The interplay of antiferromagnetism and superconductivity: new results and open questions

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Outline

1. Sign-problem free quantum Monte Carlo for the onset of antiferromagnetism in metals

2. Hole-doped cuprates:

   Where are the electron pockets in the Brillouin zone ?

   Is the pseudogap state an exotic metal with Fermi pockets which violate the Luttinger relation ? (Such a violation requires emergent gauge excitations: an example of such a metal is the Z_2-FL* state)

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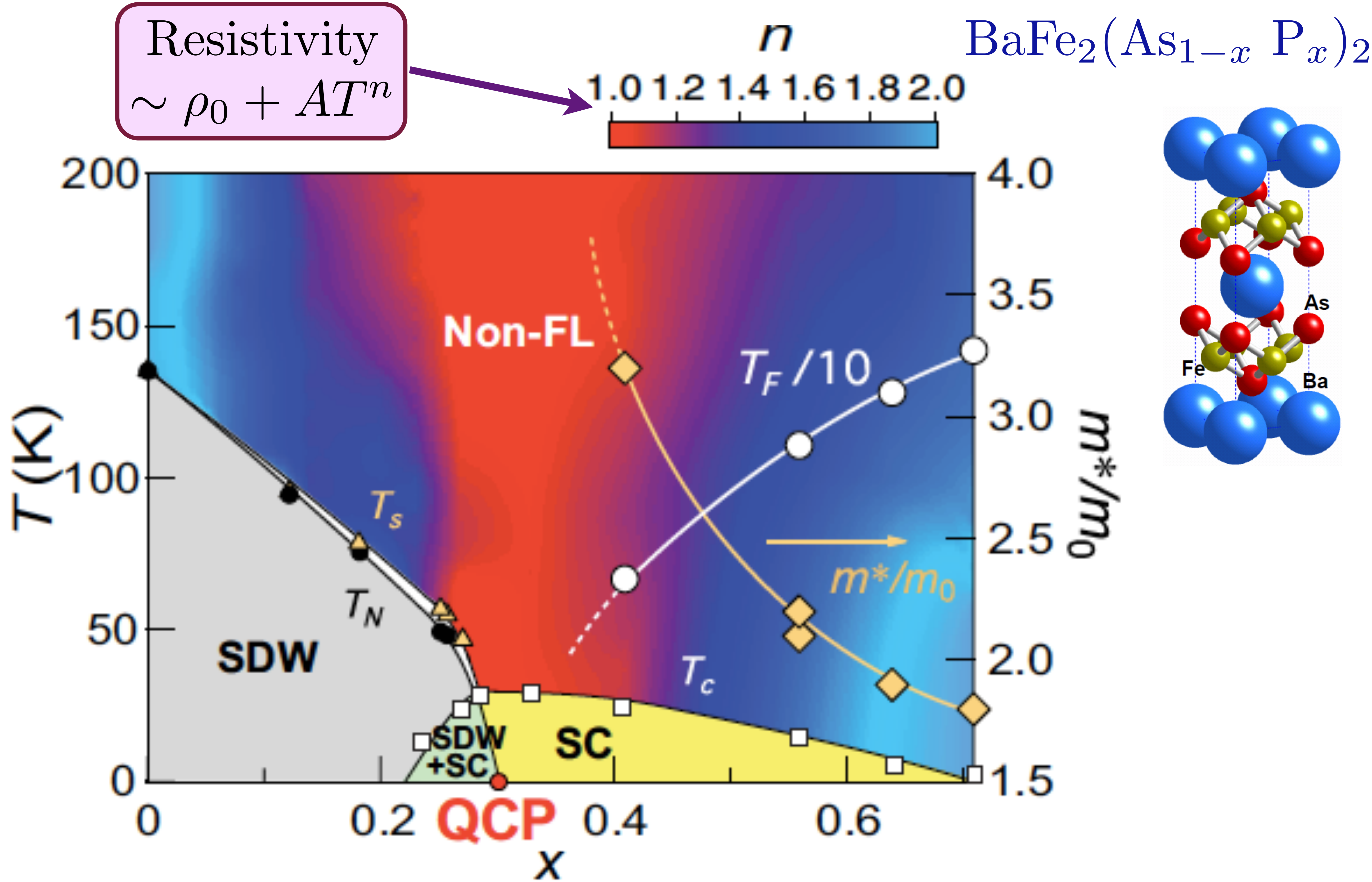
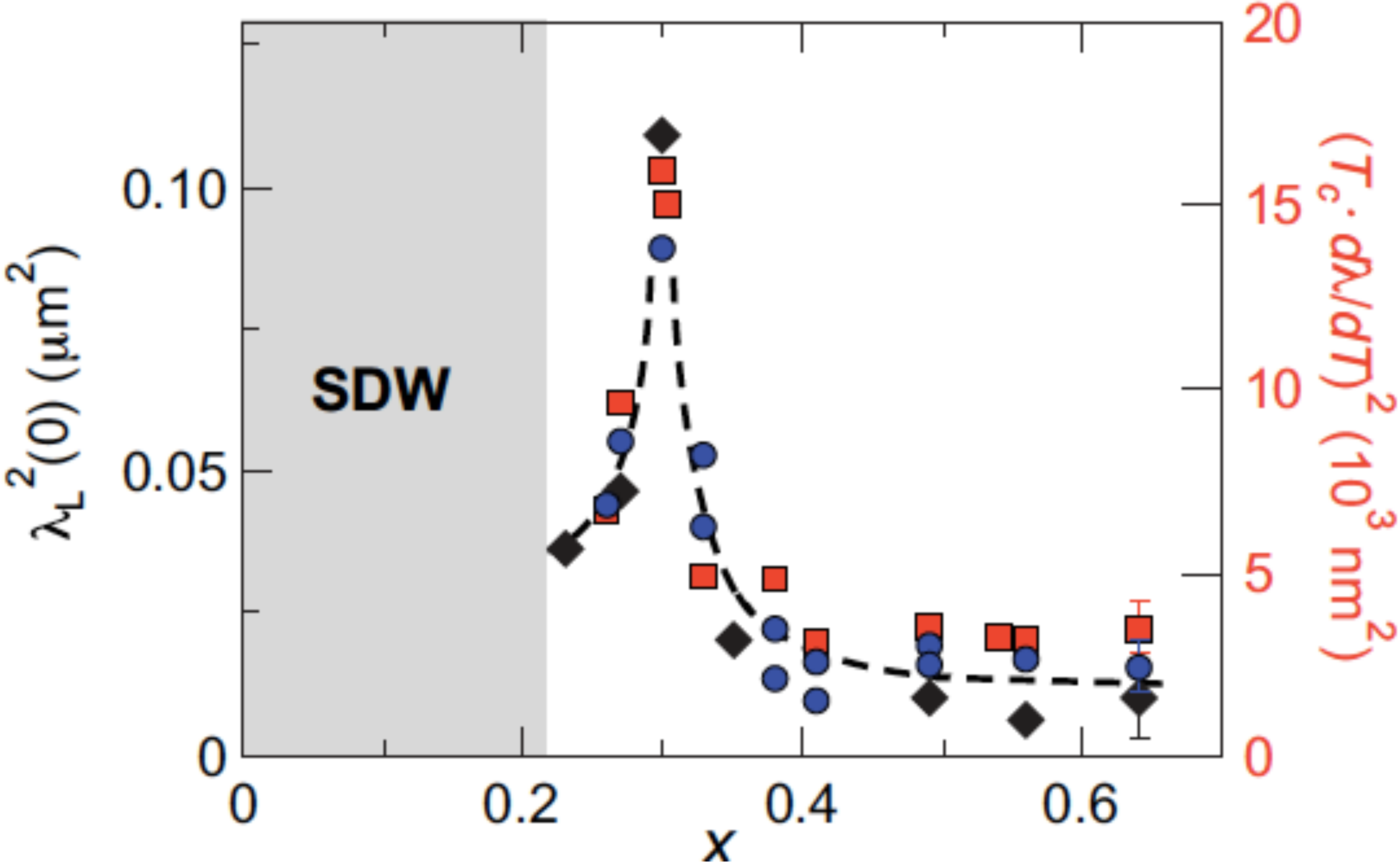
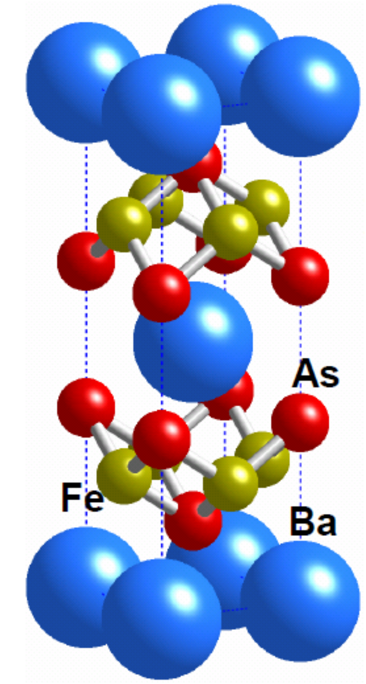


K. Hashimoto, K. Cho, T. Shibauchi, S. Kasahara, Y. Mizukami, R. Katsumata, Y. Tsuruhara, T. Terashima, H. Ikeda, M. A. Tanatar, H. Kitano, N. Salovich, R. W. Giannetta, P. Walmsley, A. Carrington, R. Prozorov, and Y. Matsuda, *Science* **336**, 1554 (2012).

$BaFe_2(As_{1-x}\ P_x)_2$





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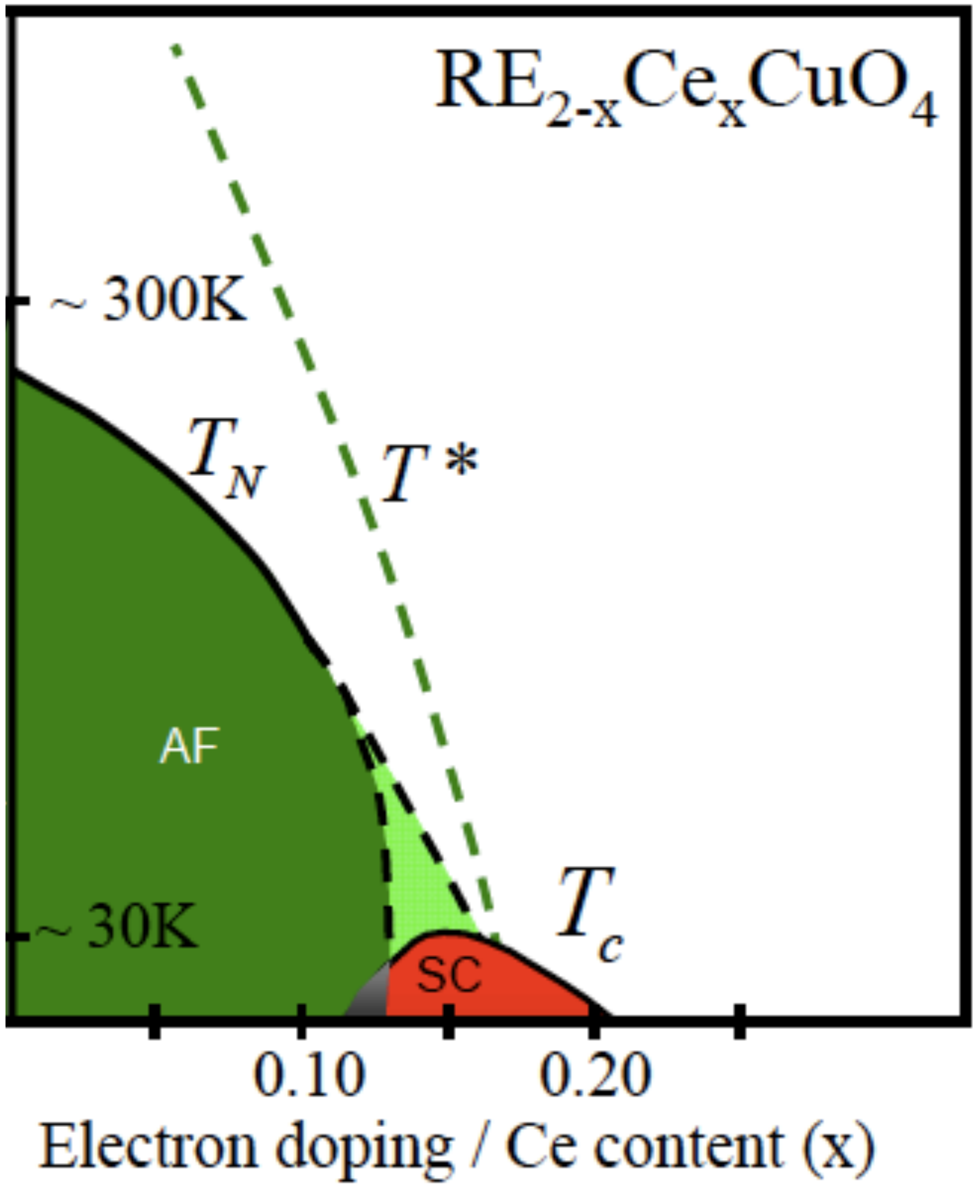
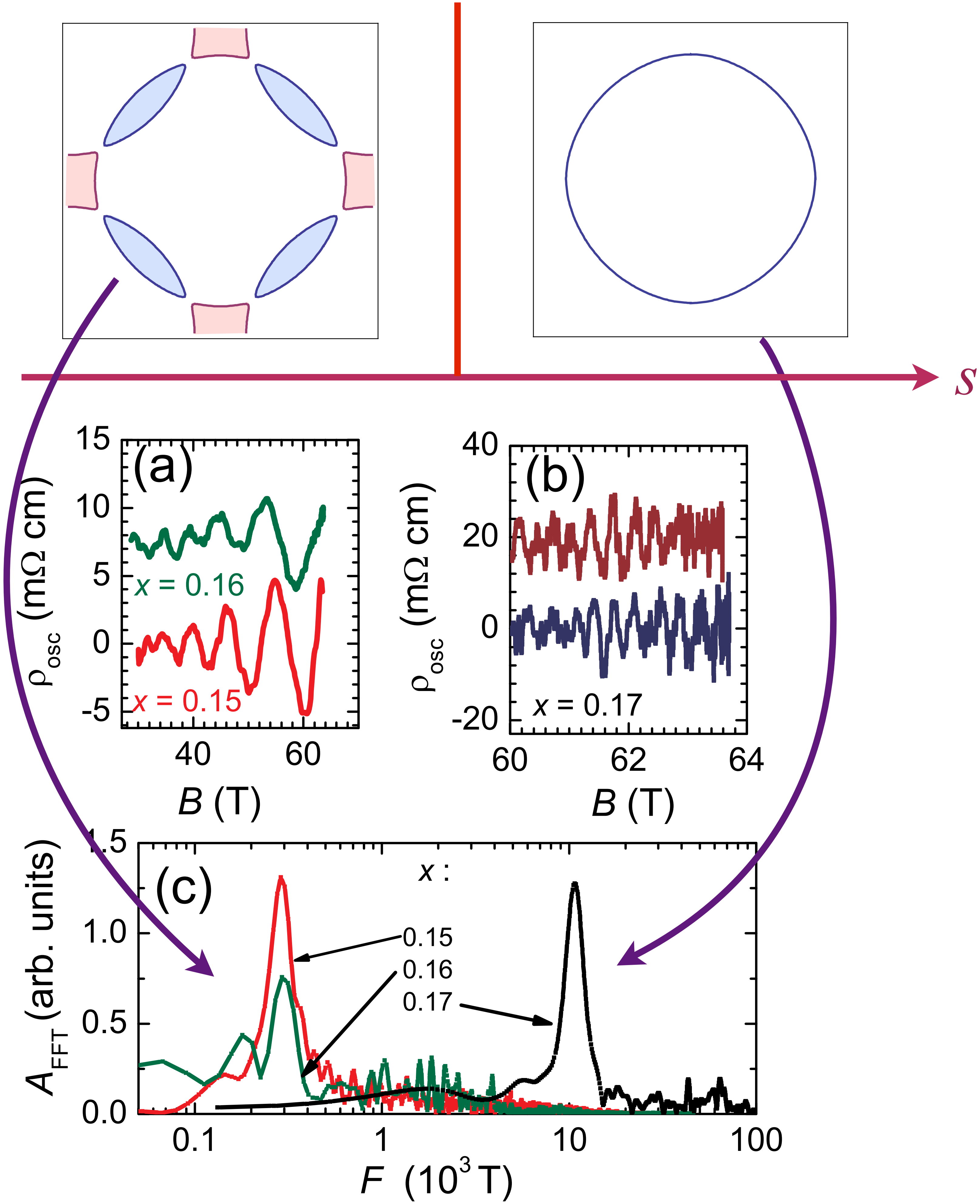


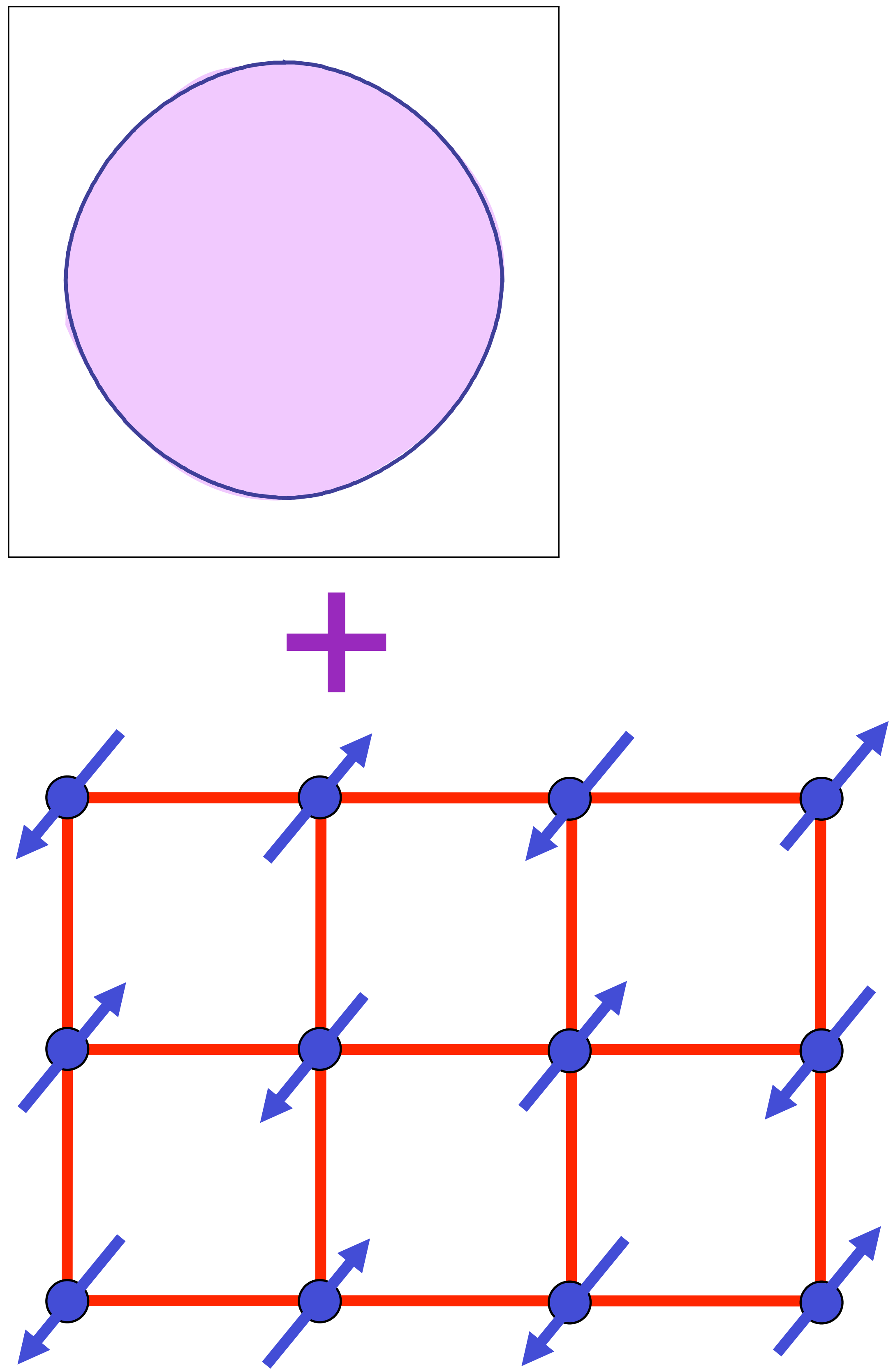


$Nd_{2-x}Ce_xCuO_4$

T. Helm, M.V. Kartsovnik,
M. Bartkowiak, N. Bittner,
M. Lambacher, A. Erb, J. Wosnitza,
and R. Gross,
Phys. Rev. Lett. **103**, 157002 (2009).

