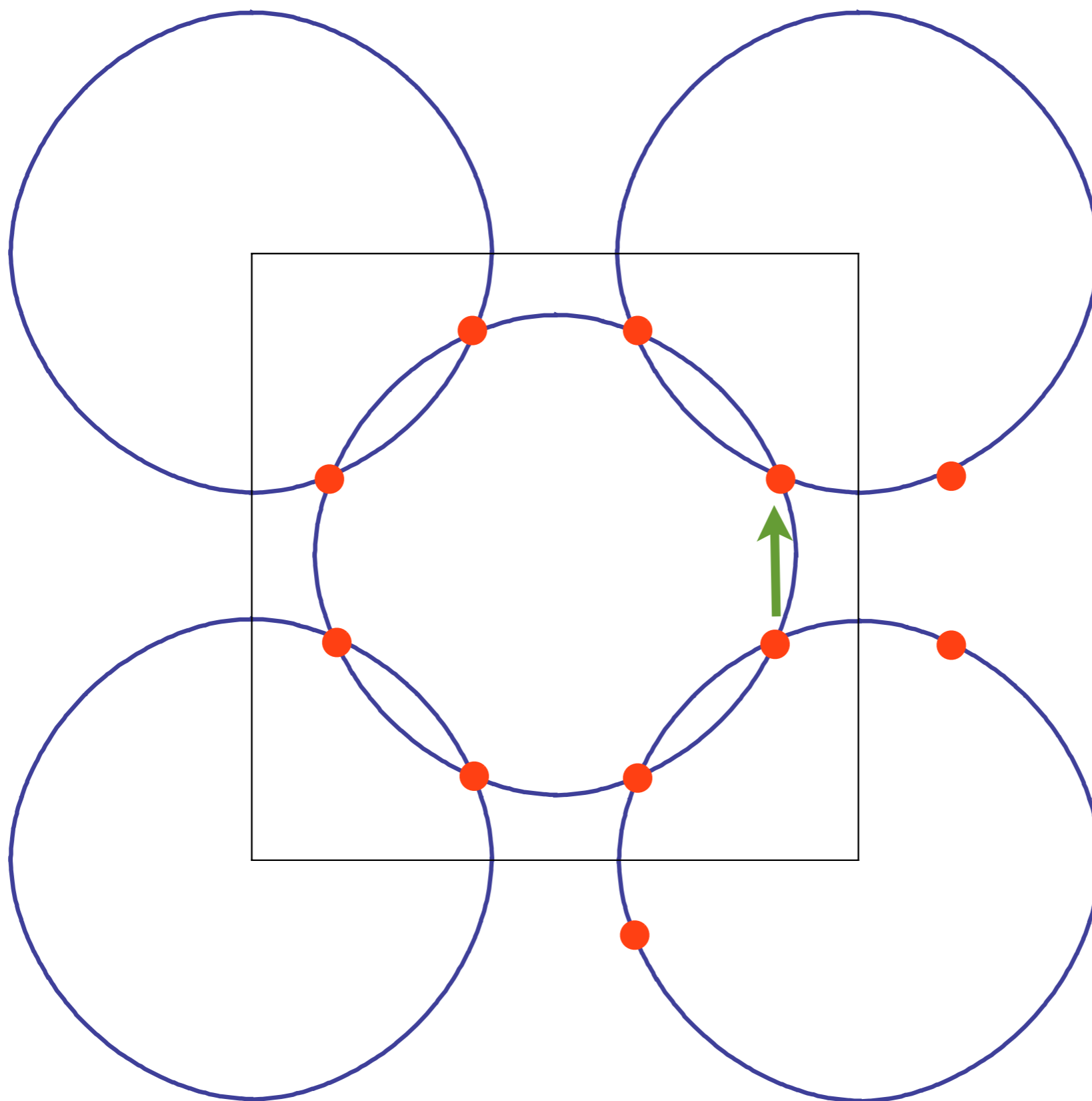
# Incommensurate $d$ -wave bond order



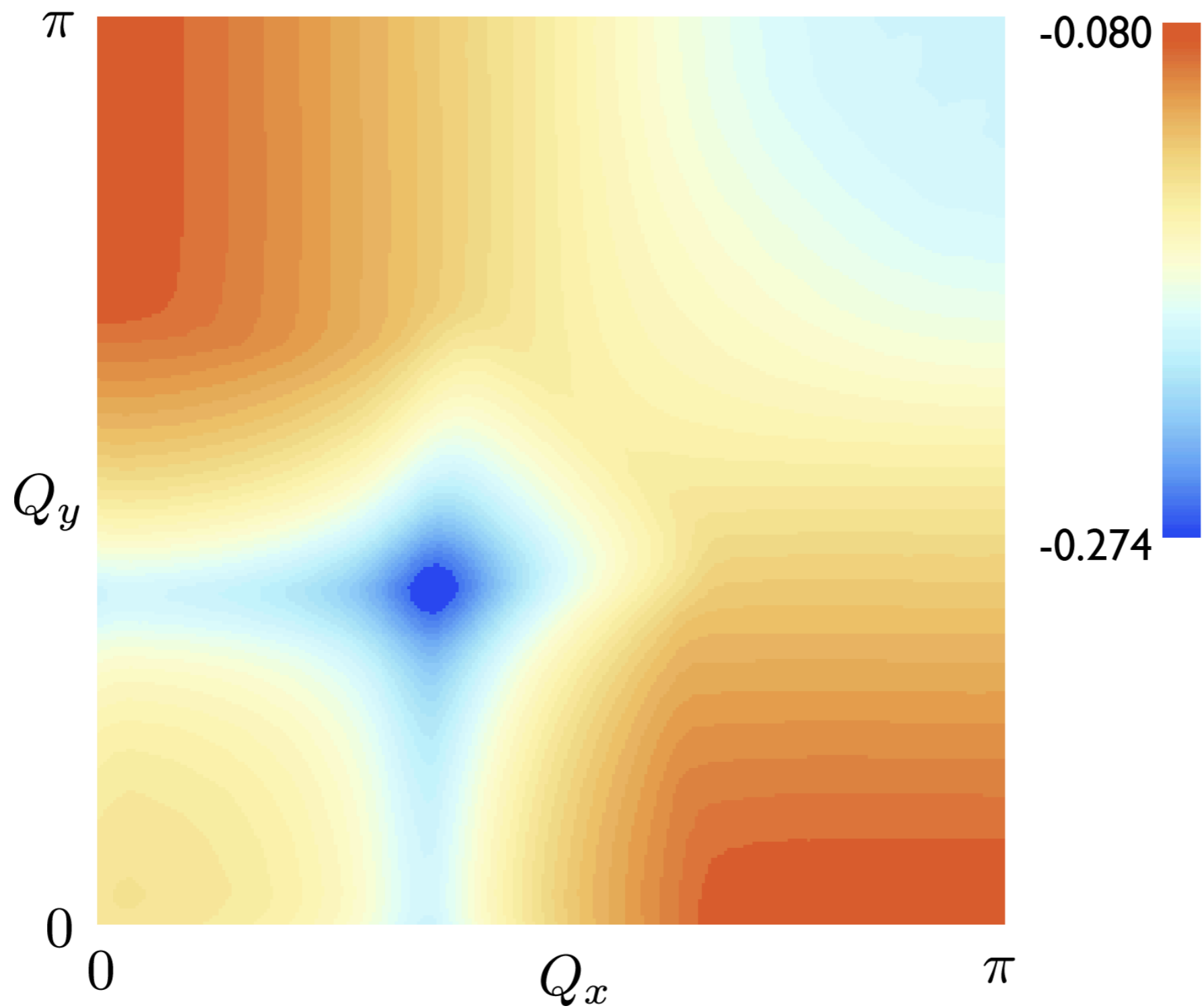
High  $T$  pseudogap:  
Fluctuating composite  
order parameter of  
nearly degenerate  
 $d$ -wave pairing and  
incommensurate  
 $d$ -wave bond order.  
(Approximate)  $SU(2)$   
symmetry of composite  
order prevents  
long-range order  $T > 0$ .