Fermi surface+antiferromagnetism

Metal with "large"
Fermi surface

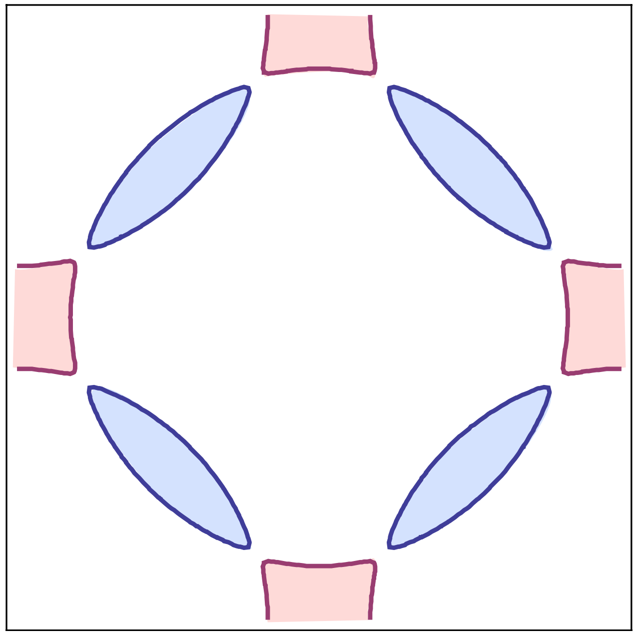


The electron spin polarization obeys

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

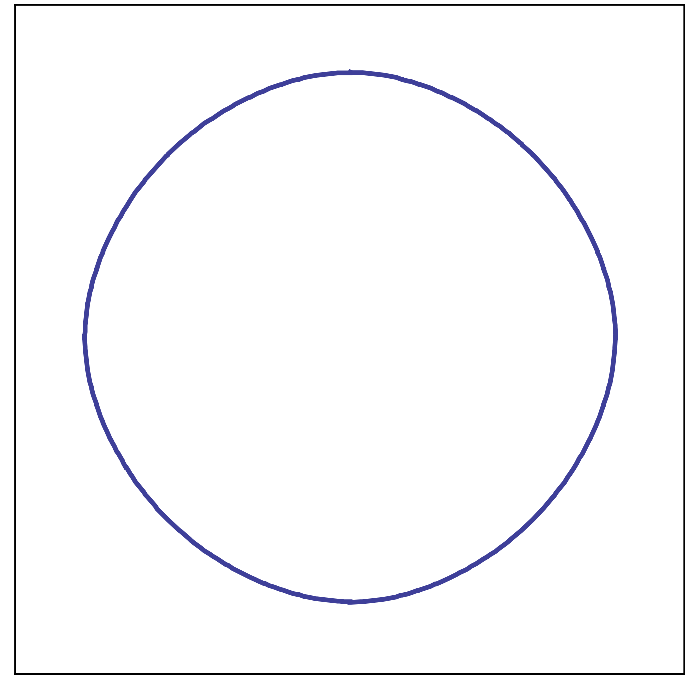
where $\mathbf{K}$ is the ordering wavevector.

Fermi surface+antiferromagnetism



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

Antiferromagnetic metal with electron and hole pockets



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

Metal with "large" Fermi surface

Increasing interaction

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

Theory for onset of antiferromagnetism

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

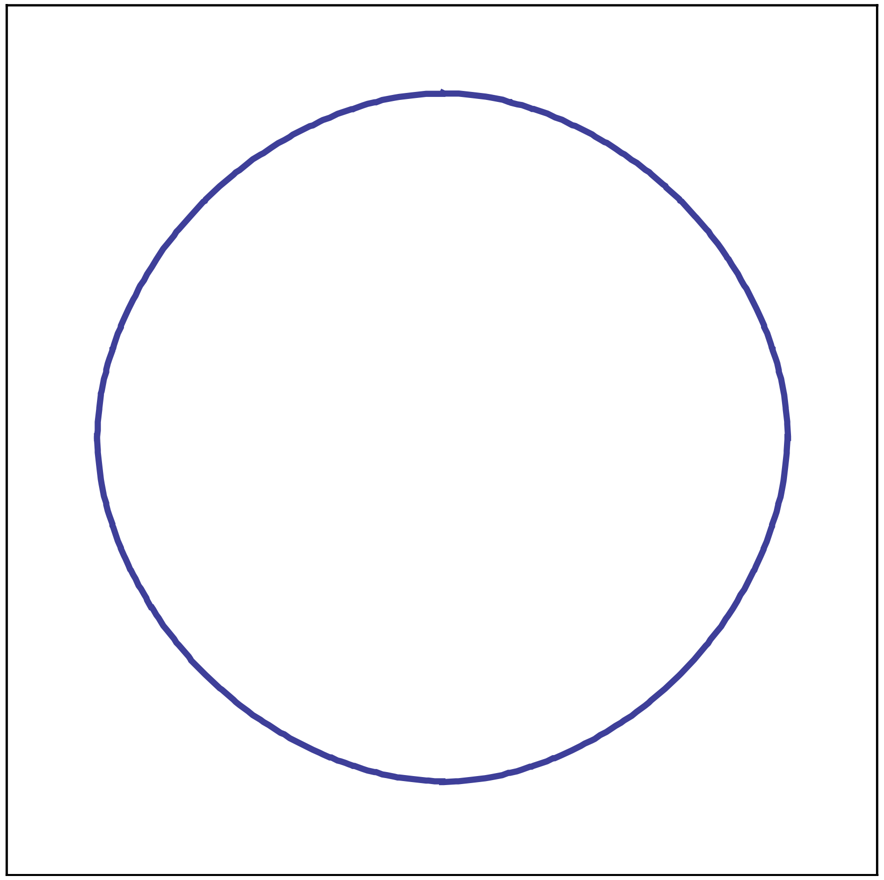
$$\mathcal{L}_c = c_a^\dagger \varepsilon(-i\boldsymbol{\nabla}) c_a$$

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

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

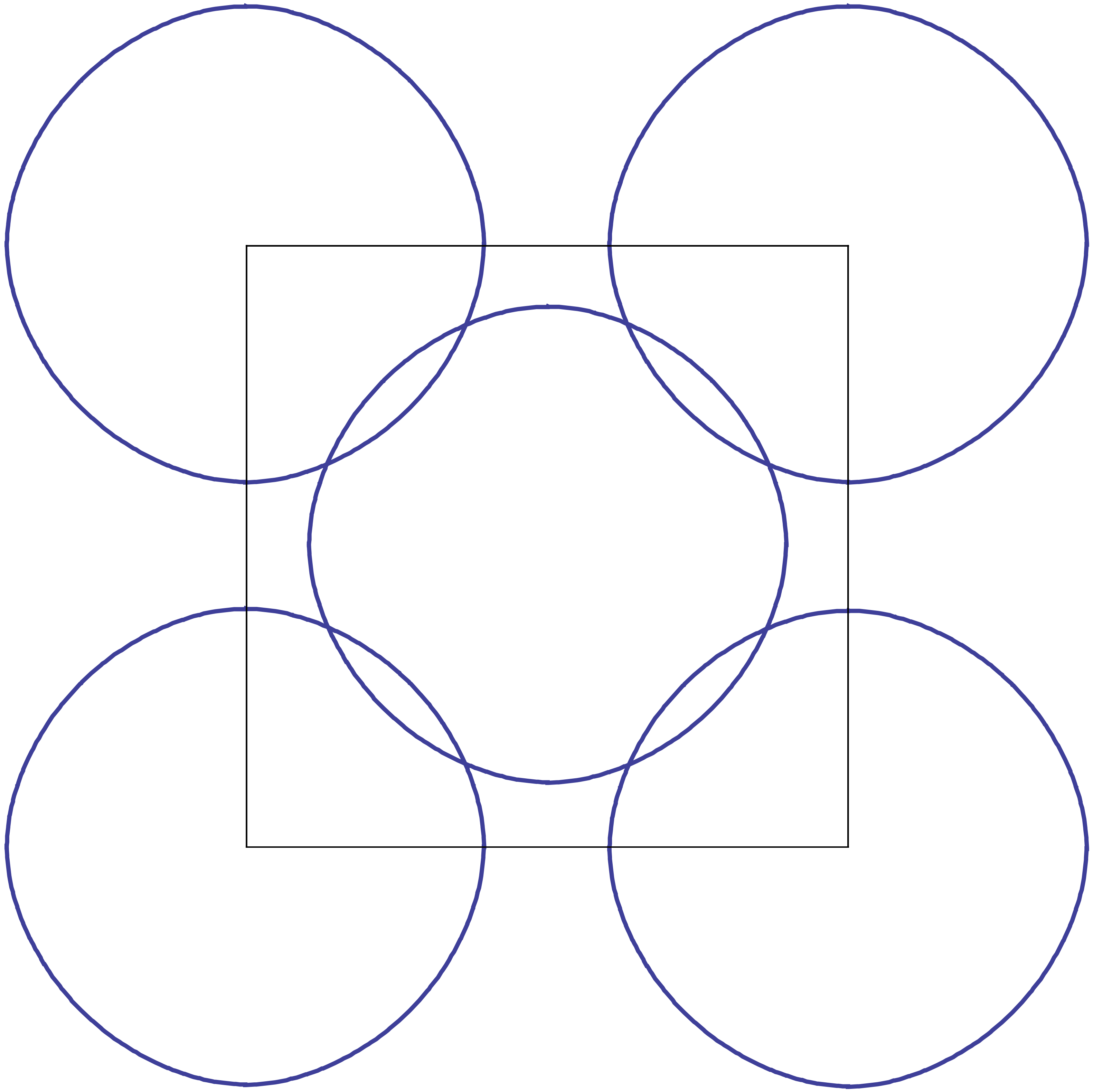
"Yukawa" coupling between fermions and antiferromagnetic order:
$\lambda^2 \sim U$, the Hubbard repulsion

Fermi surface+antiferromagnetism



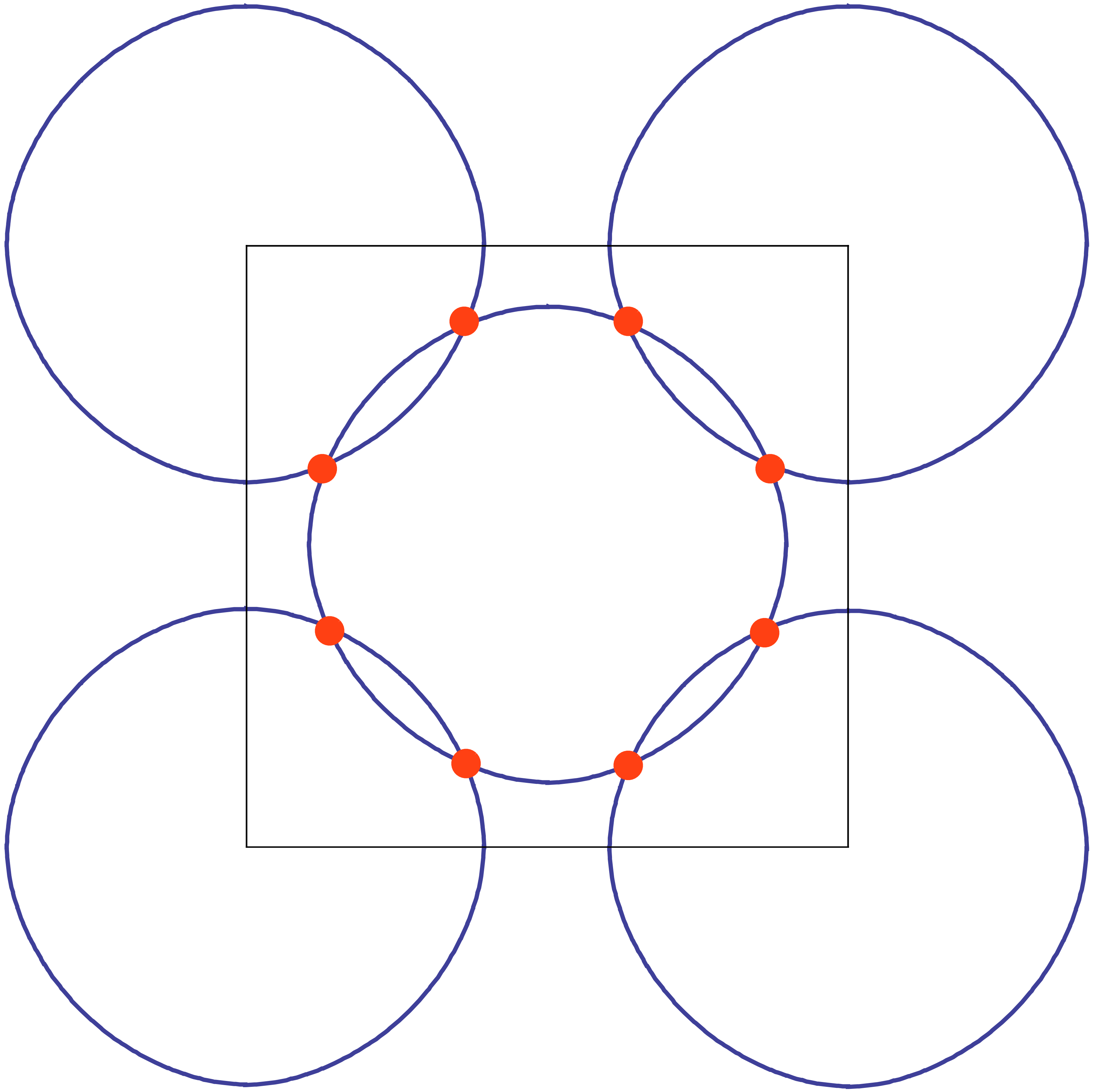
Metal with "large" Fermi surface

Fermi surface+antiferromagnetism



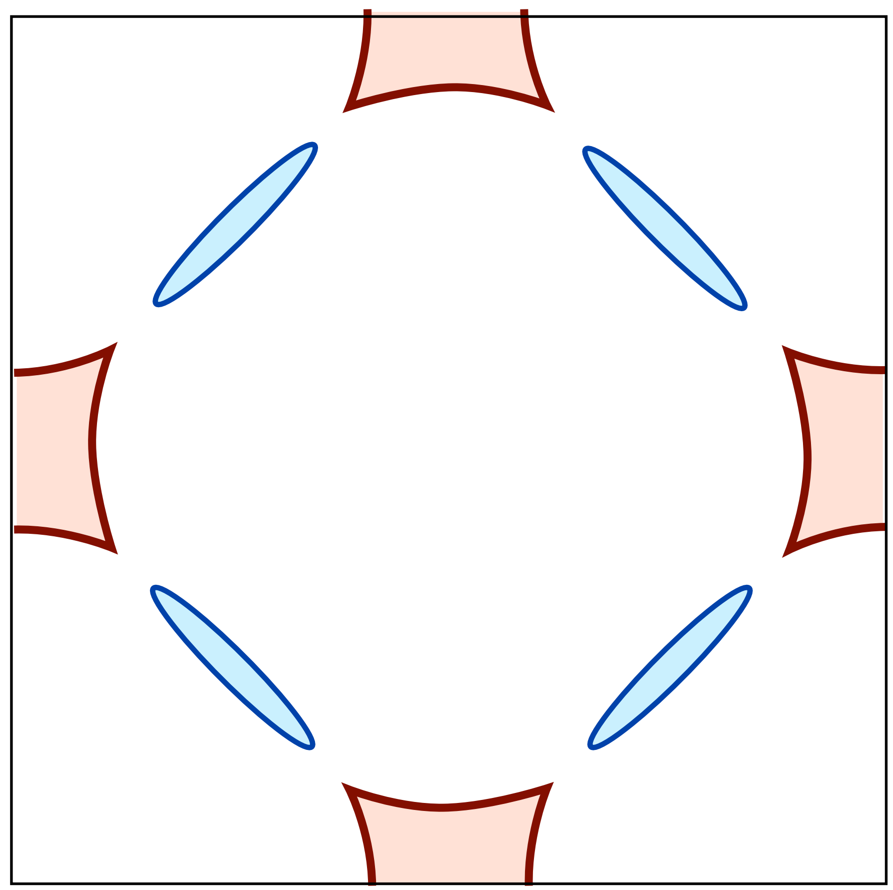
Fermi surfaces translated by $\mathbf{K} = (\pi, \pi)$.

Fermi surface+antiferromagnetism



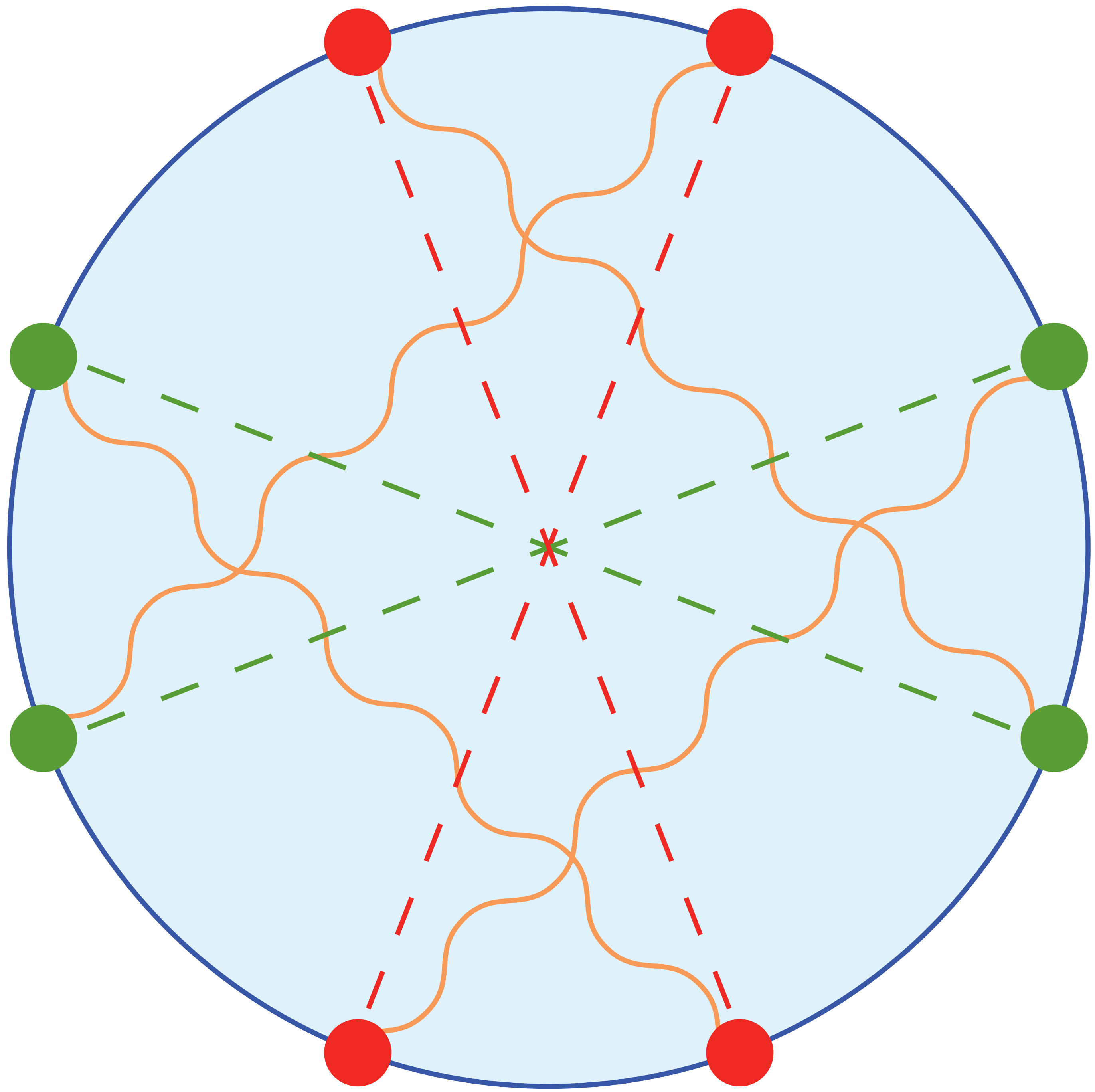
“Hot” spots

Fermi surface+antiferromagnetism



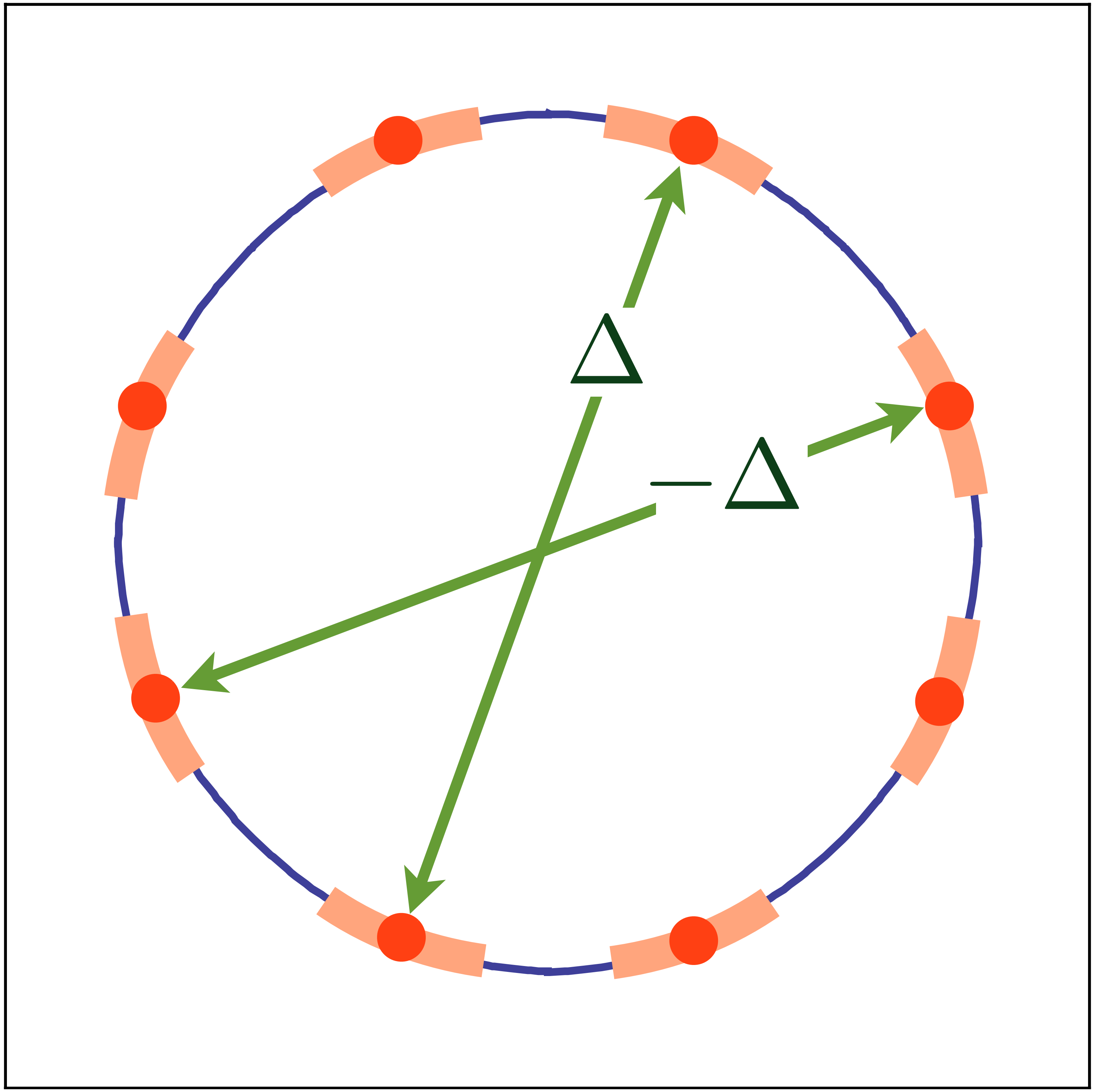
Electron and hole pockets in antiferromagnetic phase with $\langle \vec{\varphi} \rangle \neq 0$