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

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

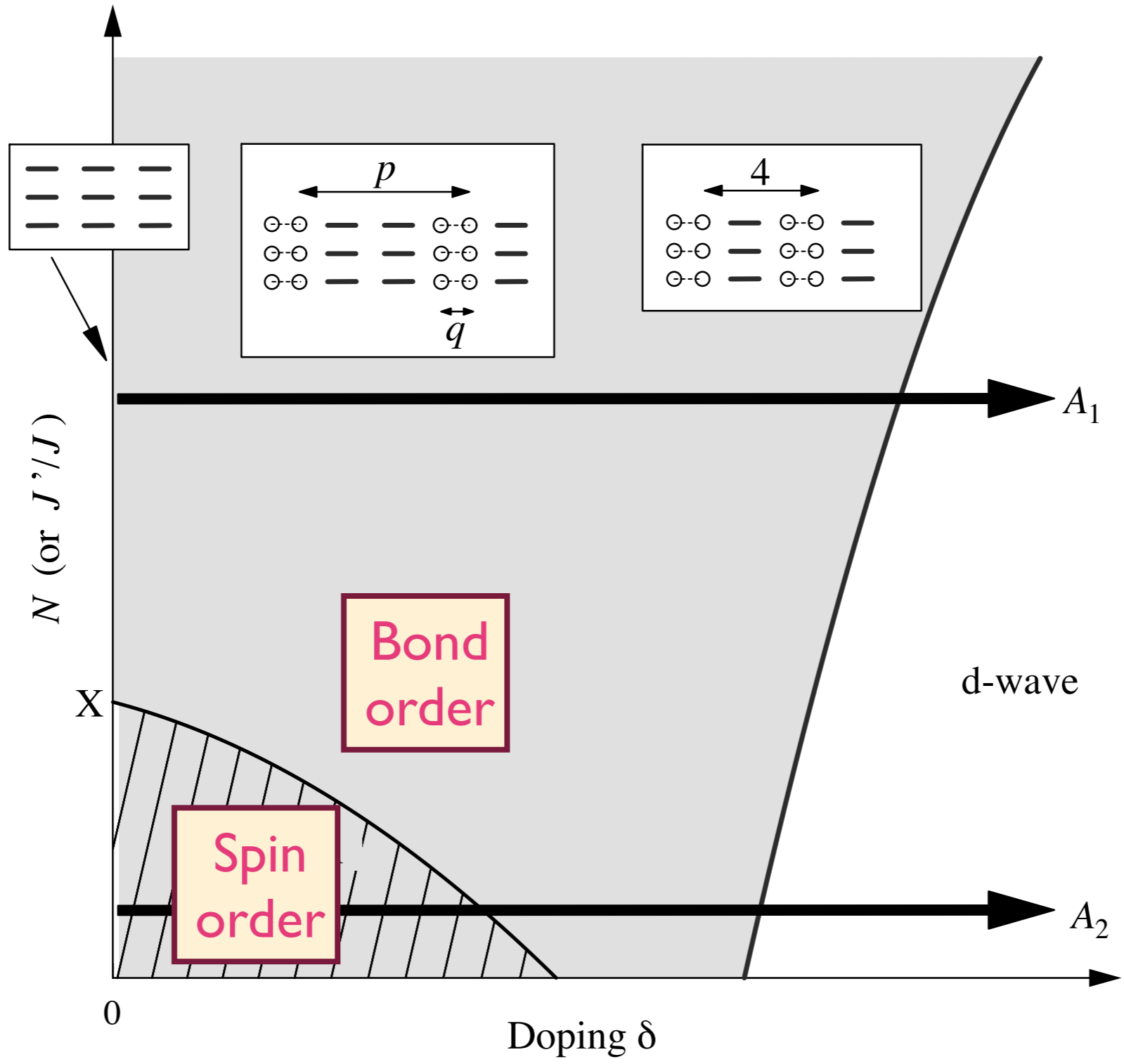


Observed  
low  $T$  ordering



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

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)

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

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

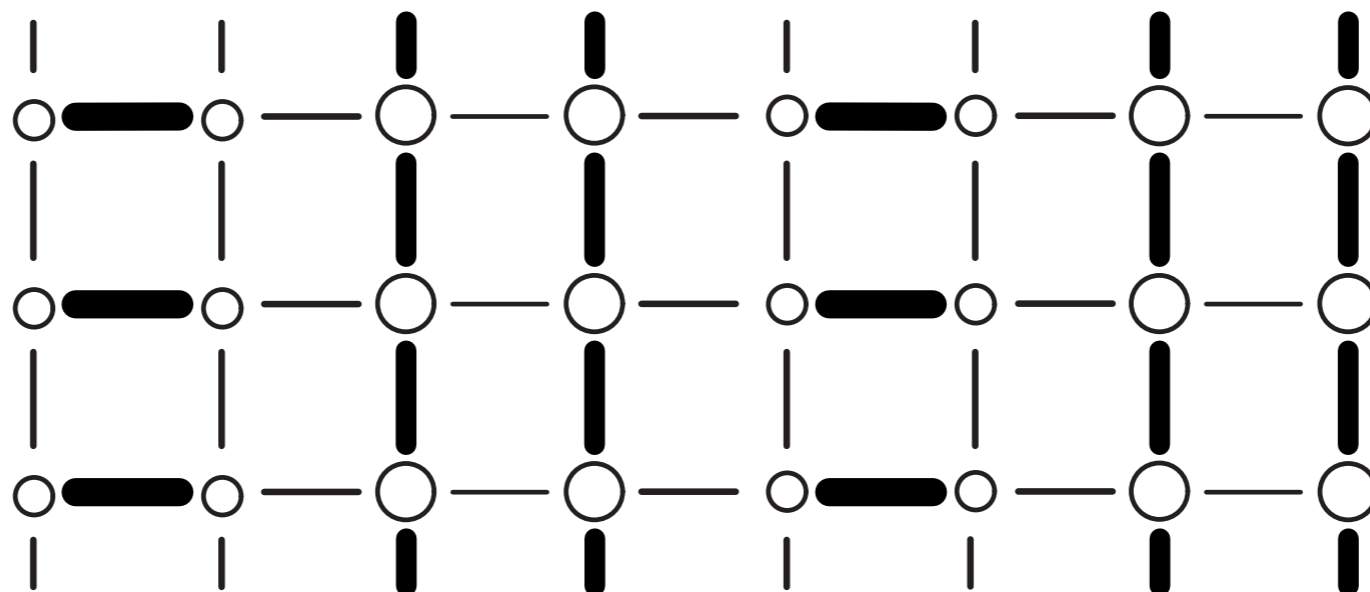
## Superconducting $d$ -wave stripes in cuprates: Valence bond order coexisting with nodal quasiparticles

Matthias Vojta and Oliver Rösch

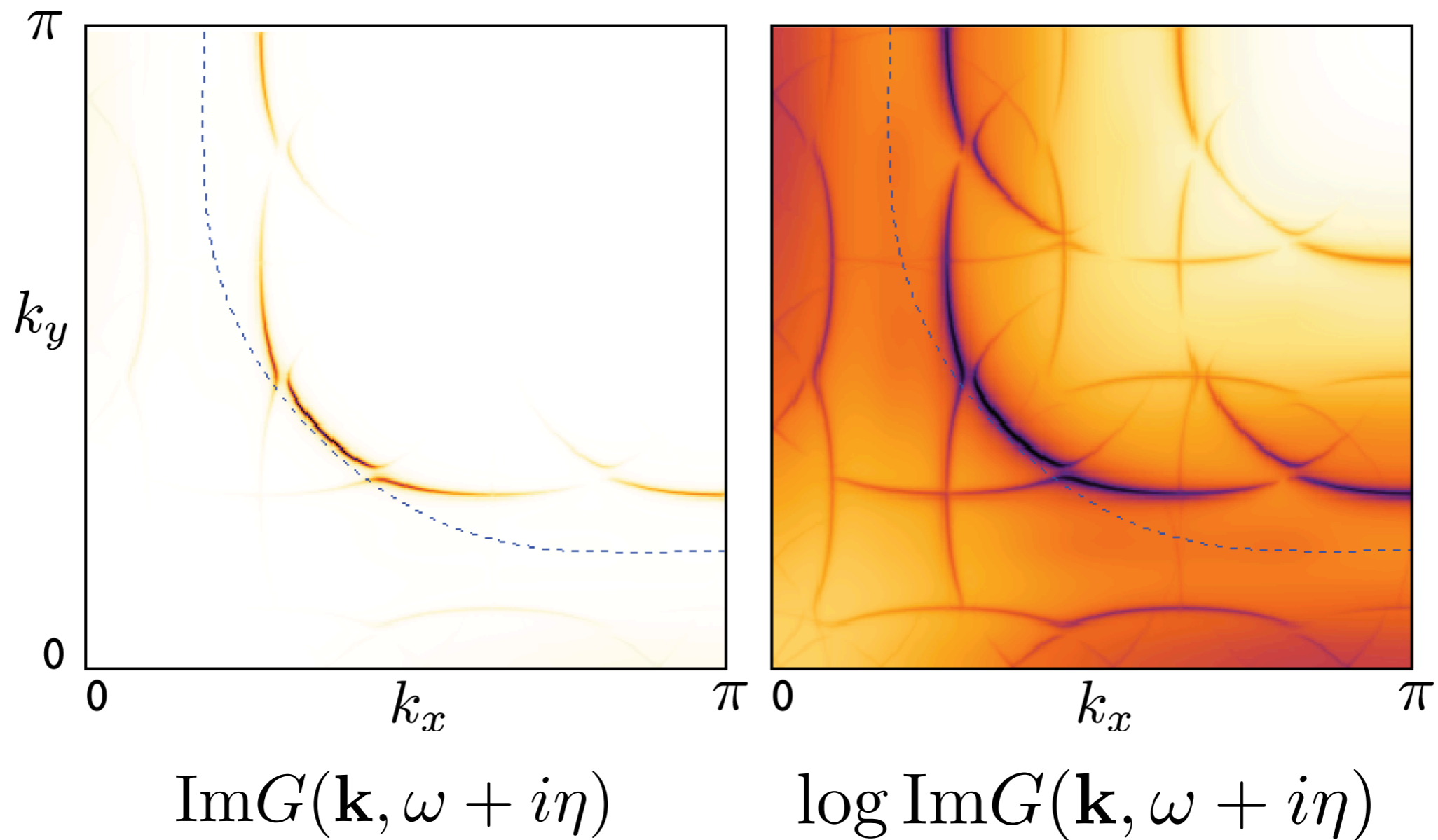
*Institut für Theoretische Physik, Universität zu Köln, Zùlpicher Straße 77, 50937 Köln, Germany*