Pairing "glue" from antiferromagnetic fluctuations



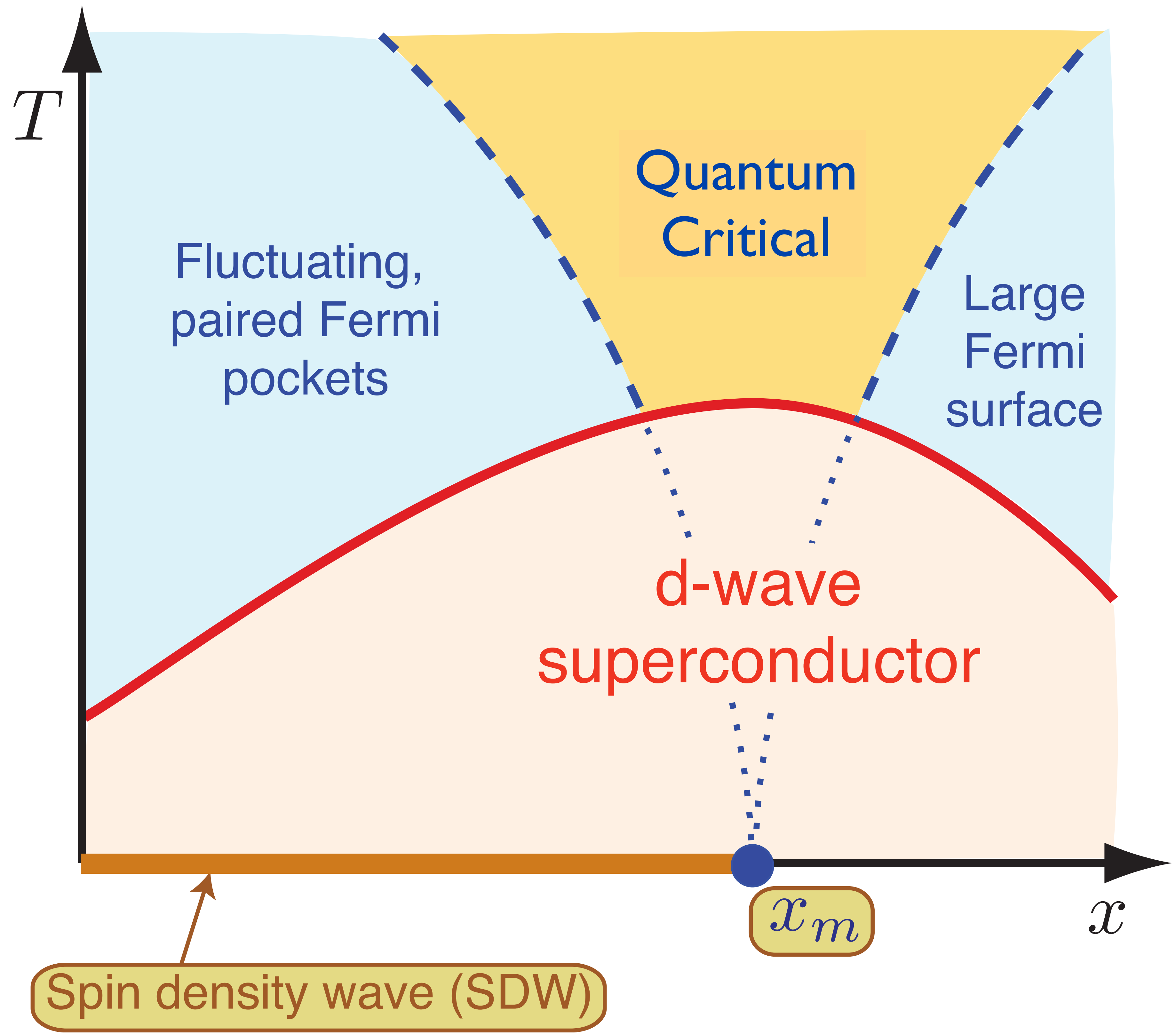
V. J. Emery, *J. Phys. (Paris) Colloq.* **44**, C3-977 (1983)
D.J. Scalapino, E. Loh, and J.E. Hirsch, *Phys. Rev. B* **34**, 8190 (1986)
K. Miyake, S. Schmitt-Rink, and C. M.Varma, *Phys. Rev. B* **34**, 6554 (1986)
S. Raghu, S.A. Kivelson, and D.J. Scalapino, *Phys. Rev. B* **81**, 224505 (2010)

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

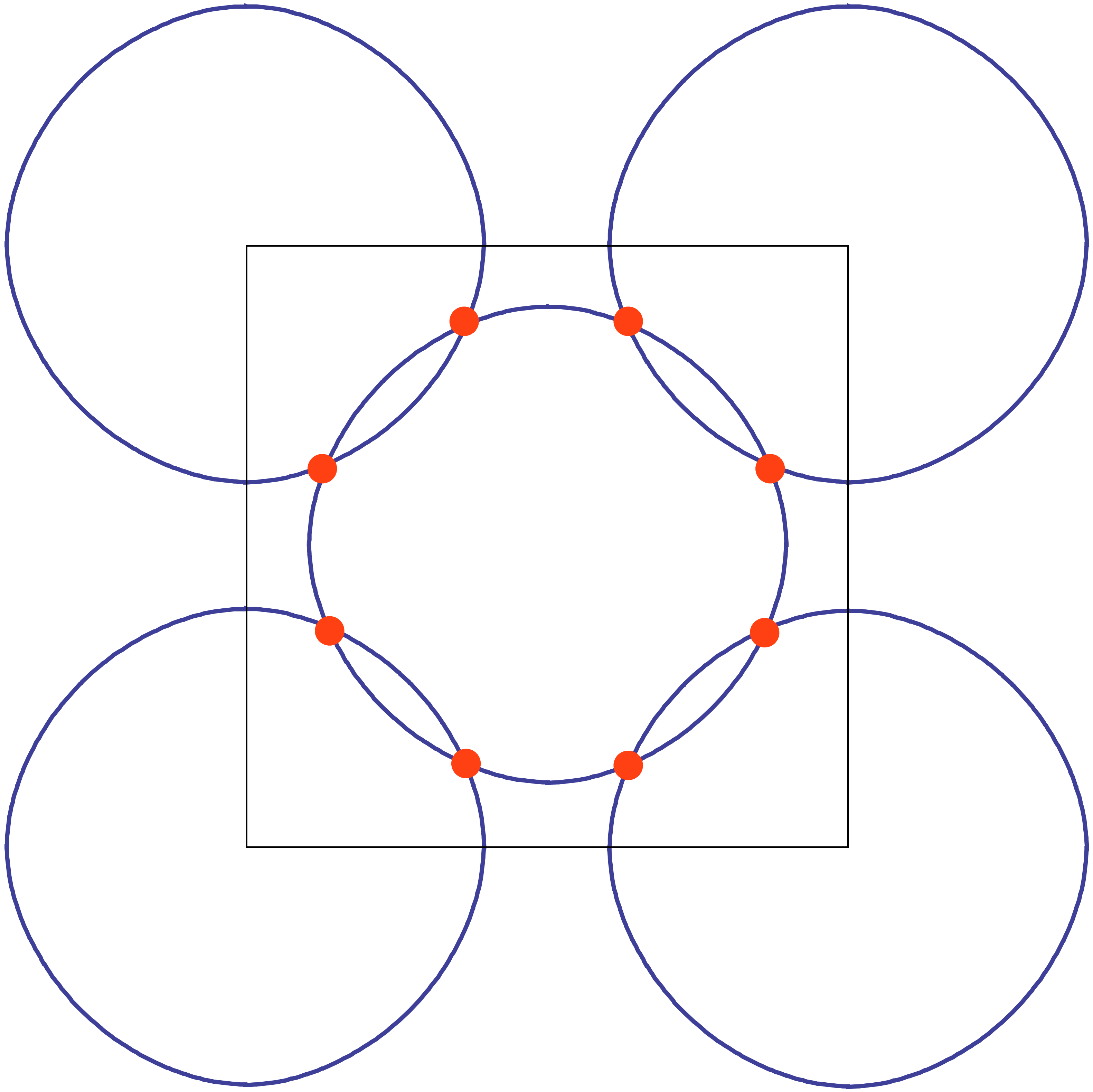


Unconventional pairing at *and near* hot spots

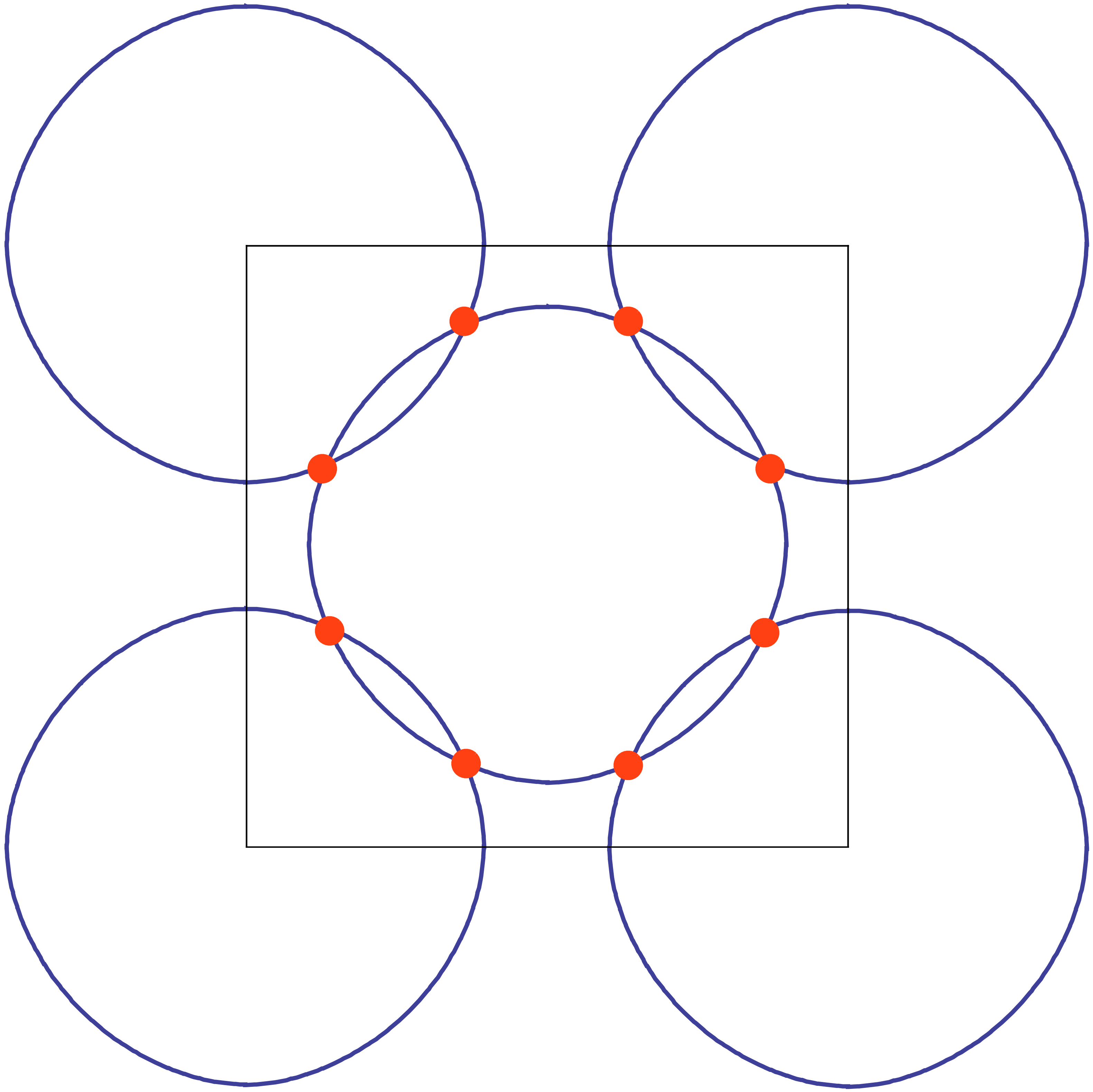
Fermi surface+antiferromagnetism



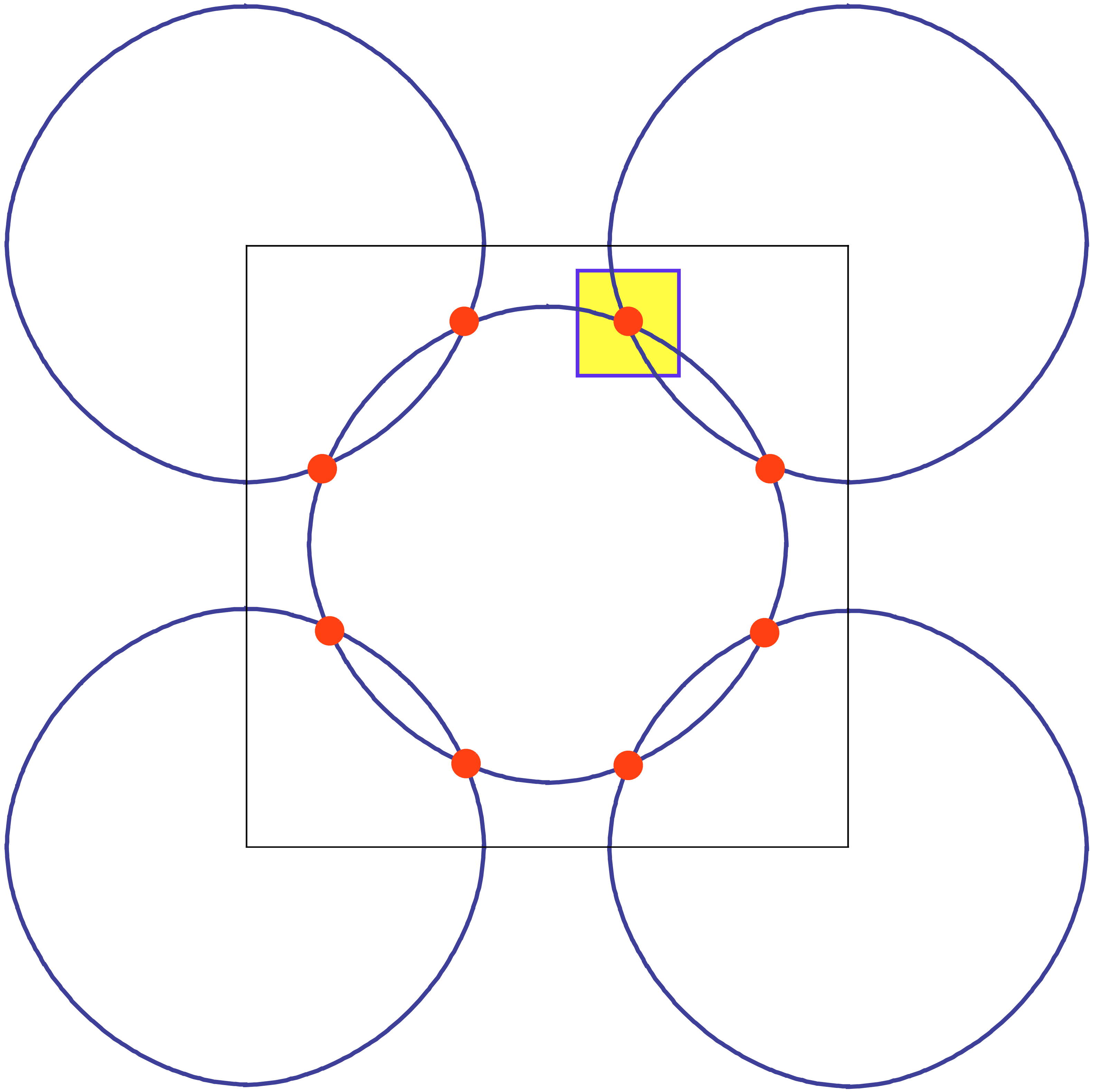
QCP for the onset of SDW order is actually within a superconductor



“Hot” spots

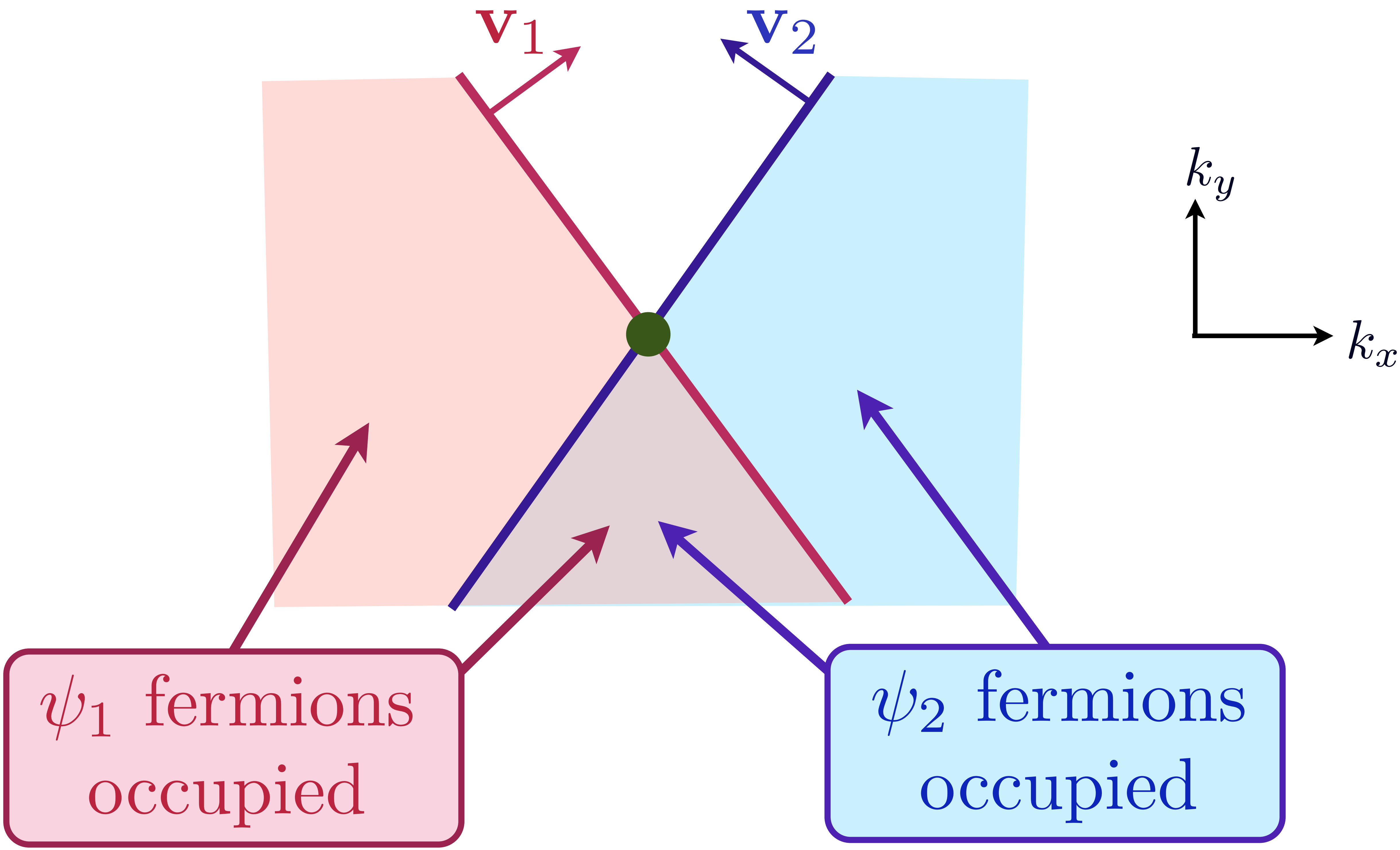


Low energy theory for critical point near hot spots



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



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

$$
\begin{aligned}
\mathcal{L} \;=\;& \psi_{1\alpha}^\dagger \left(\partial_\tau - i\mathbf{v}_1 \cdot \boldsymbol{\nabla}_r\right) \psi_{1\alpha} + \psi_{2\alpha}^\dagger \left(\partial_\tau - i\mathbf{v}_2 \cdot \boldsymbol{\nabla}_r\right) \psi_{2\alpha} \\
&+ \frac{1}{2}\left(\boldsymbol{\nabla}_r \vec{\varphi}\right)^2 + \frac{s}{2}\vec{\varphi}^2 + \frac{u}{4}\vec{\varphi}^4 \\
&- \lambda \vec{\varphi} \cdot \left(\psi_{1\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{1\beta}\right)
\end{aligned}
$$

Ar. Abanov and A.V. Chubukov, *Phys. Rev. Lett.* **93**, 255702 (2004).