(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  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  and  $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$  of Kohsaka *et al.* [Science **315**, 1380 (2007)].



# Electron spectral function



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

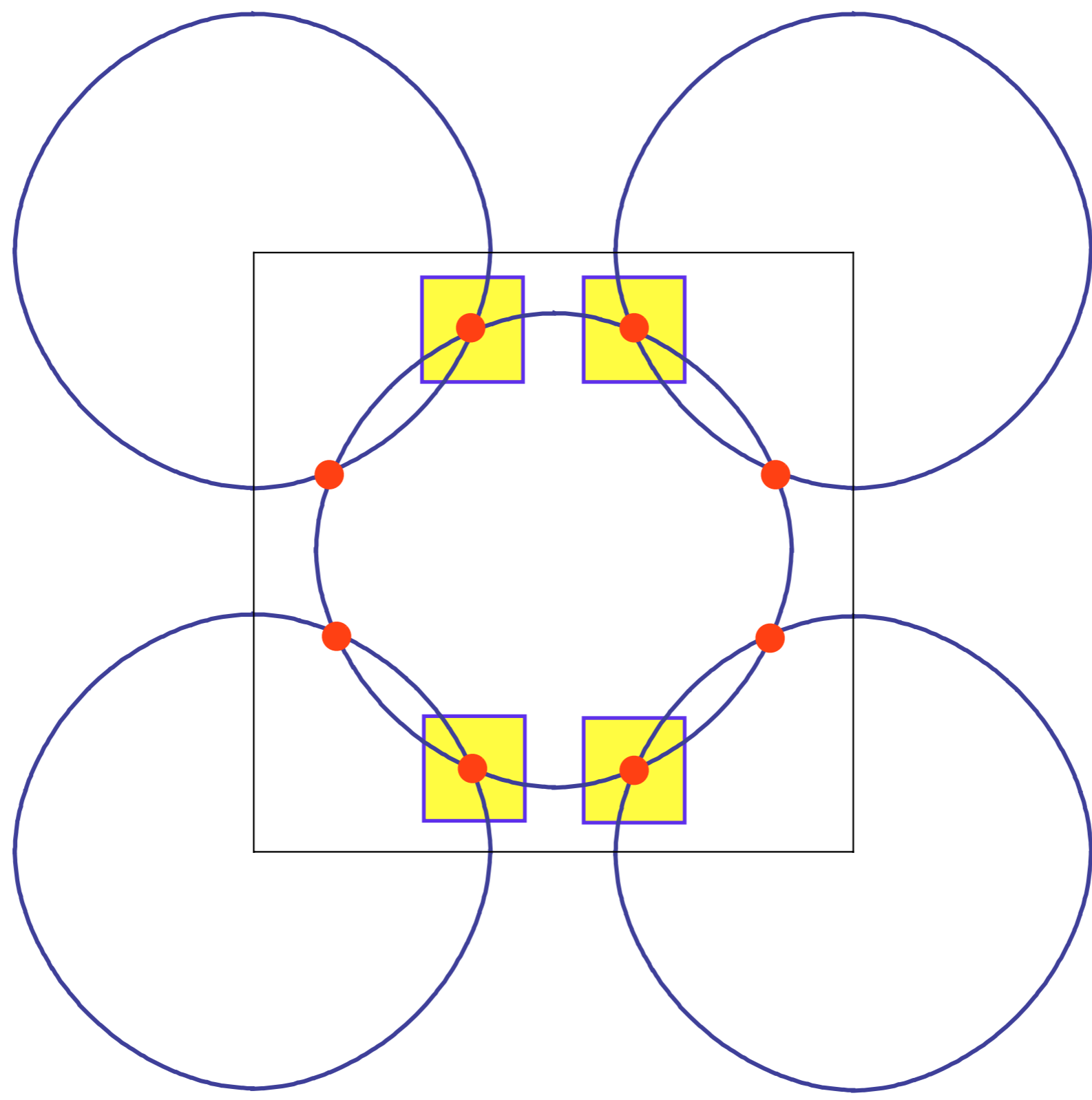
$$\text{with } \Delta_s/\Delta_d = -0.234.$$

# Outline

1. Stability of metal in Hartree-Fock-BCS theory
2. Emergent pseudospin symmetry in low energy theory of metal with antiferromagnetic interactions
3. Quantum Monte Carlo without the sign problem

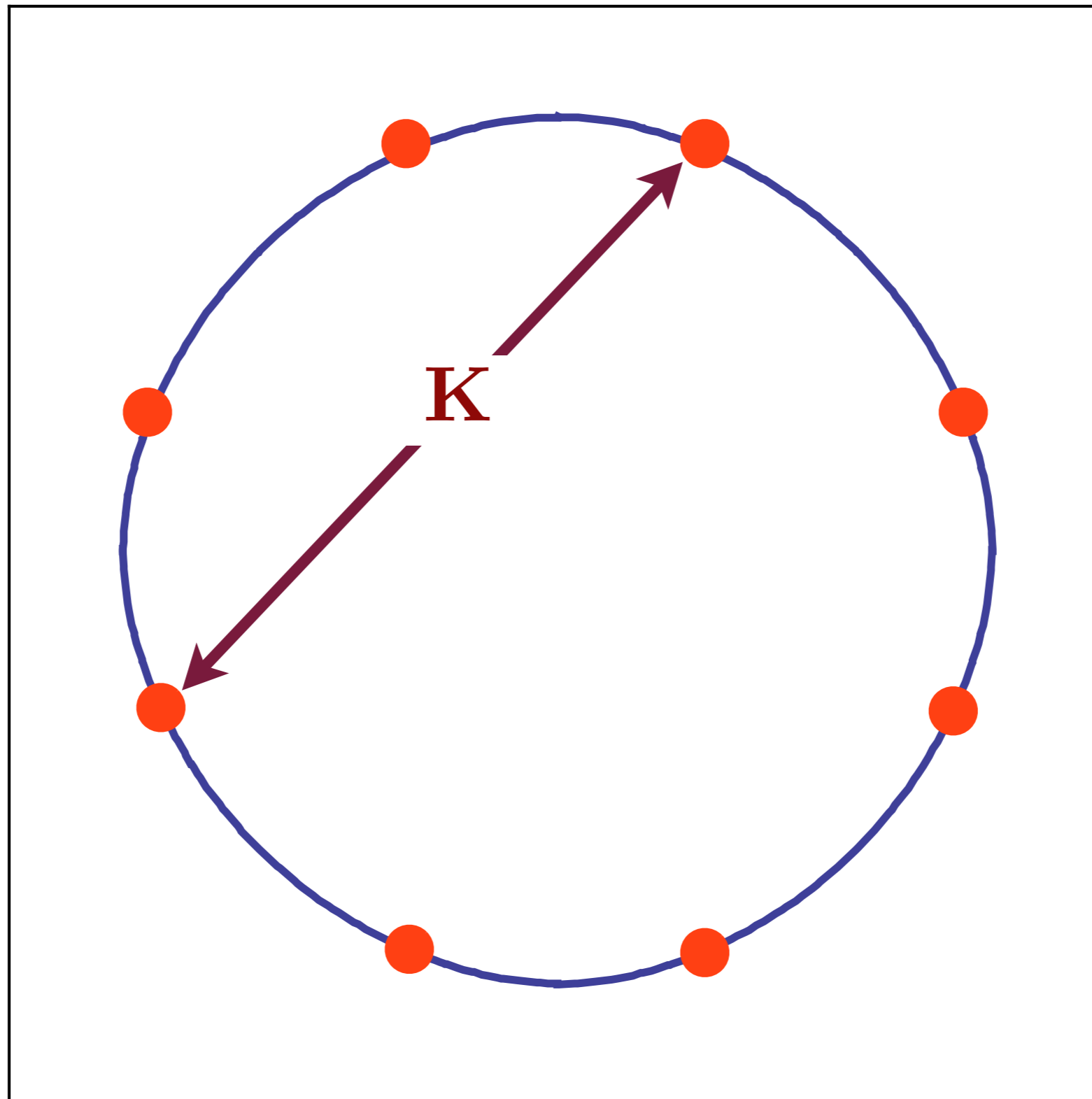
# Outline

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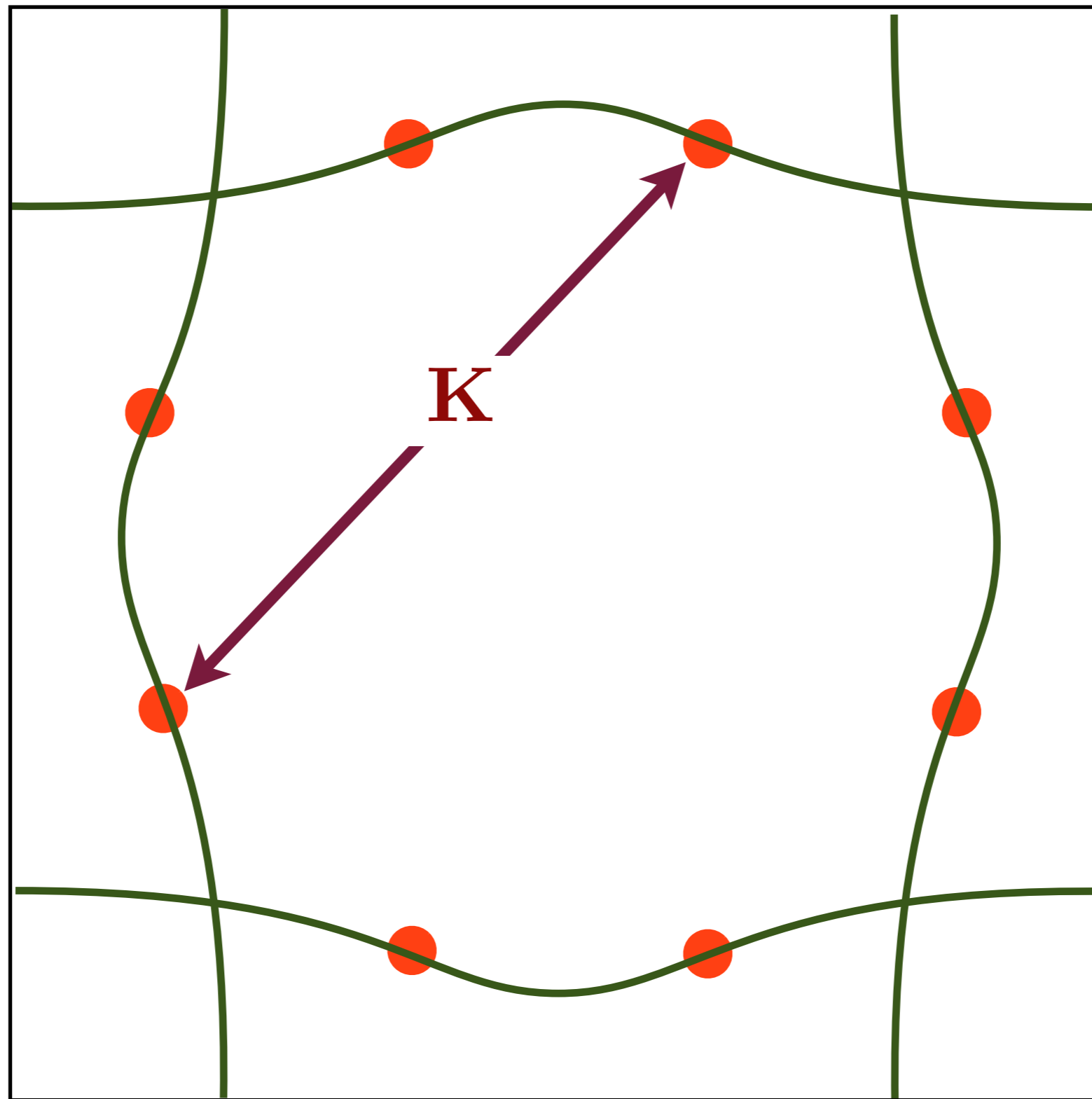
# Low energy theory for critical point near hot spots

# QMC for the onset of antiferromagnetism



Hot spots in a single band model

# QMC for the onset of antiferromagnetism

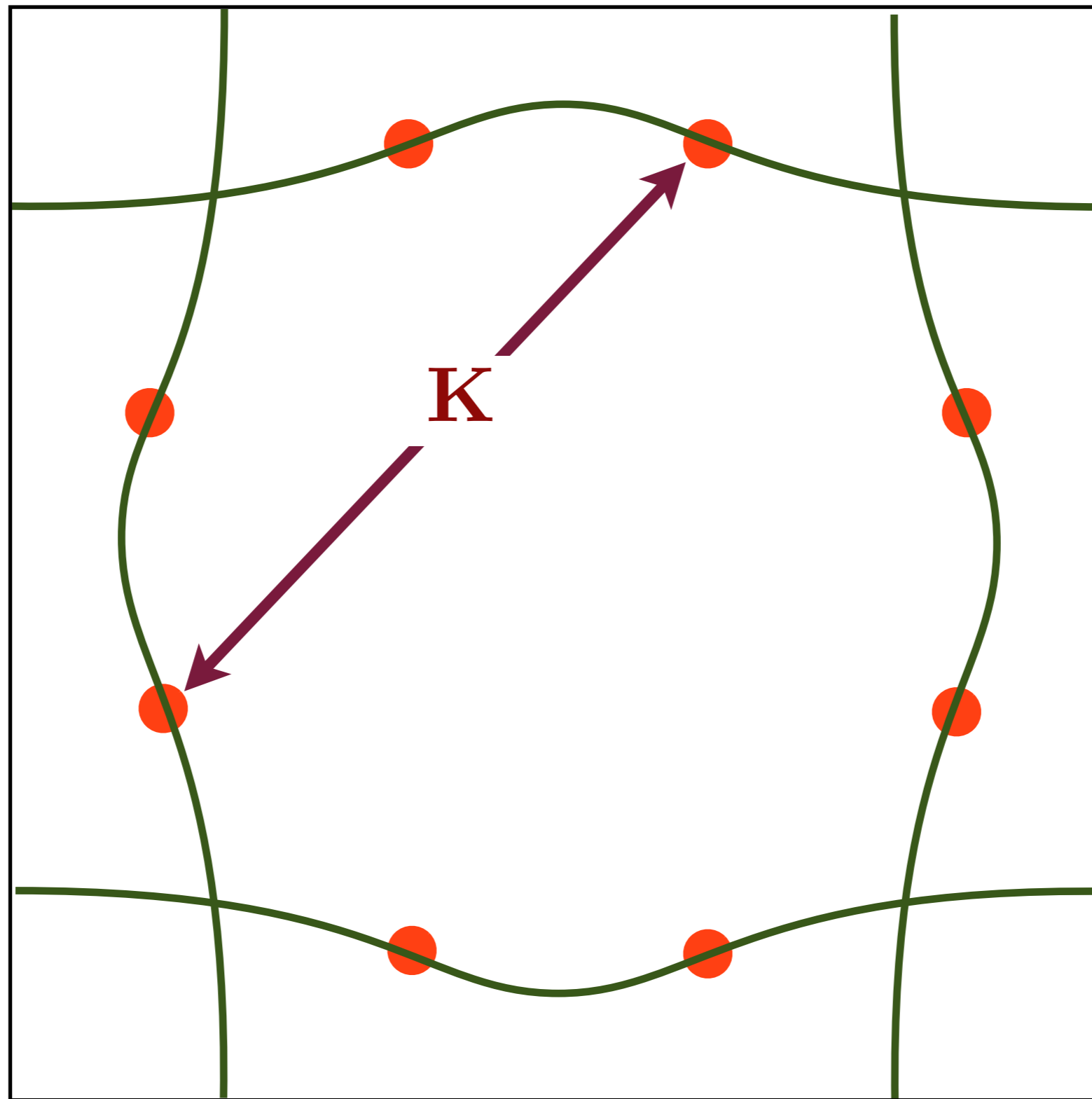


E. Berg,  
M. Metlitski, and  
S. Sachdev,  
*Science* **338**, 1606  
(2012).

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 antiferromagnetism.