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

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&+\frac{1}{2}\left(\boldsymbol{\nabla}_r\vec{\varphi}\right)^2 + \frac{s}{2}\vec{\varphi}^2 + \frac{u}{4}\vec{\varphi}^4 \\
&-\lambda\vec{\varphi}\cdot\left(\psi^\dagger_{1\alpha}\vec{\sigma}_{\alpha\beta}\psi_{2\beta} + \psi^\dagger_{2\alpha}\vec{\sigma}_{\alpha\beta}\psi_{1\beta}\right)
\end{aligned}
$$

Note fermion spectrum has *lines* of zero energy excitations in momentum space.
If fermions are replaced by massless Dirac fermions with *points* of zero energy excitations, then critical theory is well-understood

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

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\begin{aligned}
\mathcal{L} \;=\;& \psi_{1\alpha}^{\dagger}\left(\partial_{\tau} - i\mathbf{v}_1 \cdot \boldsymbol{\nabla}_r\right)\psi_{1\alpha} + \psi_{2\alpha}^{\dagger}\left(\partial_{\tau} - i\mathbf{v}_2 \cdot \boldsymbol{\nabla}_r\right)\psi_{2\alpha} \\
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M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **82**, 075128 (2010)
S.A. Hartnoll, D.M. Hofman, M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **84**, 125115 (2011)

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

$$\begin{aligned}\mathcal{L} \; = \; & \psi_{1\alpha}^\dagger \left(\partial_\tau - i\mathbf{v}_1 \cdot \boldsymbol{\nabla}_r\right) \psi_{1\alpha} + \psi_{2\alpha}^\dagger \left(\partial_\tau - i\mathbf{v}_2 \cdot \boldsymbol{\nabla}_r\right) \psi_{2\alpha} \\ & + \frac{1}{2} \left(\boldsymbol{\nabla}_r \vec{\varphi}\right)^2 + \frac{s}{2} \vec{\varphi}^2 + \frac{u}{4} \vec{\varphi}^4 \\ & - \lambda \vec{\varphi} \cdot \left(\psi_{1\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{1\beta} \right)\end{aligned}$$

Theory flows to strong-coupling in $d = 2$.

M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **82**, 075128 (2010)
S.A. Hartnoll, D.M. Hofman, M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **84**, 125115 (2011)

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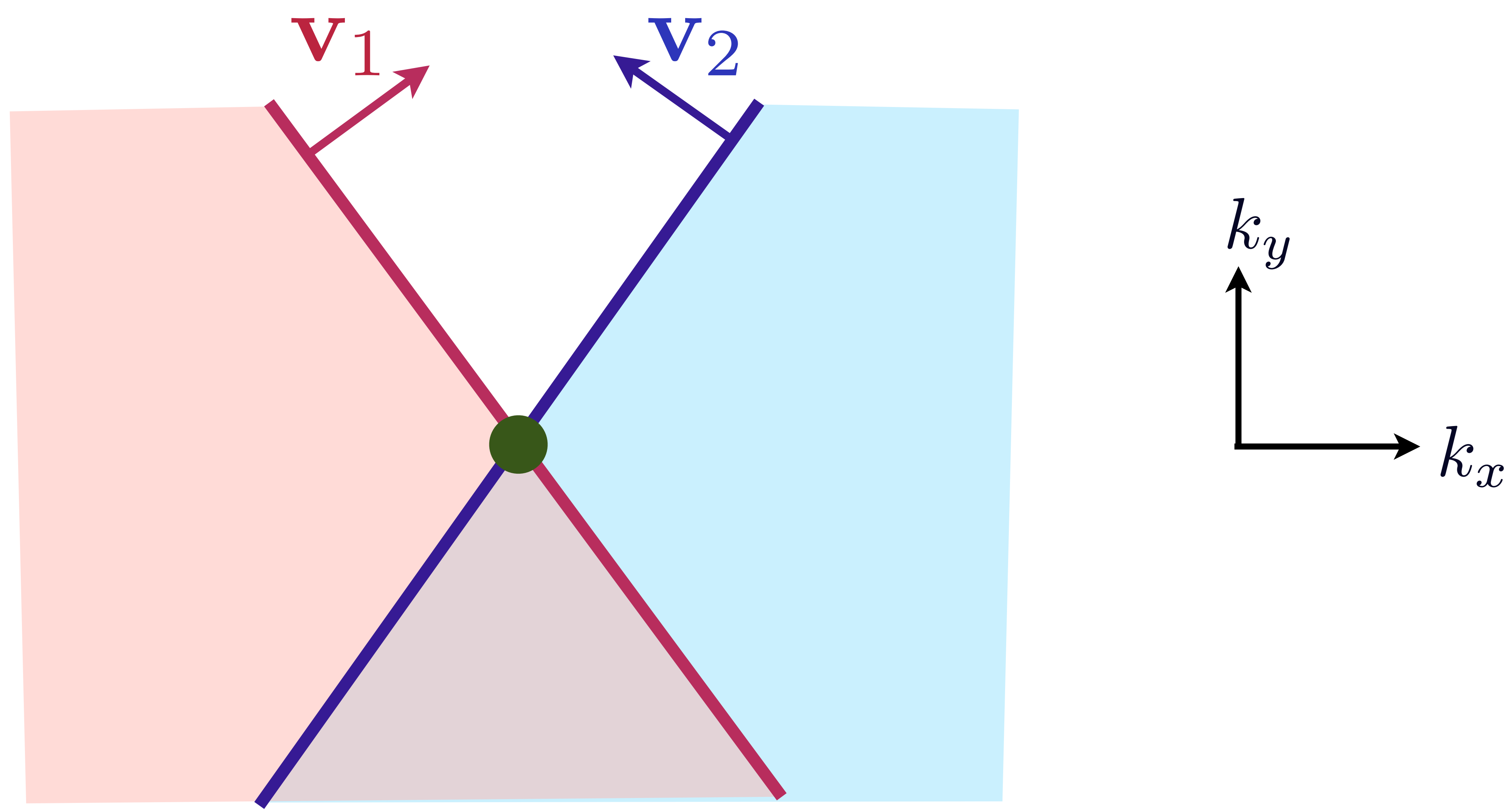
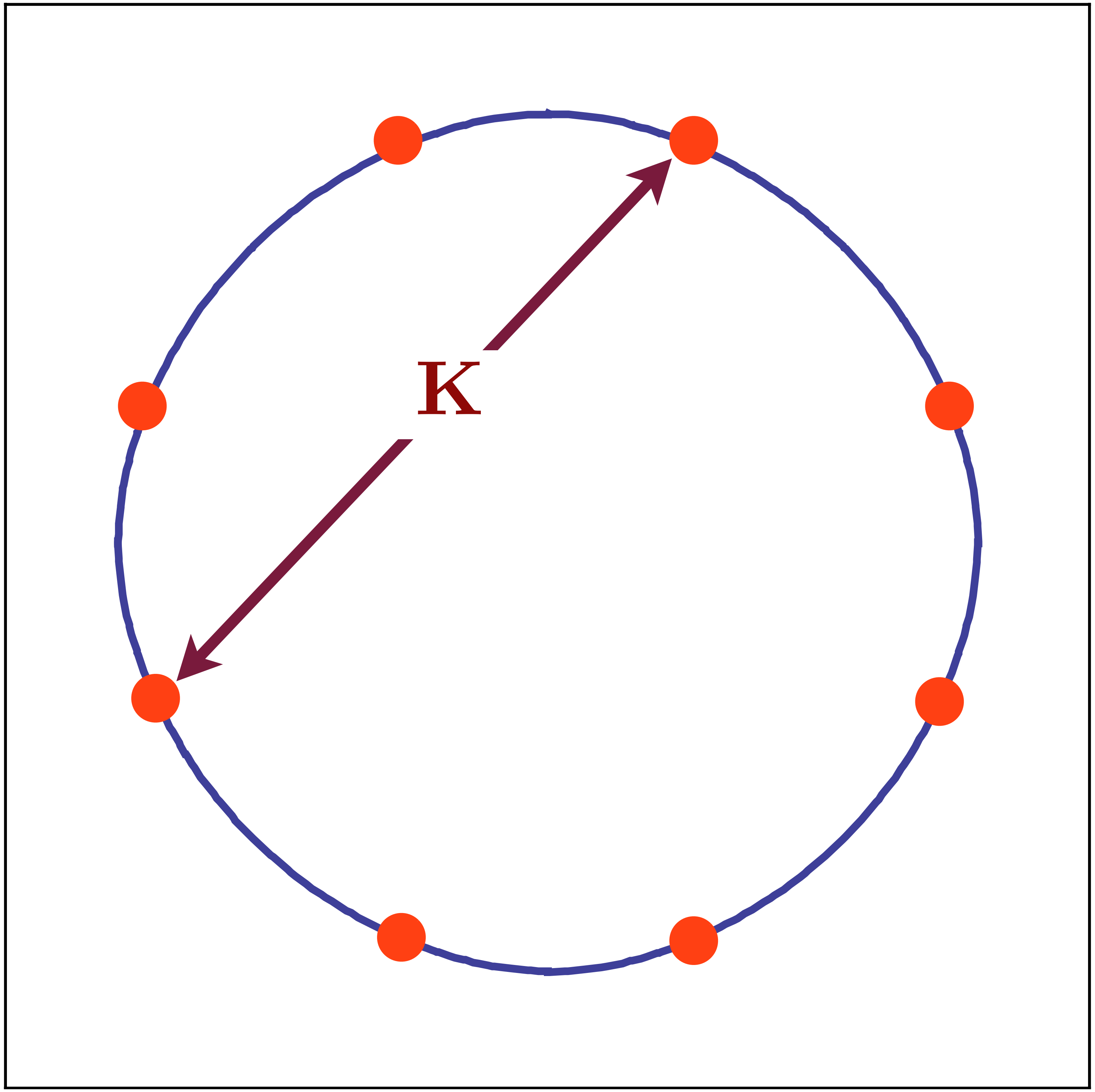


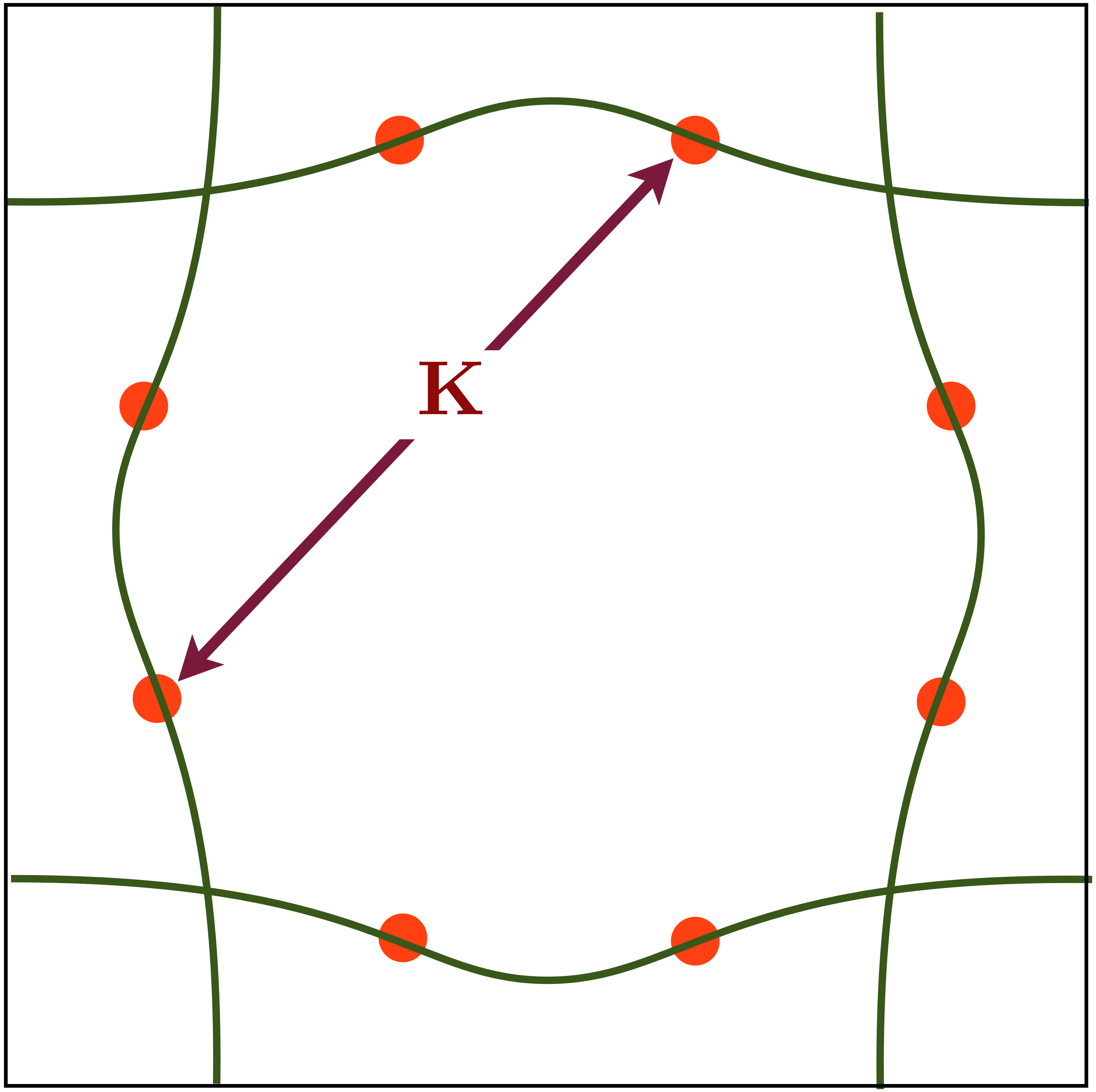
To faithfully realize low energy theory in quantum Monte Carlo, we need a UV completion in which Fermi lines don't end and all weights are positive.

QMC for the onset of antiferromagnetism



Hot spots in a single band model

QMC for the onset of antiferromagnetism

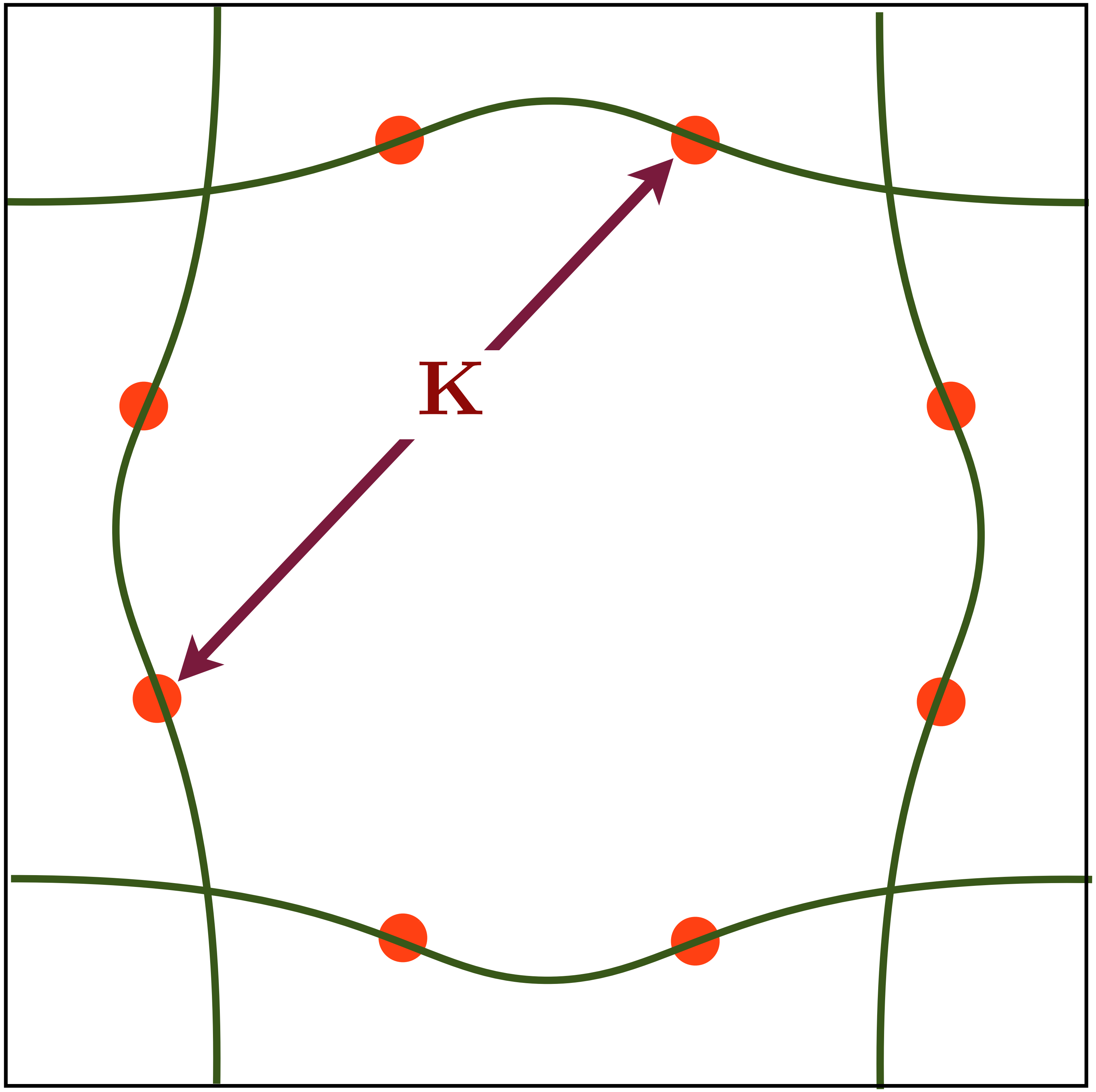


Hot spots in a two band model

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

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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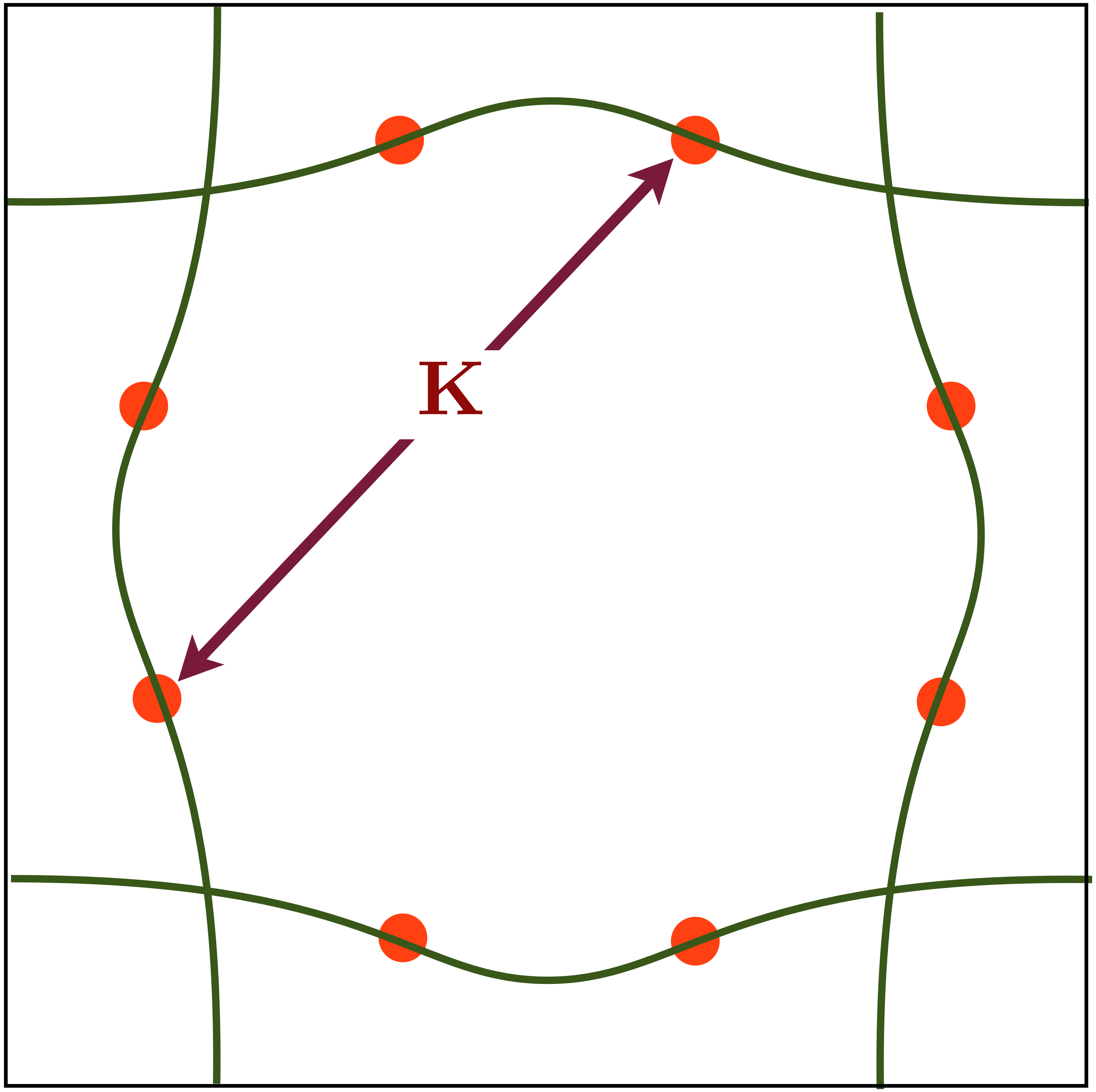

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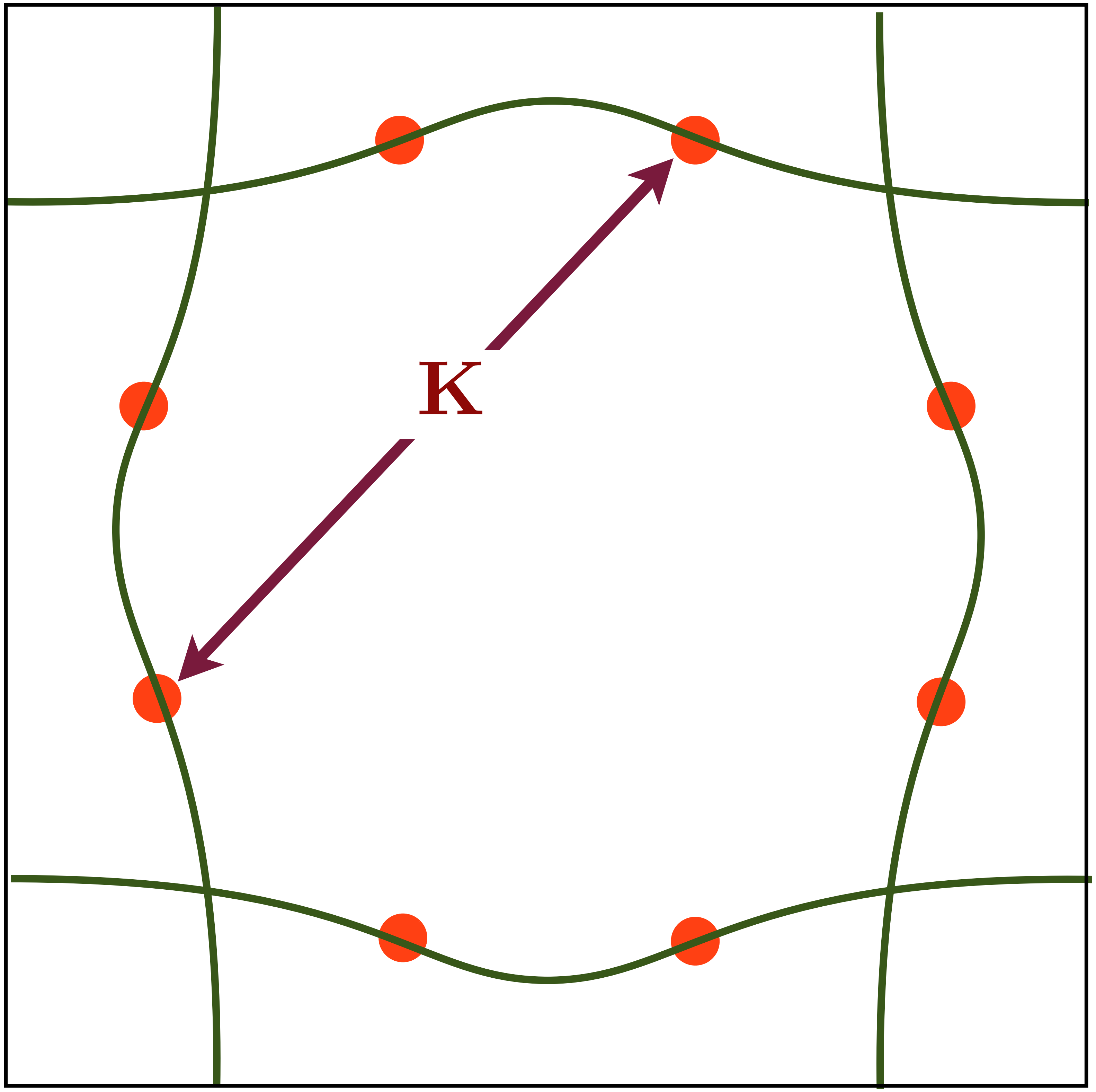
QMC for the onset of antiferromagnetism

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



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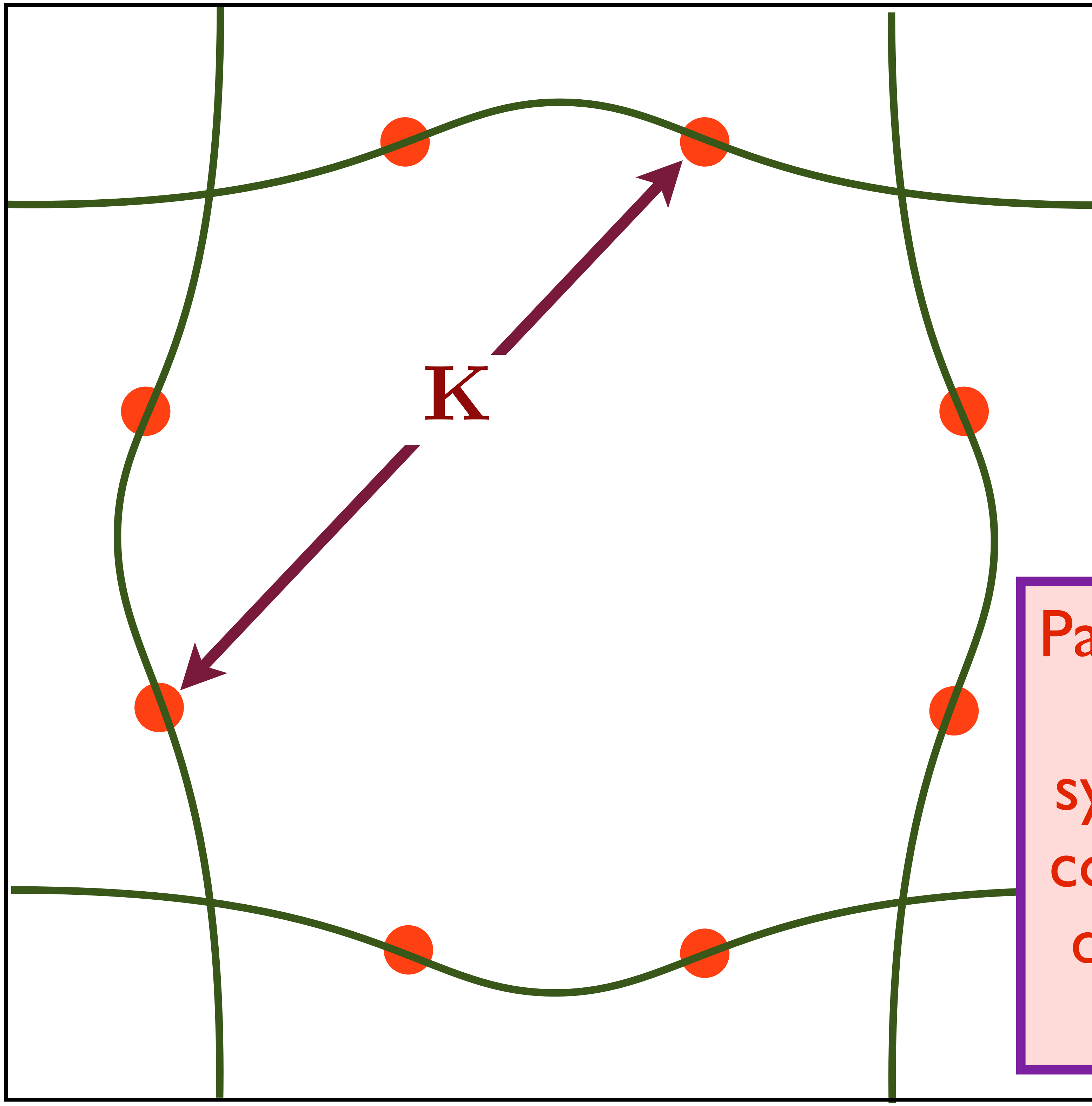

Hot spots in a two band model

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

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 $\vec{\varphi}$.

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

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

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

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

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 $\vec{\varphi}$.

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

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

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

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E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

QMC for the onset of antiferromagnetism

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S. Sachdev,
arXiv:1206.0742

No sign problem !

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

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

QMC for the onset of antiferromagnetism

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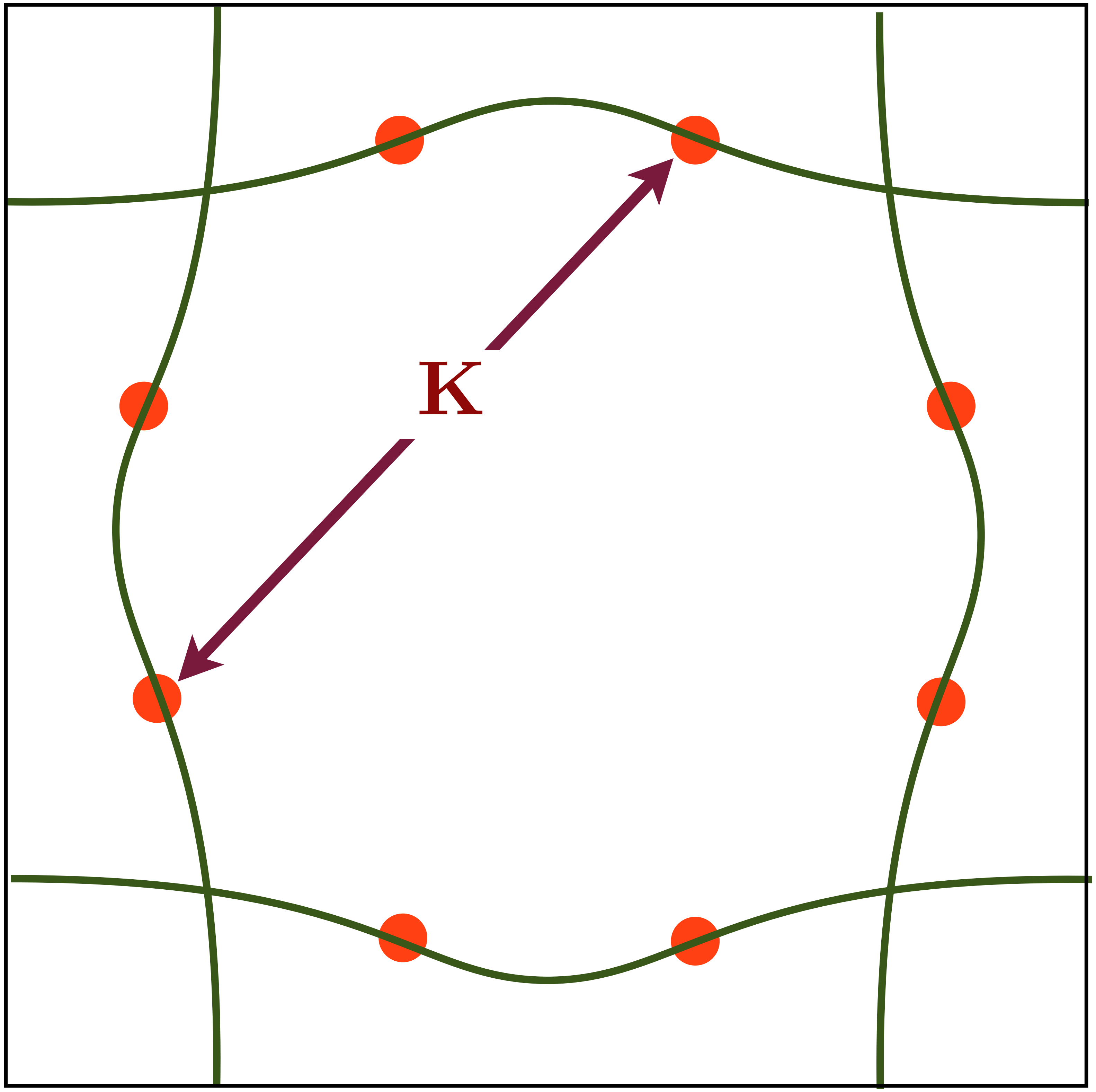
Can integrate out $\vec{\varphi}$ to obtain an extended Hubbard model. The interactions in this model only couple electrons in separate bands.

QMC for the onset of antiferromagnetism



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M. Metlitski, and
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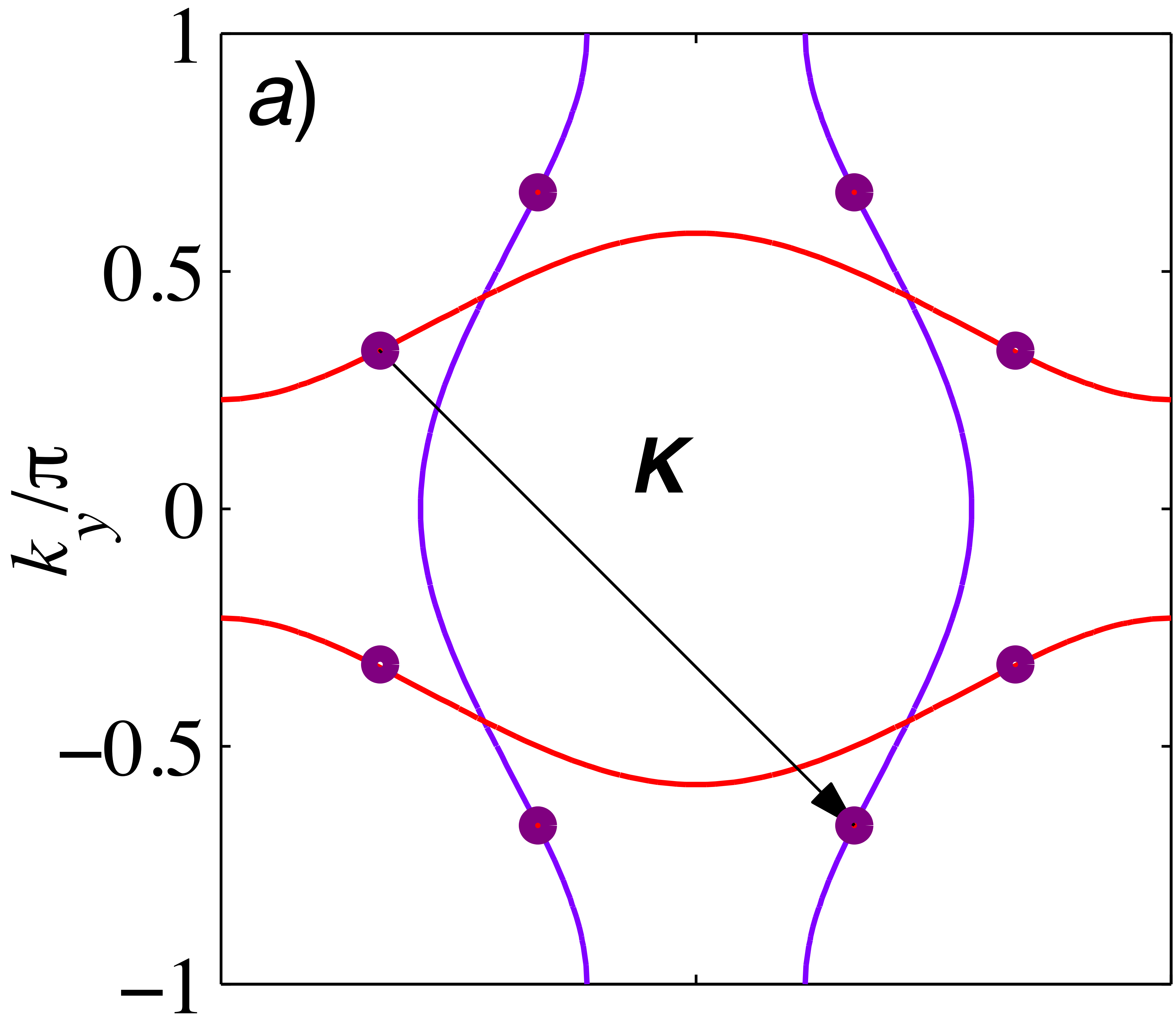
Hot spots in a two band model

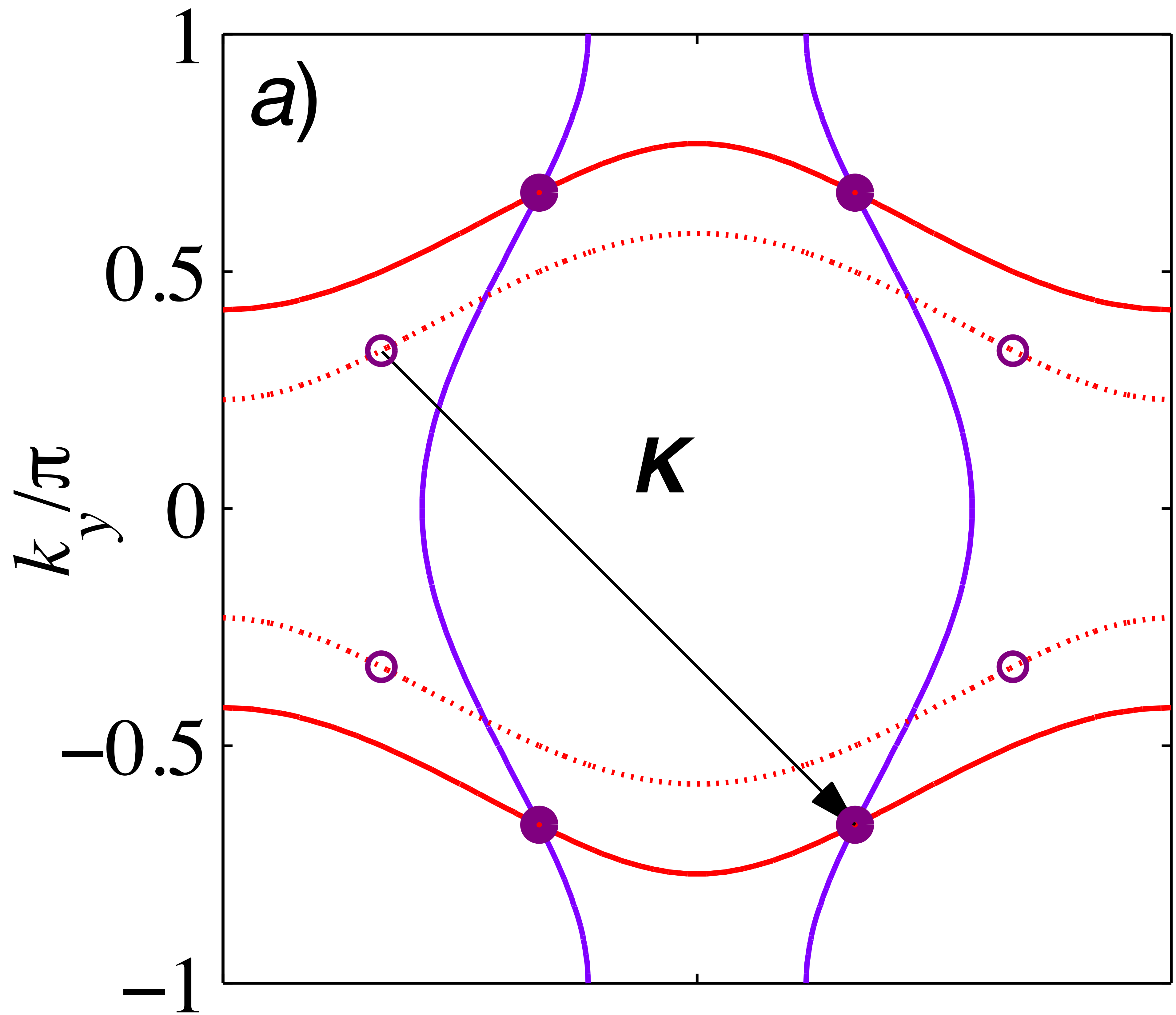
QMC for the onset of antiferromagnetism



Center Brillouin zone at (π,π,)