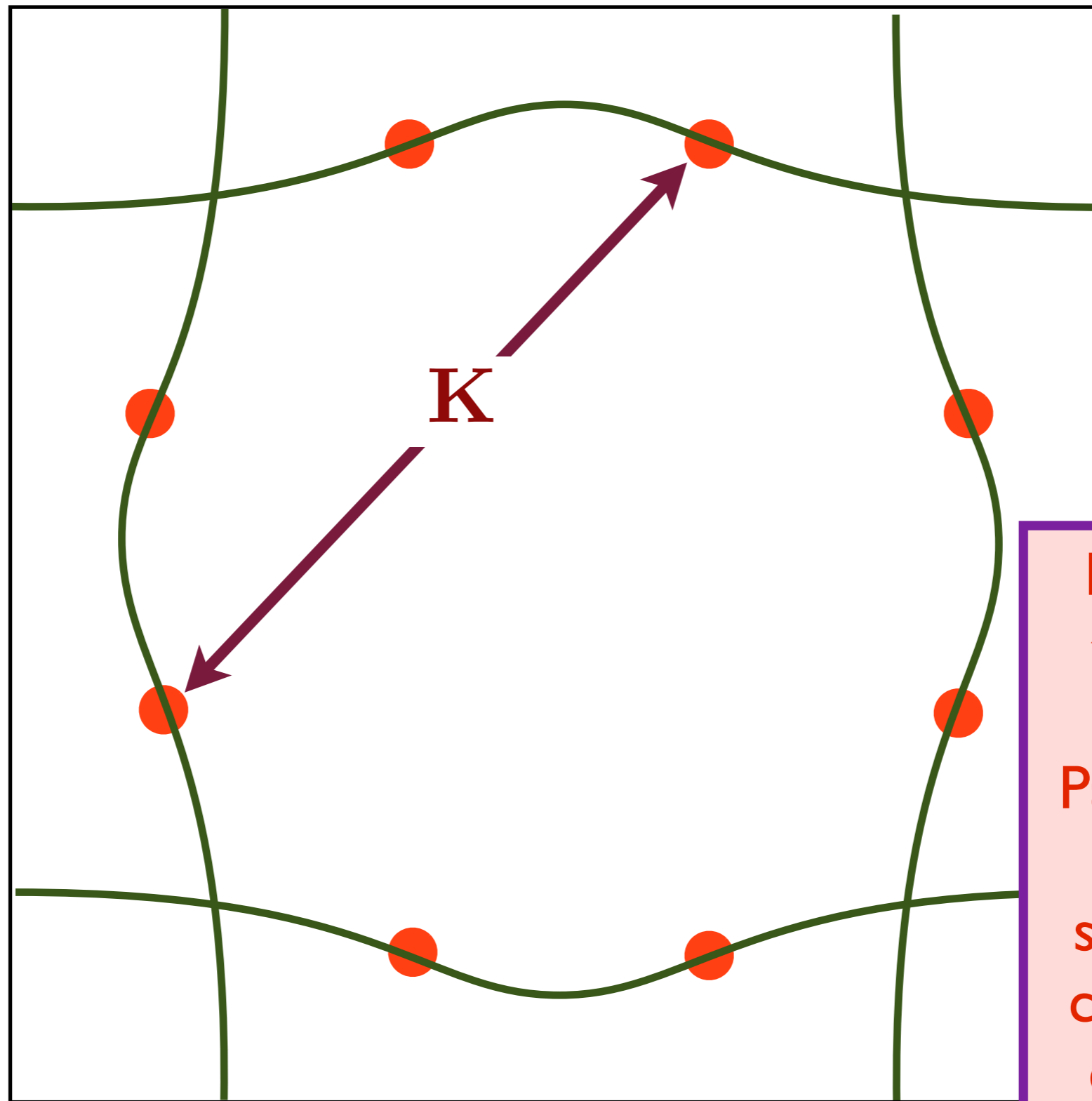


Hot spots in a two band model

E. Berg,  
M. Metlitski, and  
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*Science* **338**, 1606  
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# QMC for the onset of antiferromagnetism

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



E. Berg,  
M. Metlitski, and  
S. Sachdev,  
*Science* **338**, 1606  
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Requires only time-reversal symmetry. Particle-hole or point-group symmetries or commensurate densities **not** required !

Hot spots in a two band mod

# 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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E. Berg,  
M. Metlitski, and  
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E. Berg,  
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*Science* **338**, 1606  
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No sign problem !

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E. Berg,  
M. Metlitski, and  
S. Sachdev,  
*Science* **338**, 1606  
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Applies without changes to the microscopic band structure in the iron-based superconductors

# QMC for the onset of antiferromagnetism

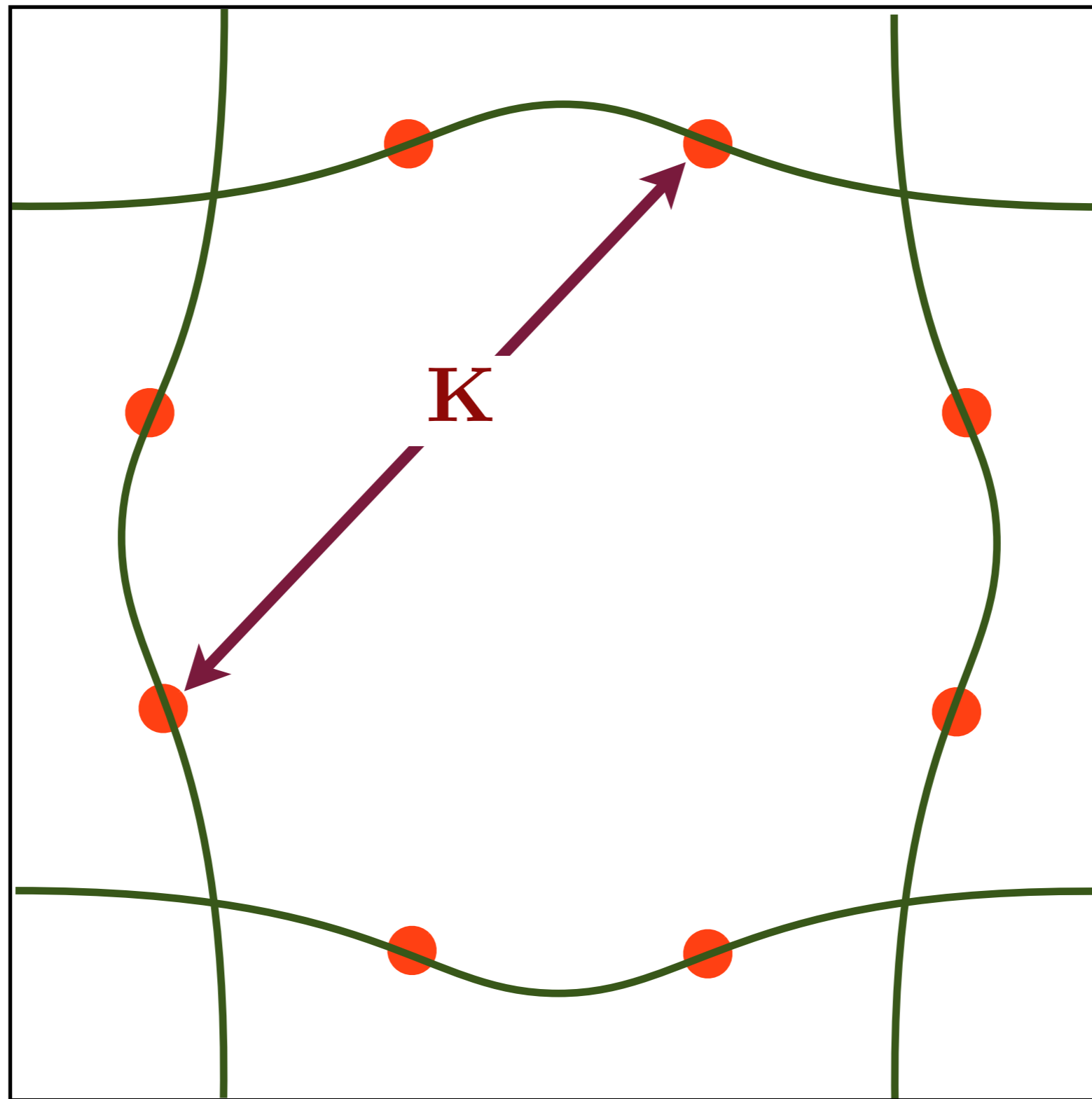
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E. Berg,  
M. Metlitski, and  
S. Sachdev,  
*Science* **338**, 1606  
(2012).

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

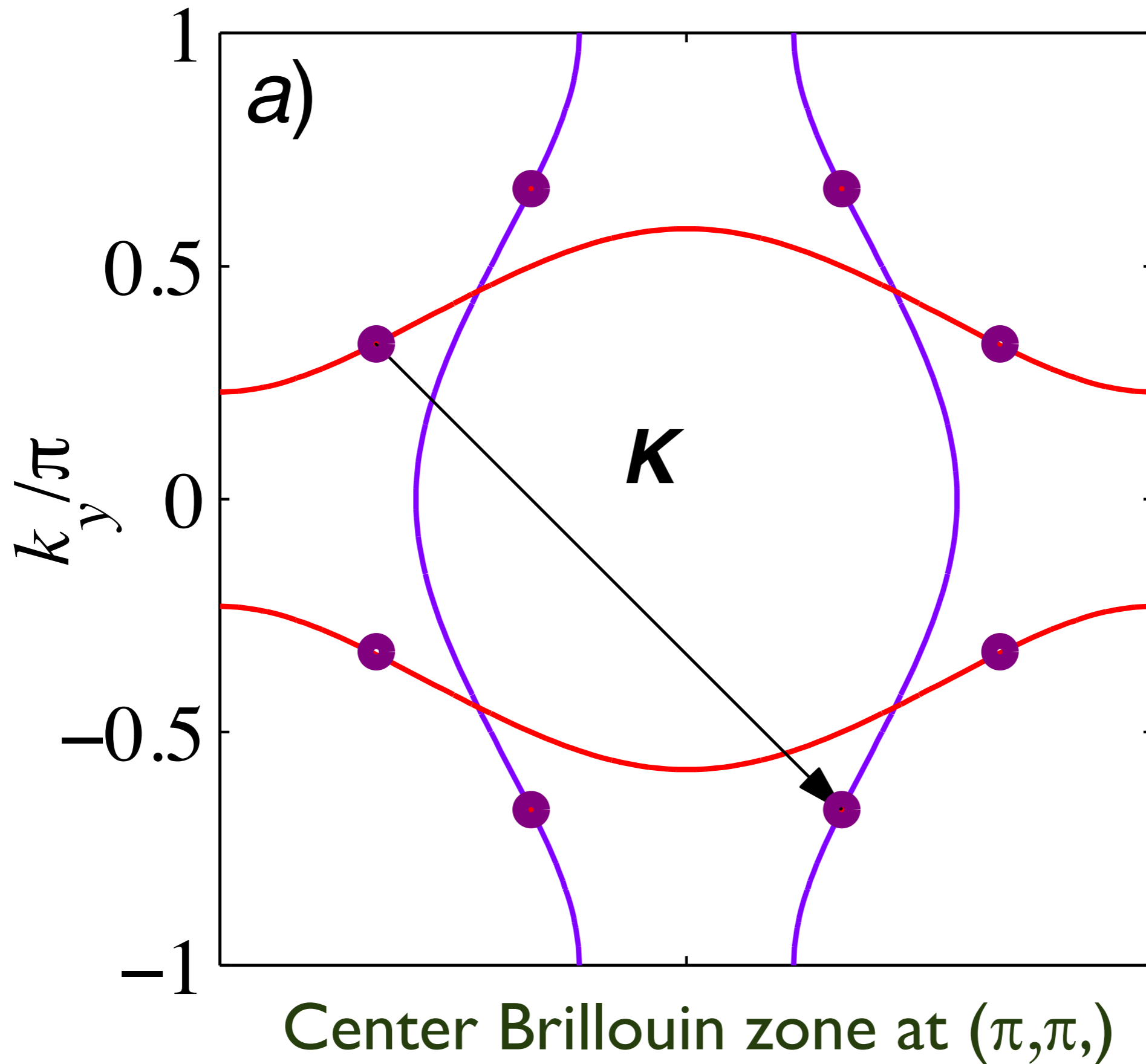
# QMC for the onset of antiferromagnetism



E. Berg,  
M. Metlitski, and  
S. Sachdev,  
*Science* **338**, 1606  
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Hot spots in a two band model

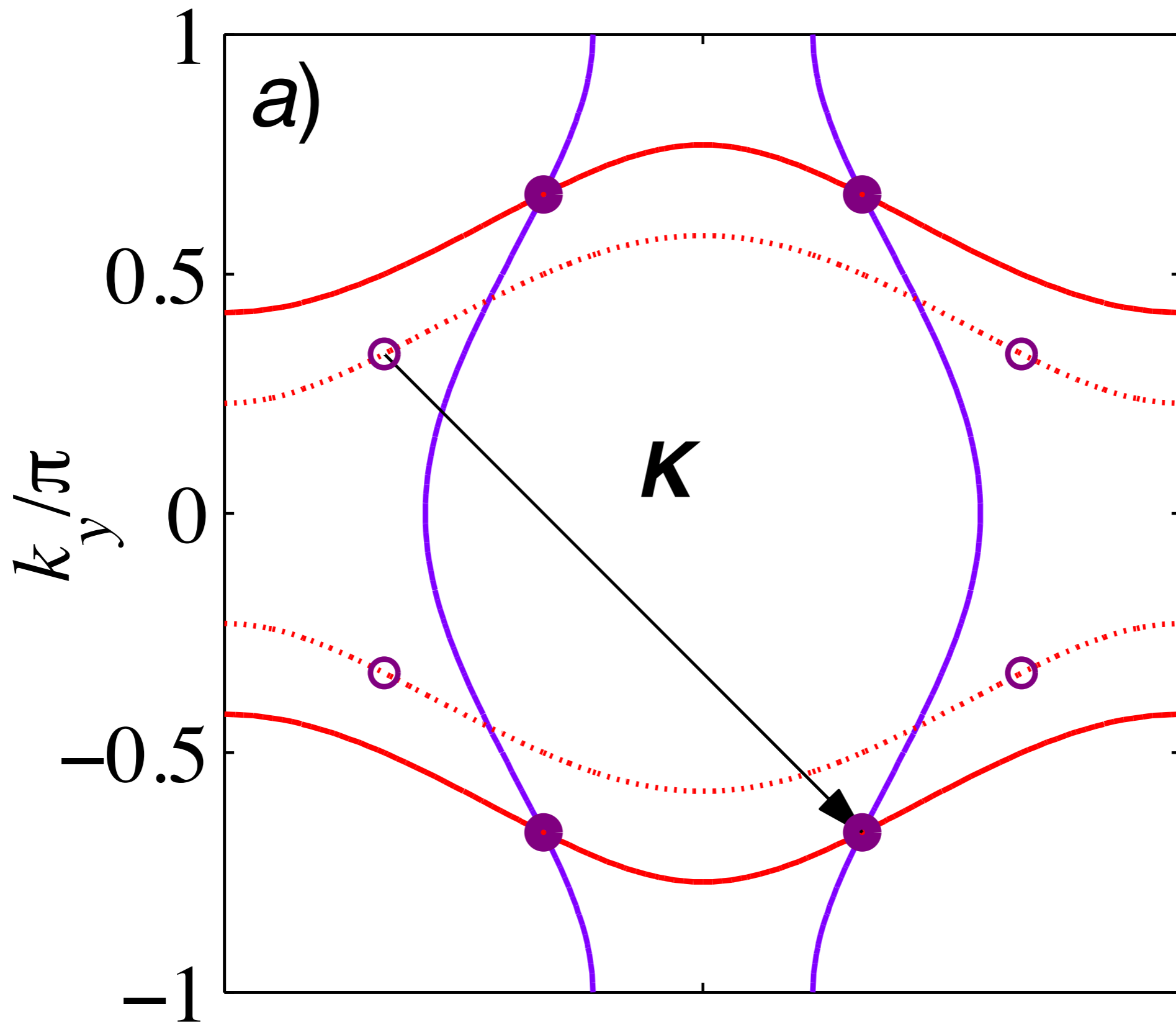
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E. Berg,  
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*Science* **338**, 1606  
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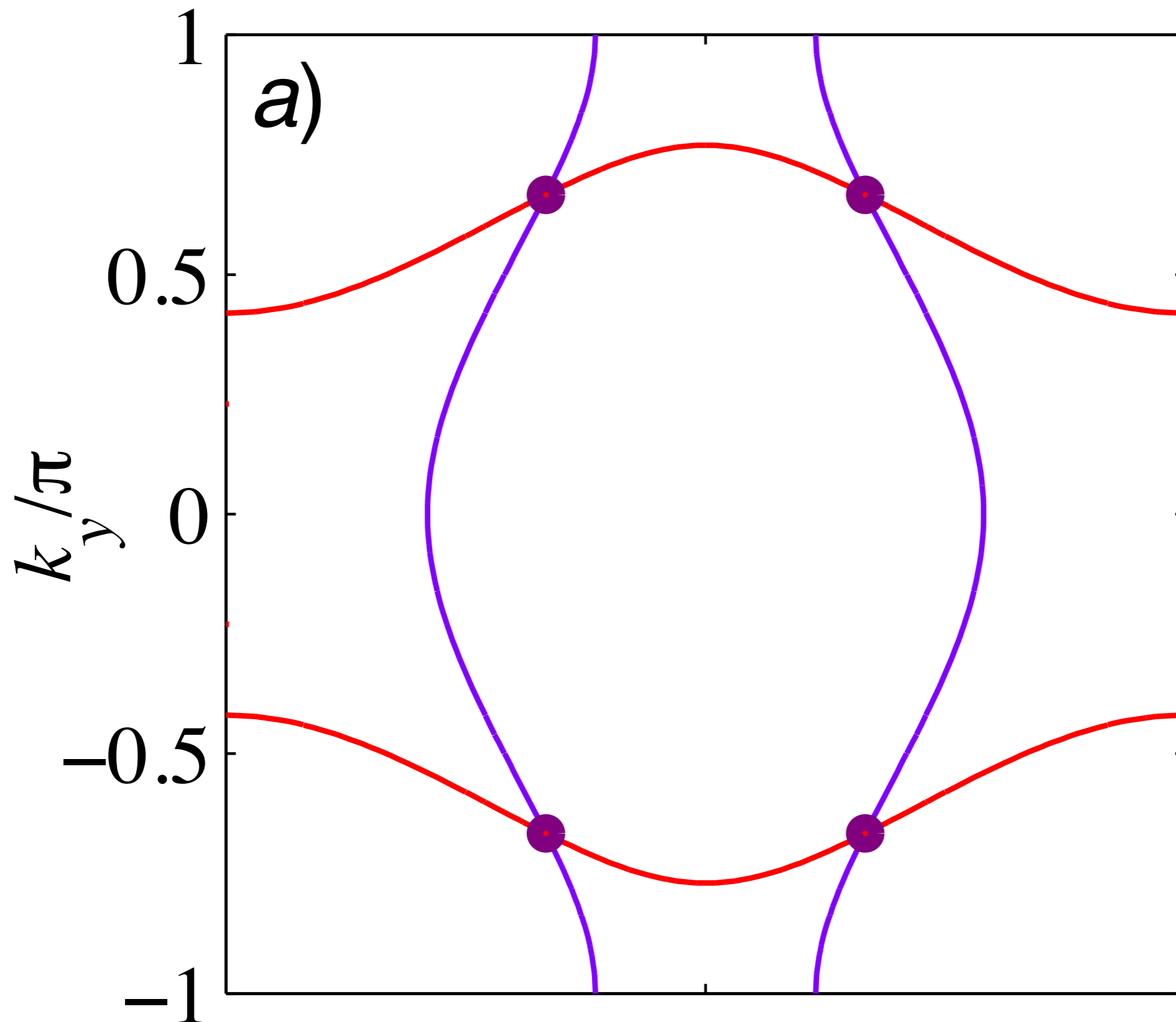
# QMC for the onset of antiferromagnetism