E. Berg,
M. Metlitski, and
S. Sachdev,
arXiv:1206.0742

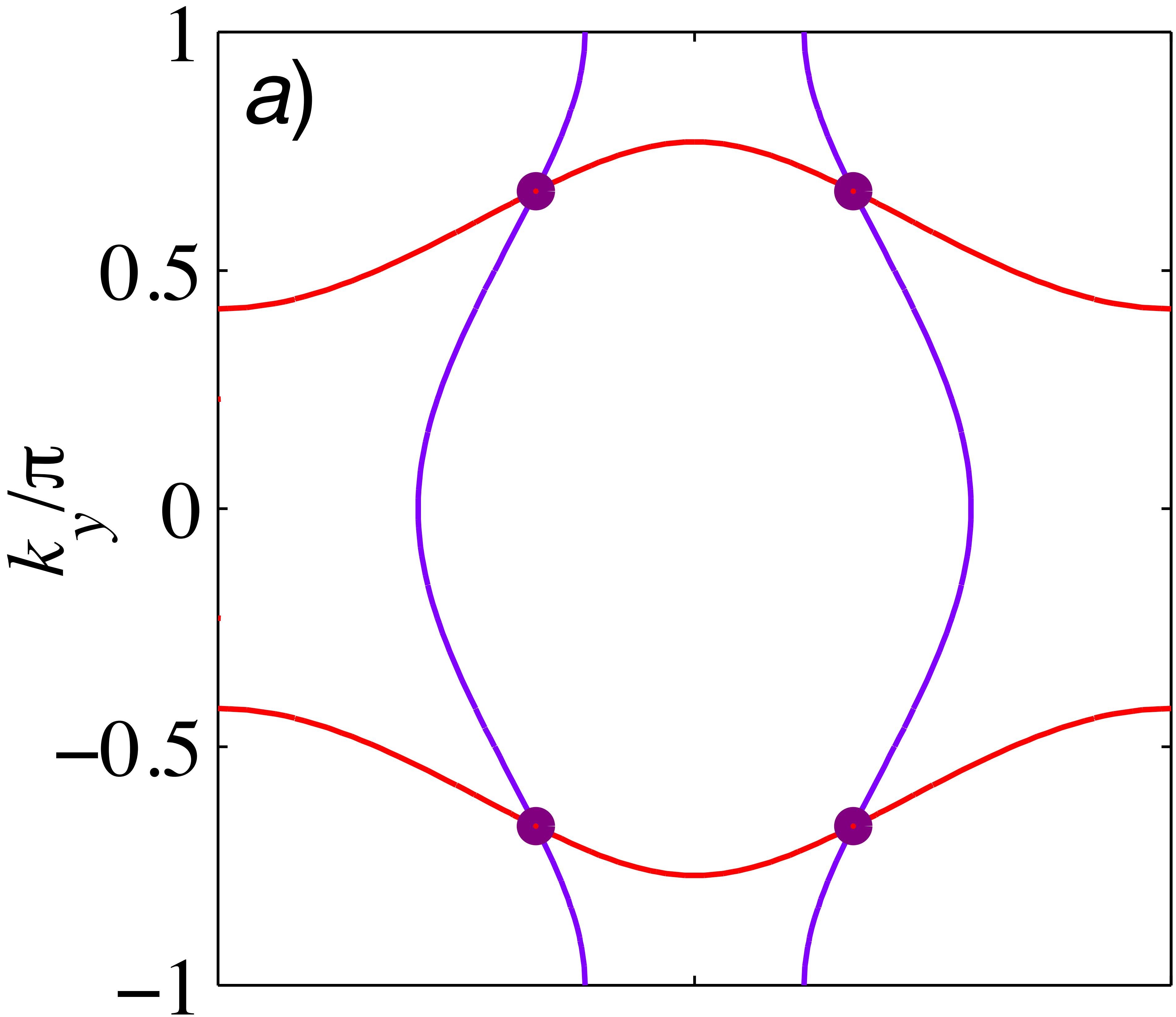
QMC for the onset of antiferromagnetism



E. Berg,
M. Metlitski, and
S. Sachdev,
arXiv:1206.0742

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

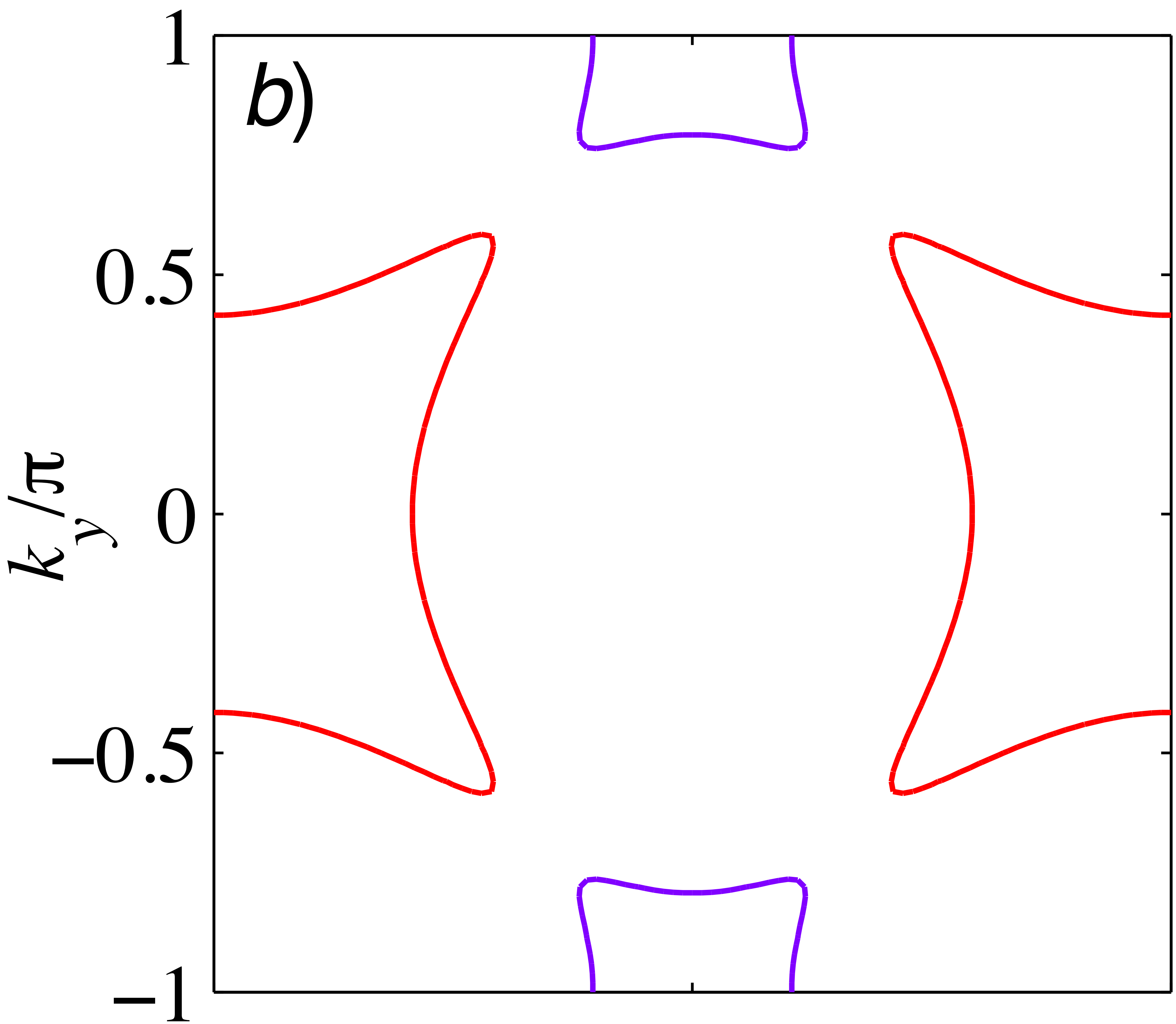
QMC for the onset of antiferromagnetism



E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

Now hot spots are at Fermi surface intersections

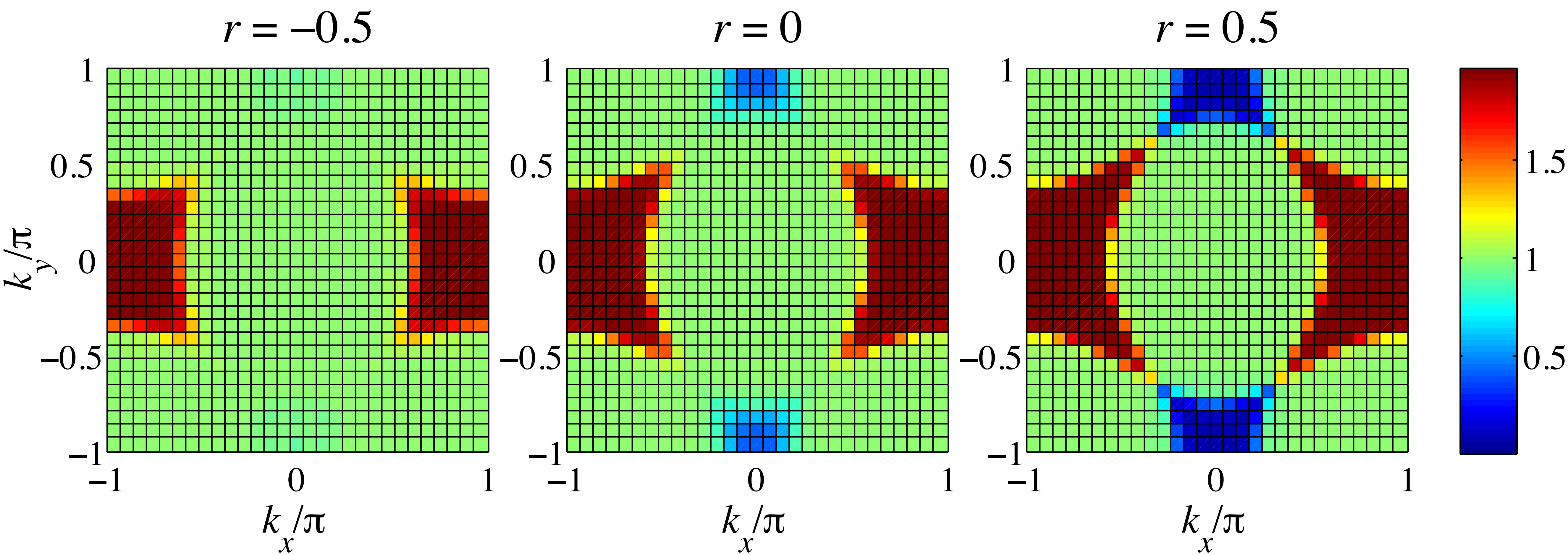
QMC for the onset of antiferromagnetism



E. Berg,
M. Metlitski, and
S. Sachdev,
arXiv:1206.0742

Expected Fermi surfaces in the AFM ordered phase

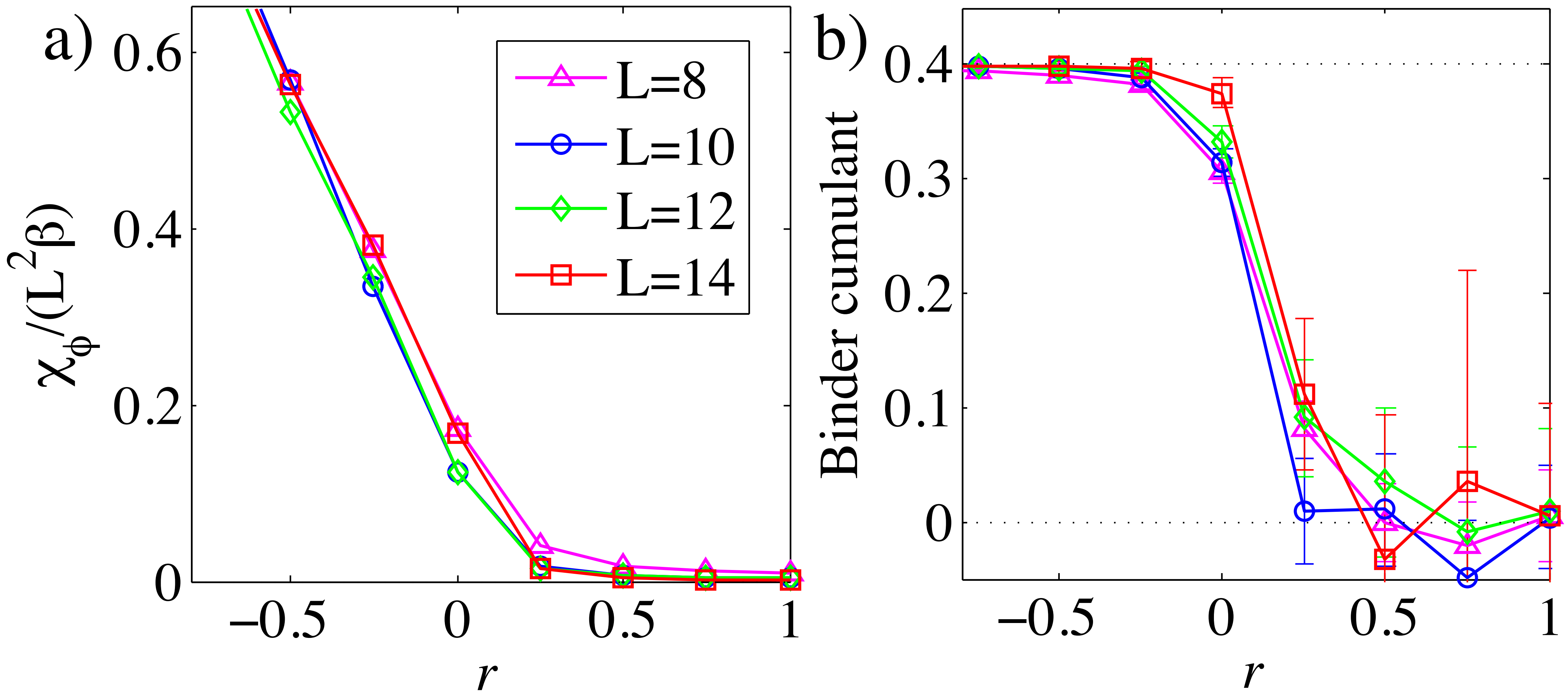
QMC for the onset of antiferromagnetism



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

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

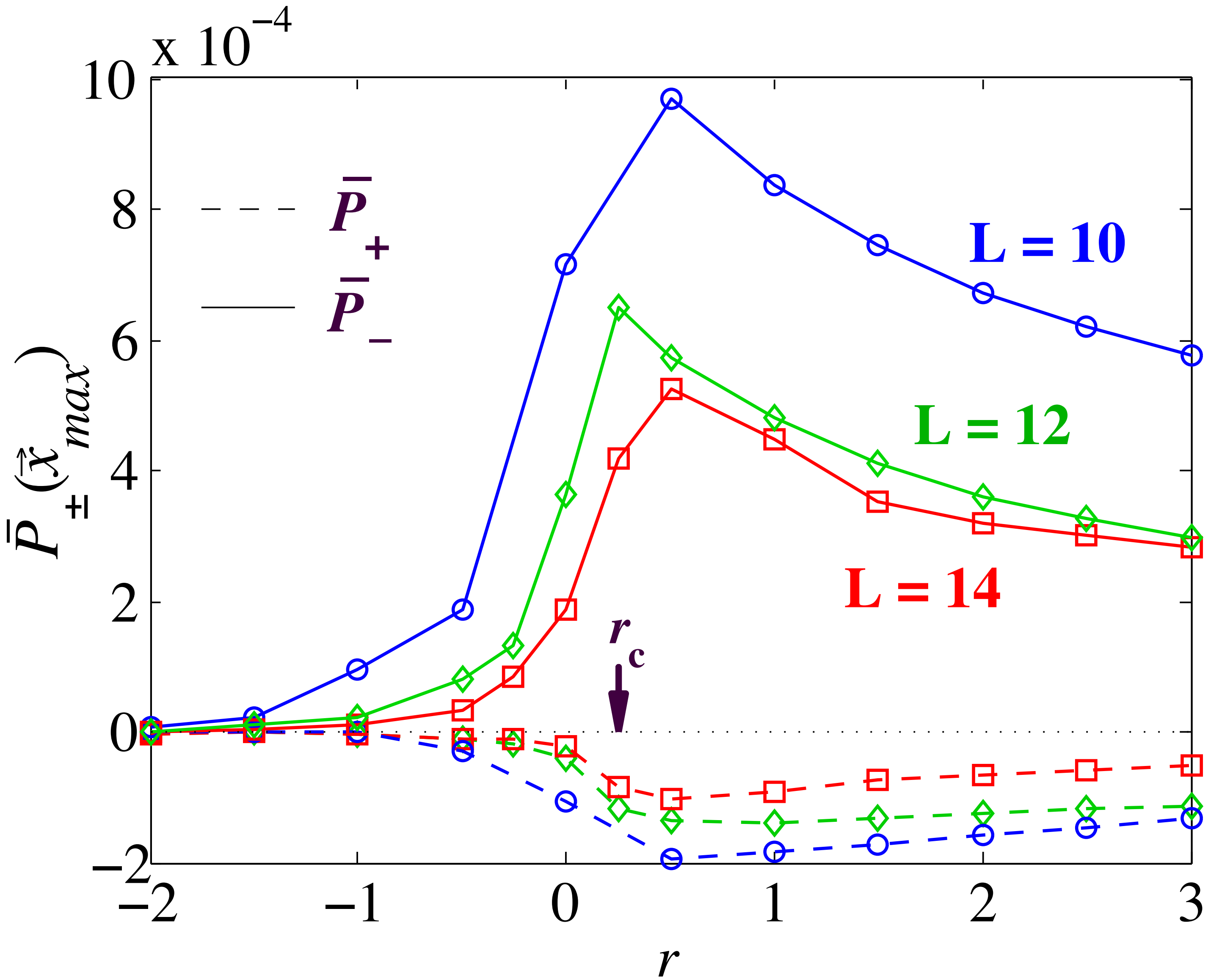
QMC for the onset of antiferromagnetism



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

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

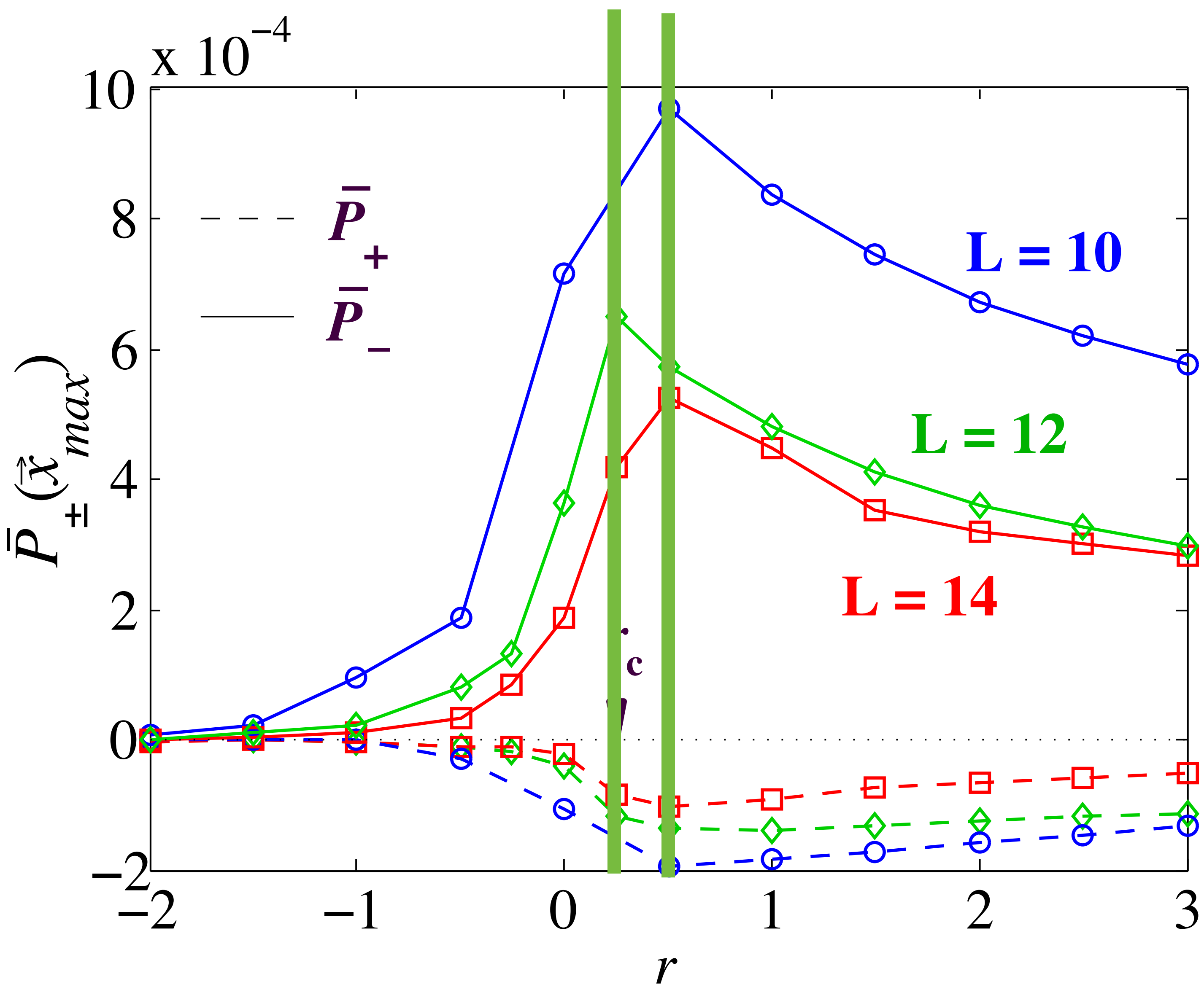
QMC for the onset of antiferromagnetism



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

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

QMC for the onset of antiferromagnetism



Notice shift between the position of the QCP in the superconductor, and the position of maximum pairing. This is found in numerous experiments.