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

# QMC for the onset of antiferromagnetism

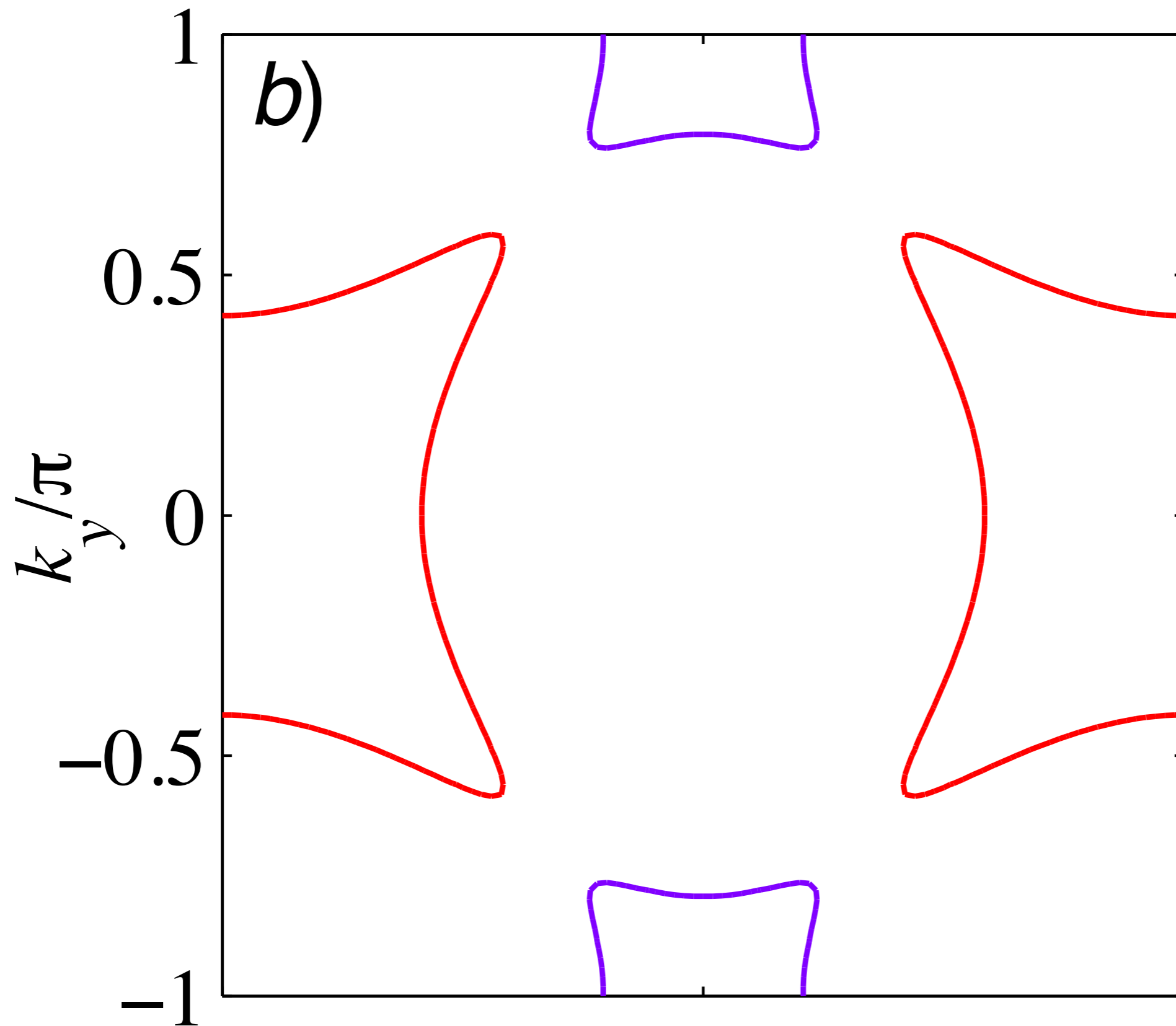


E. Berg,  
M. Metlitski, and  
S. Sachdev,  
*Science* **338**, 1606  
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Now hot spots are at Fermi surface intersections

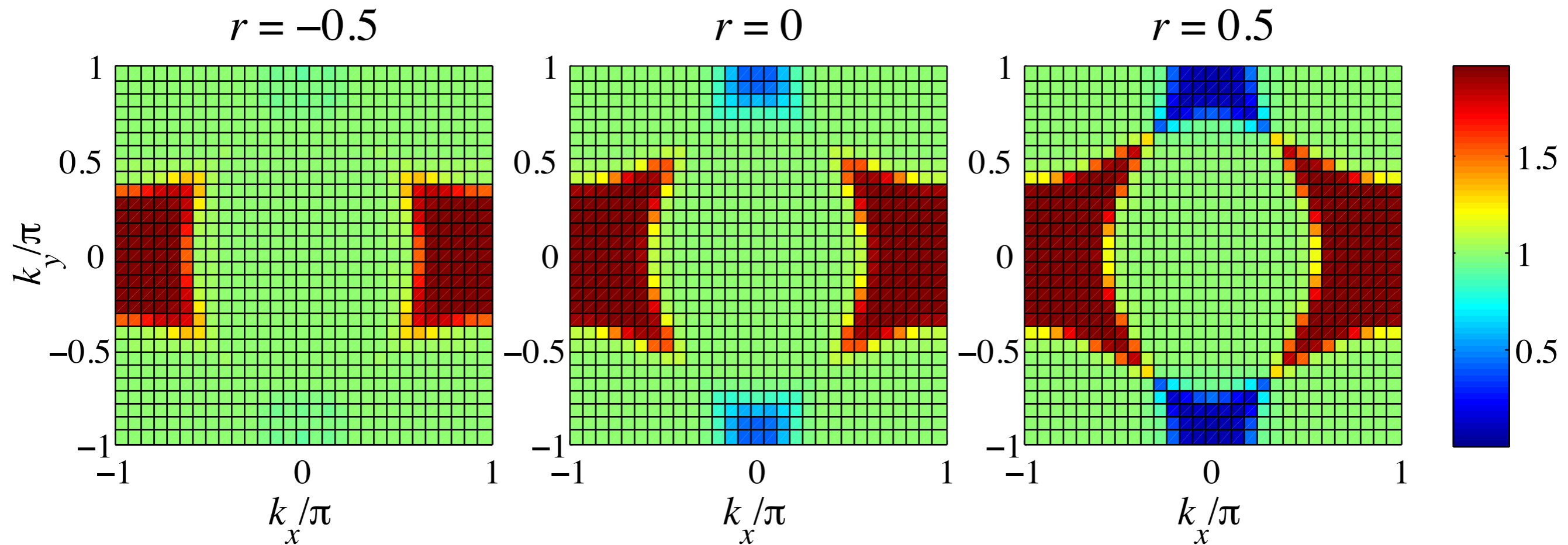
# QMC for the onset of antiferromagnetism