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

Outline

1. Sign-problem free quantum Monte Carlo for the onset of antiferromagnetism in metals

2. Hole-doped cuprates:

Where are the electron pockets in the Brillouin zone ?

Is the pseudogap state an exotic metal with Fermi pockets which violate the Luttinger relation ? (Such a violation requires emergent gauge excitations: an example of such a metal is the $\mathcal{Z}_2$-FL* state)

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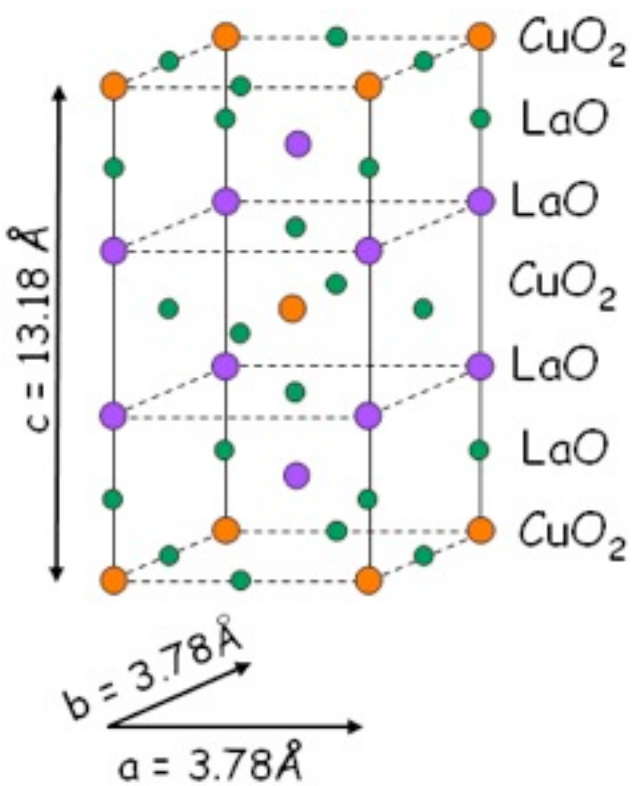
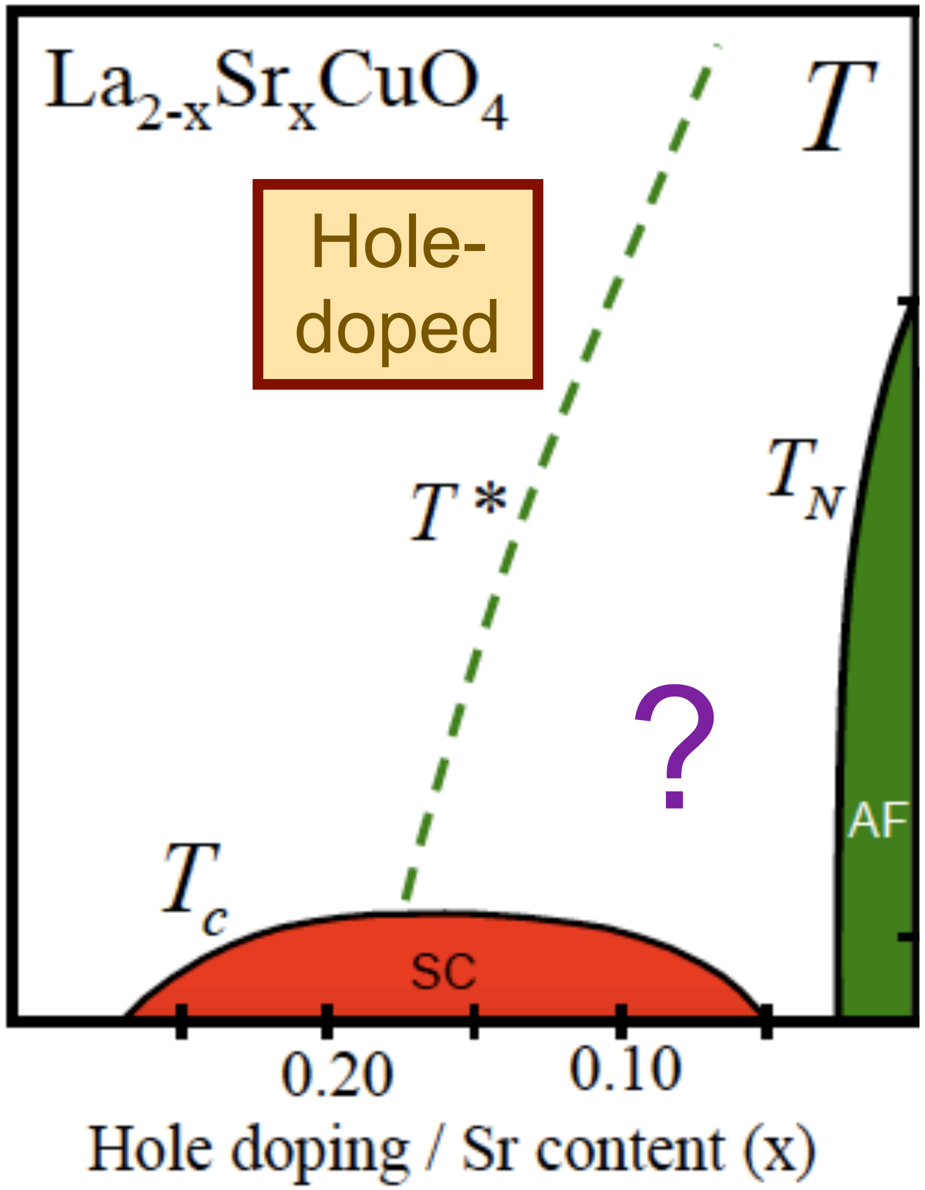
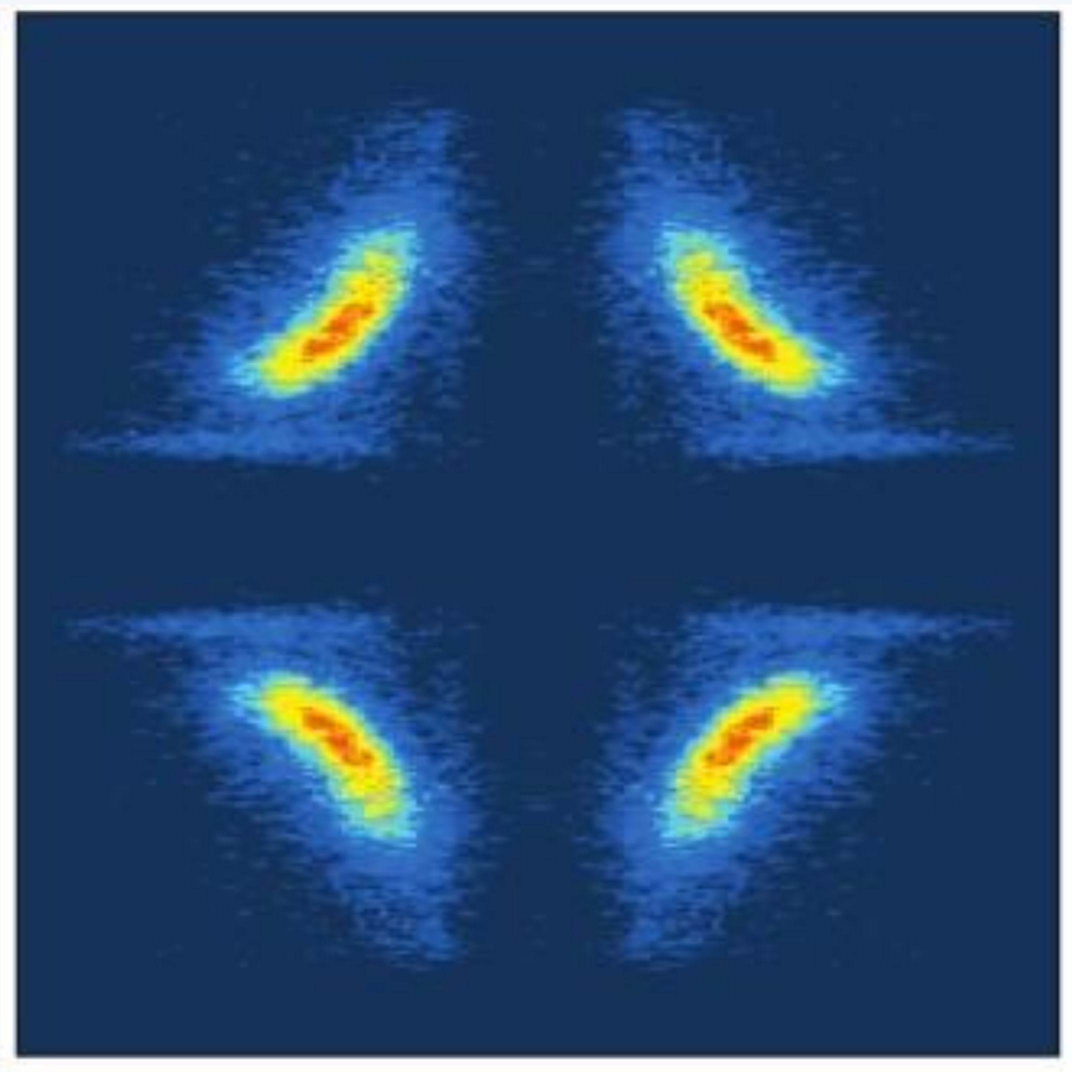

CuO2
LaO
LaO
CuO2
LaO
LaO
CuO2
c = 13.18 Å
b = 3.78Å
a = 3.78Å

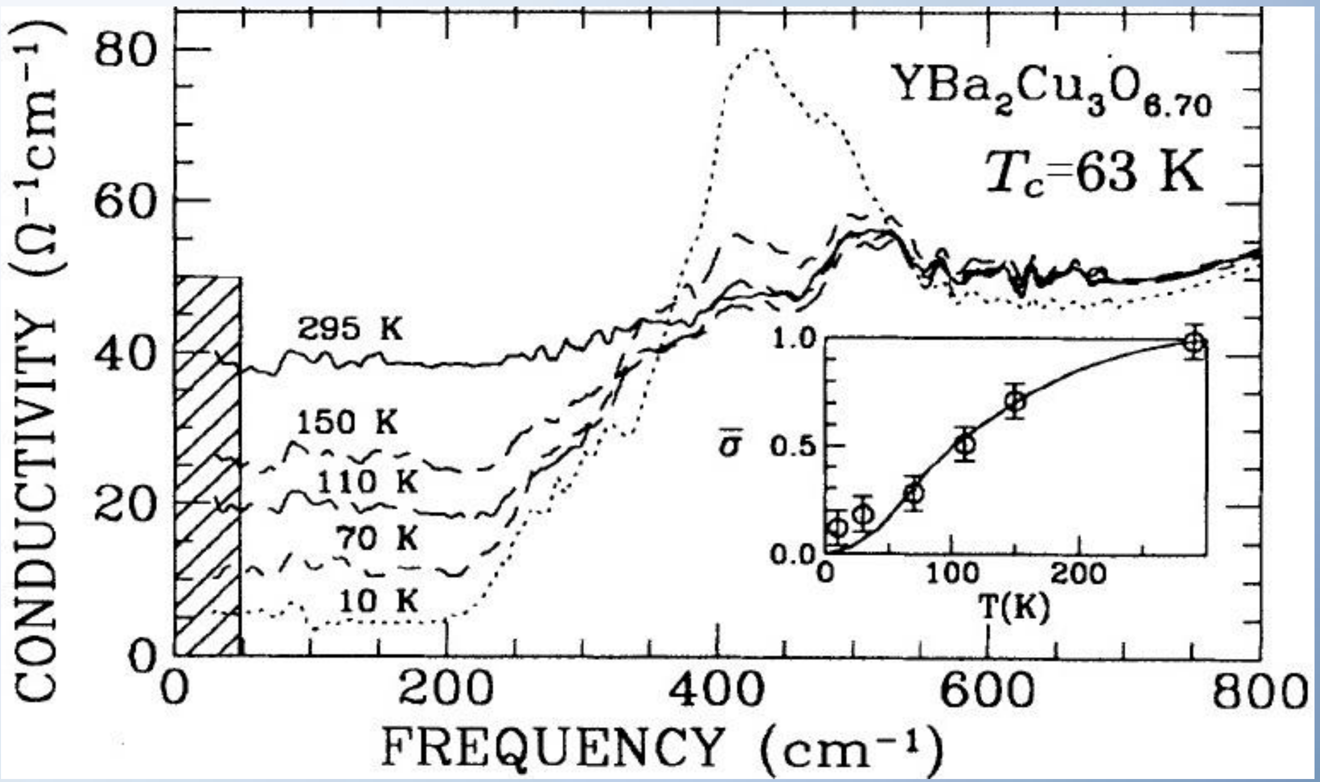

La2-xSrxCuO4
Hole-
doped
T
T*
TN
?
AF
Tc
SC
0.20
0.10
Hole doping / Sr content (x)

Pseudogap state has no low energy fermions in the antinodal region

YBCO$_{6+x}$

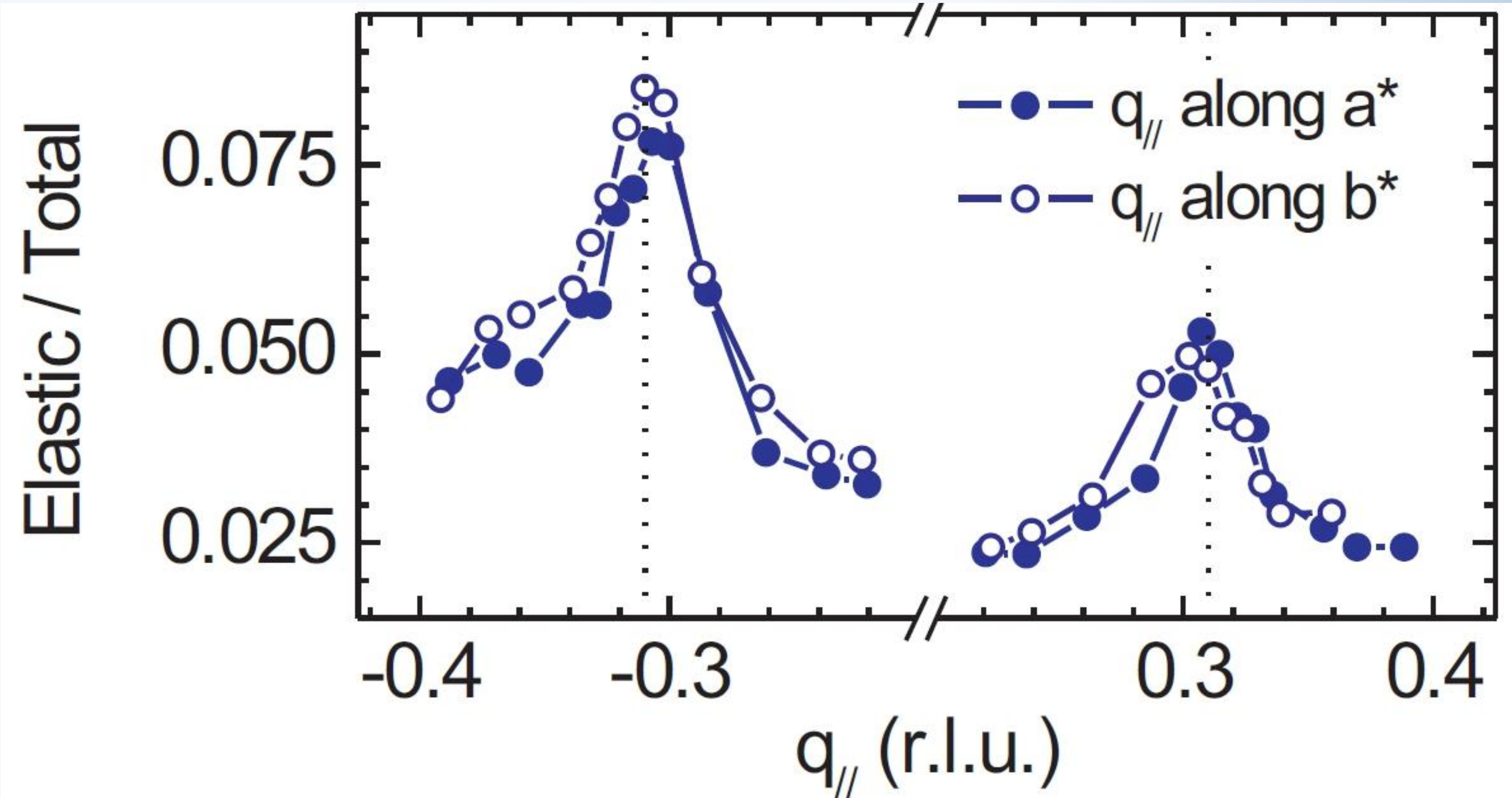


Peets D C… Damascelli A *New J. Phys.* **9** 28 (2007)