E. Berg,  
M. Metlitski, and  
S. Sachdev,  
*Science* **338**, 1606  
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Expected Fermi surfaces in the AFM ordered phase

# QMC for the onset of antiferromagnetism

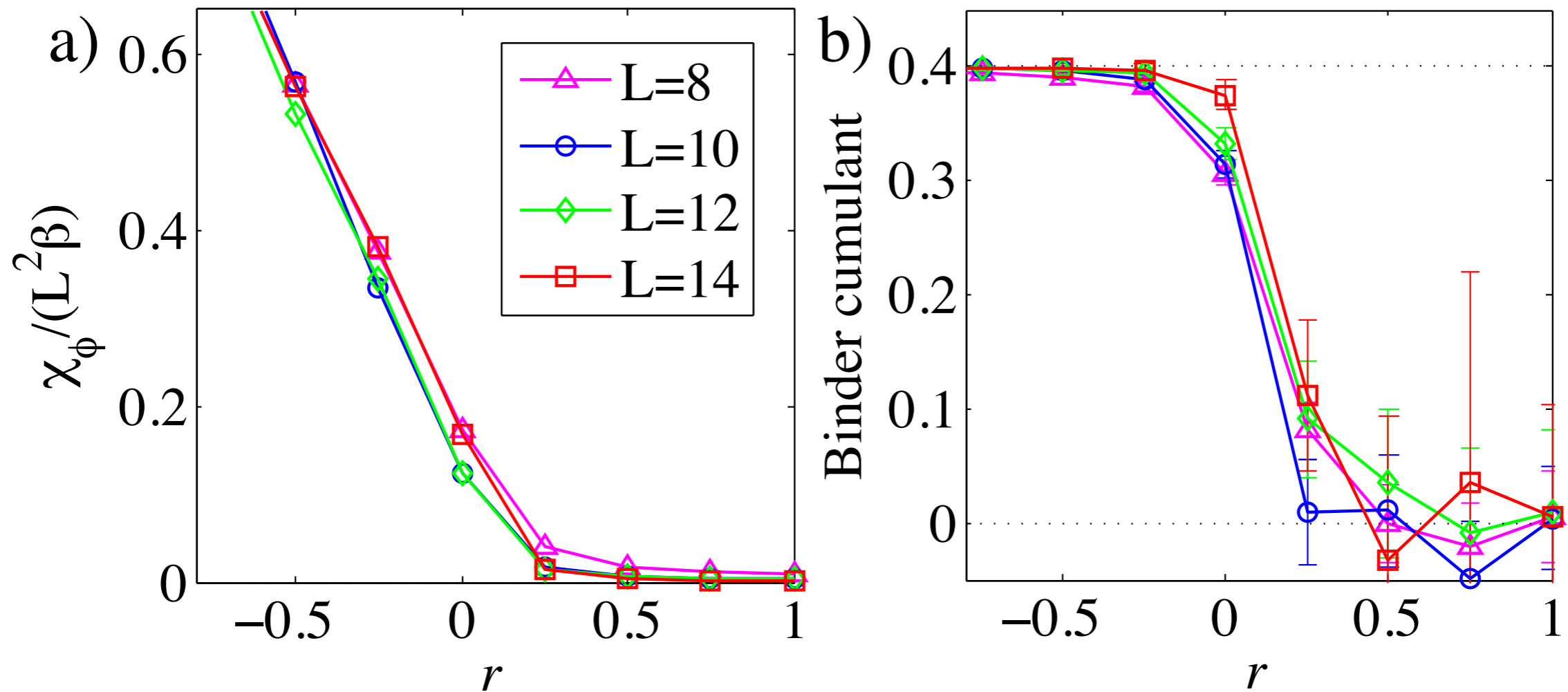


Electron occupation number  $n_{\mathbf{k}}$   
as a function of the tuning parameter  $r$

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



# QMC for the onset of antiferromagnetism

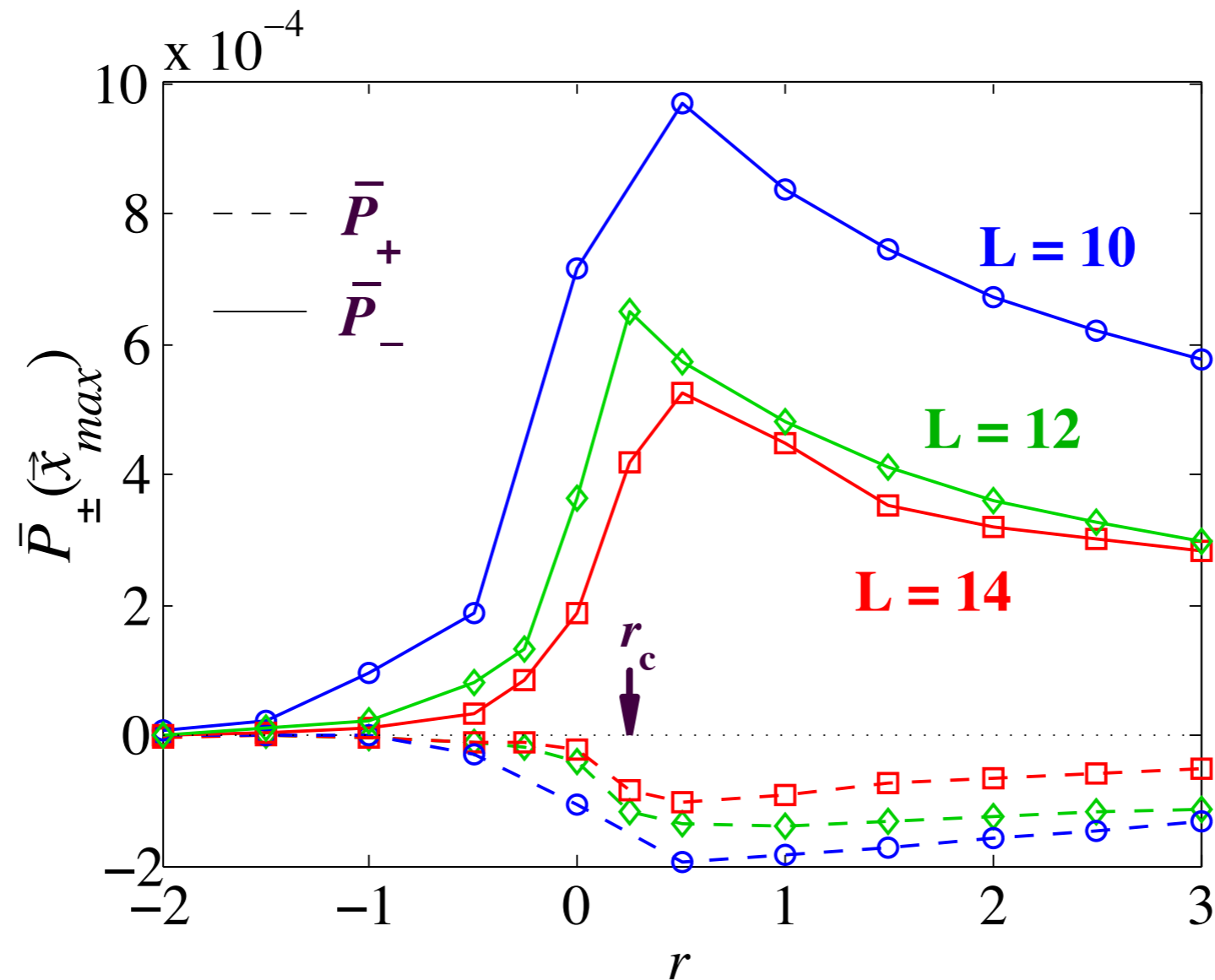


AF susceptibility,  $\chi_\phi$ , and Binder cumulant  
as a function of the tuning parameter  $r$

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



# 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

- 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.
- 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.