C. C. Holmes et al. Phys. Rev. Lett. 71, 1645 **(1993)**

Resonant x-ray scattering
Surprise – wavevectors ≈ 3.3a, biaxial



$YBa_2Cu_3O_{6.6}$

$E \simeq 931$ eV

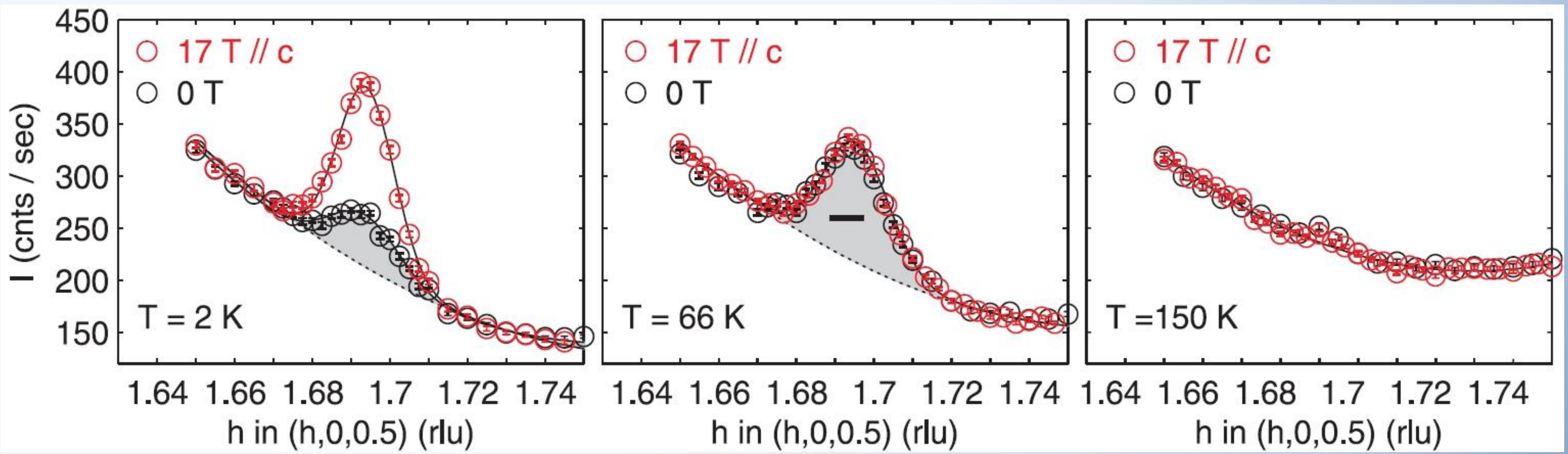
Q = (0.31, 0) and (0, 0.31)

Correlation length ξ≈ 60Å

$Q_{CDW} \neq 2Q_{SDW}$

Ghiringelli et al. (http://dx.doi.org/10.1126/science.1223532)

Hard x-ray scattering in agreement with results from resonant x-ray scattering



J. Chang et al. arXiv: 1206.4333

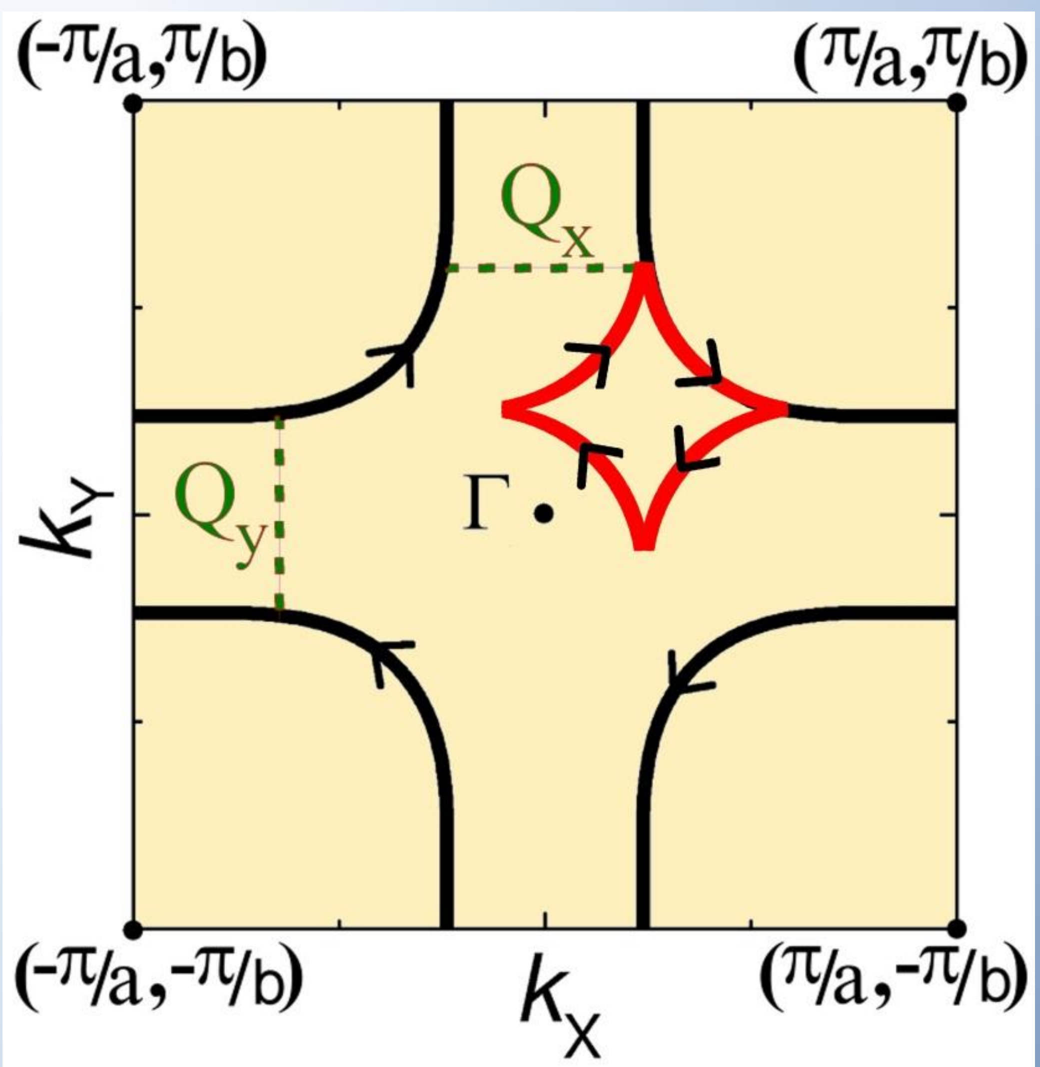
$E \simeq 100$ keV

$YBa_2Cu_3O_{6.67}$ (ortho-VIII)

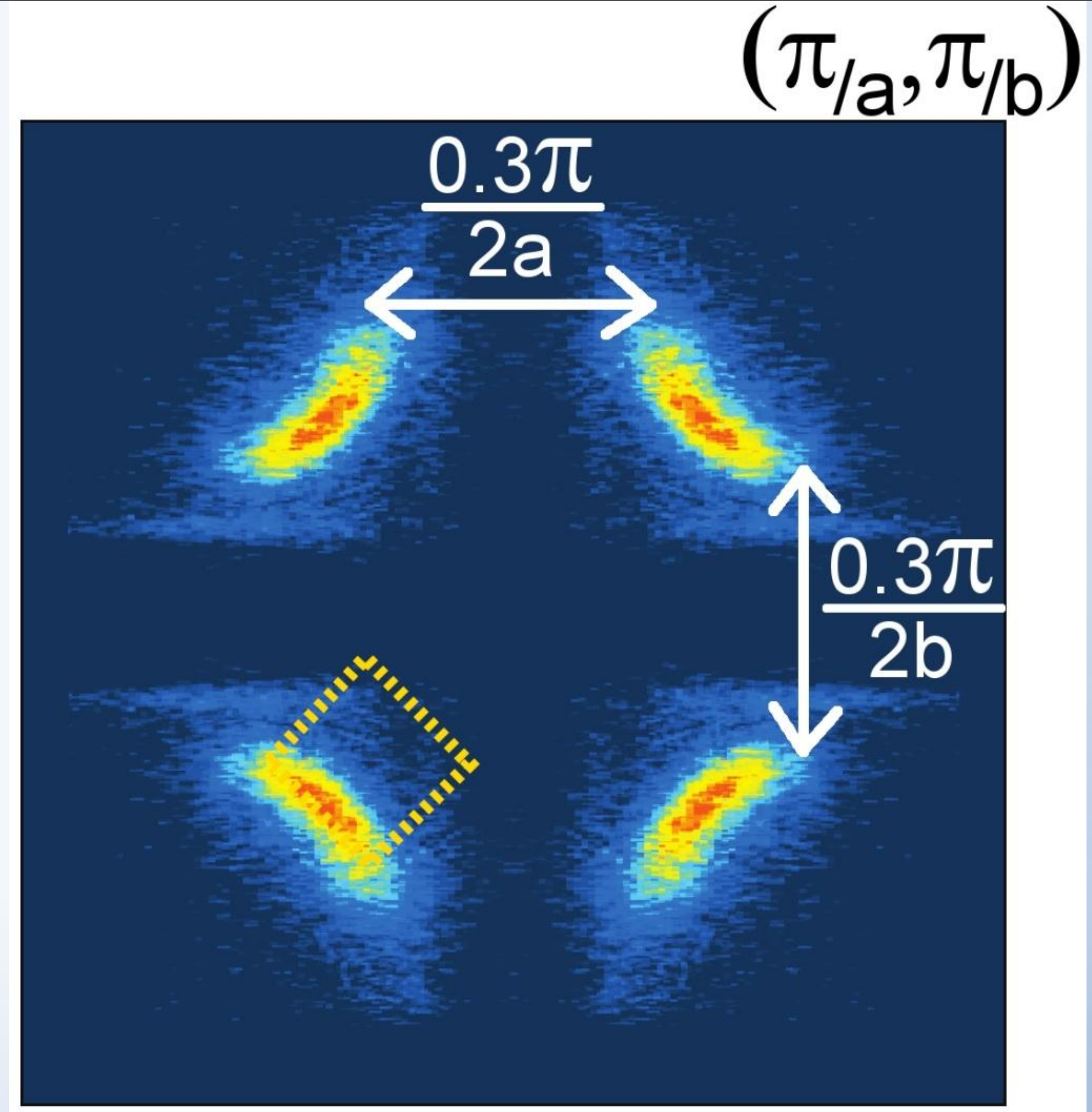
Correlation length $\xi \approx 98$Å (at 2K and 17T)

$\boldsymbol{q}_{CDW} = \boldsymbol{q}_1 = (\delta_1, 0, 0.5)$ and $\boldsymbol{q}_2 = (0, \delta_2, 0.5)$, where $\delta_1 \approx 0.30$ and $\delta_2 \approx 0.31$.

Nodal pocket with electron-like direction of cyclotron motion



N. Harrison & SES Phys. Rev. Lett. 106, 226402 (2011)
S. E. Sebastian et al., Rep. Prog. Physics (in press, 2012)

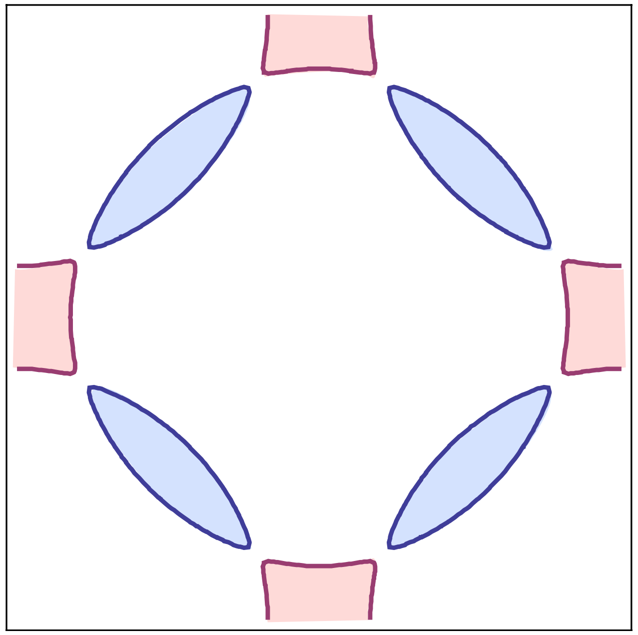


S. E. Sebastian et al., Rep. Prog. Physics (in press, 2012)

In reality, such an electron pocket is a reconstruction of a parent state which has no Fermi surface in the anti-nodal region. So if we accept this picture, the parent state is very exotic !

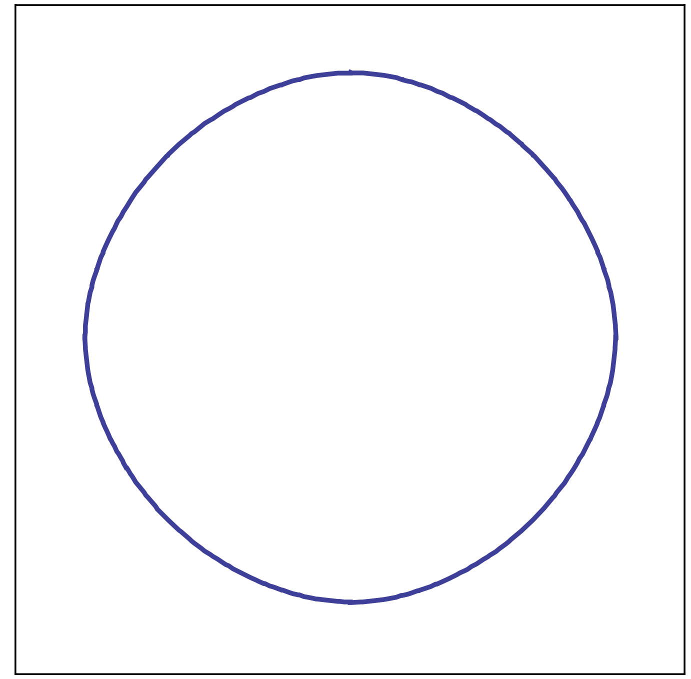
A metal with Fermi surfaces only near the nodes, and no broken symmetry, which violates the Luttinger relation.

Quantum phase transition with Fermi surface reconstruction



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

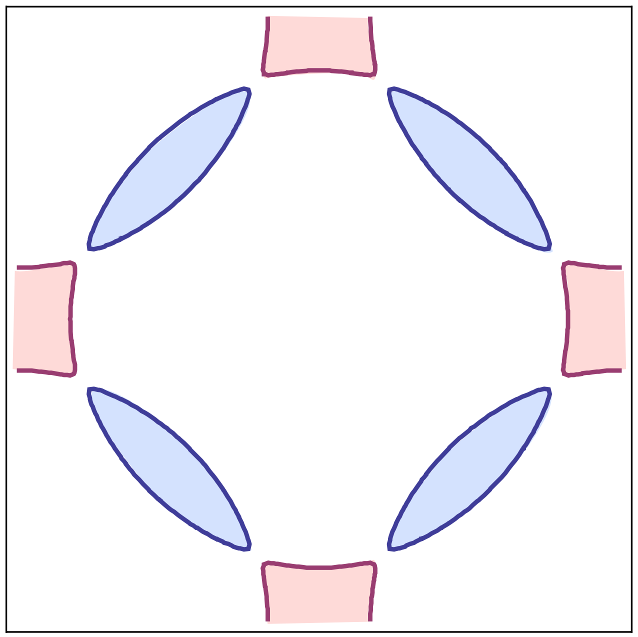
Metal with electron and hole pockets



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

Metal with "large" Fermi surface

Separating onset of SDW order and Fermi surface reconstruction



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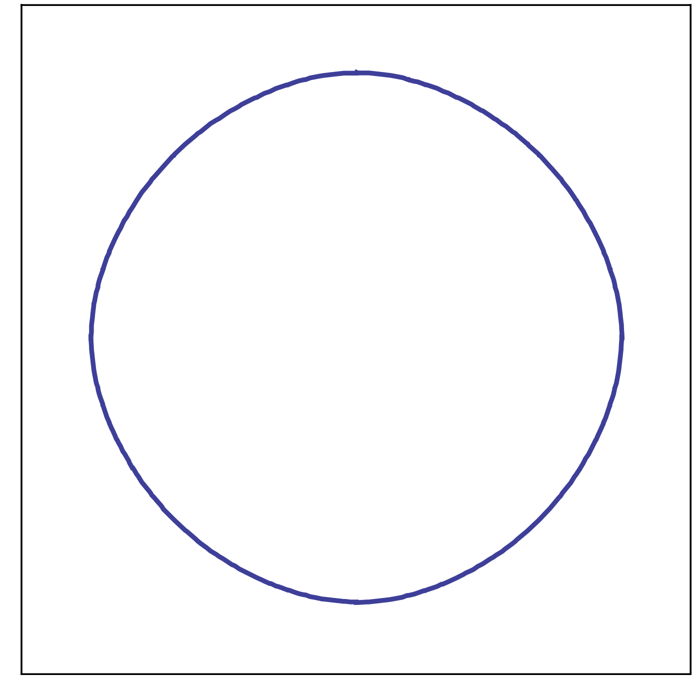

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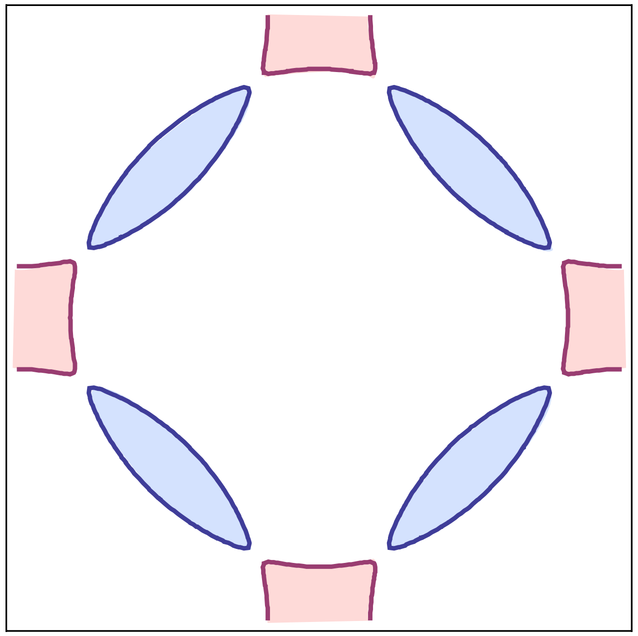

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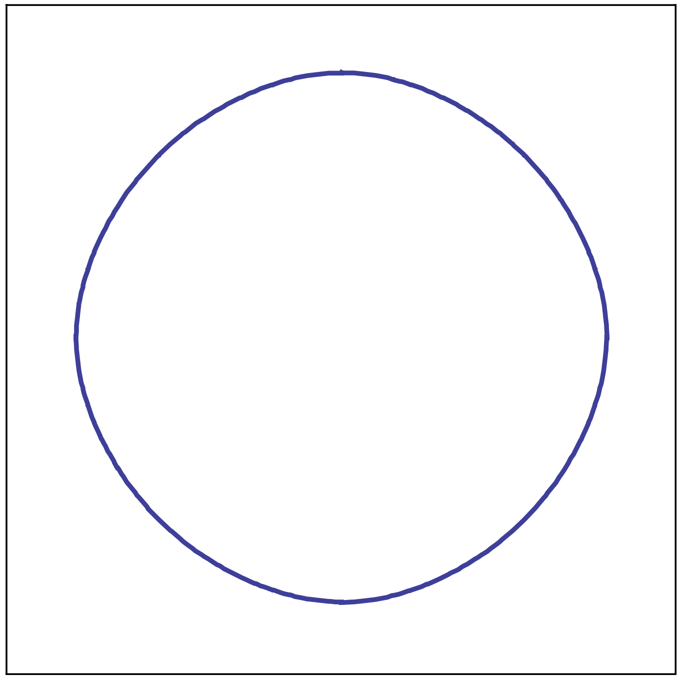
Fractionalized Fermi liquid (FL*) phase with no symmetry breaking and "small" Fermi surface



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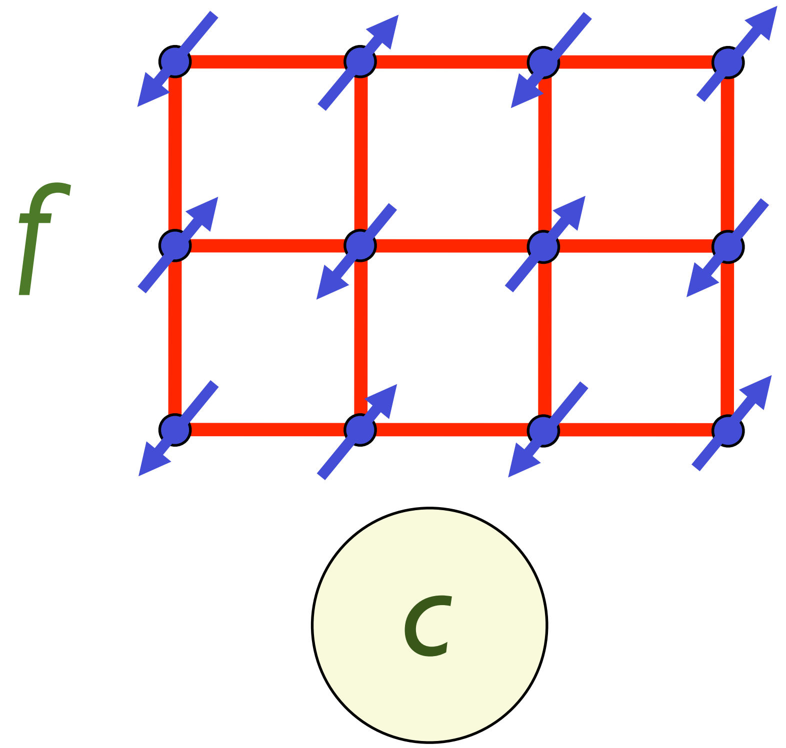
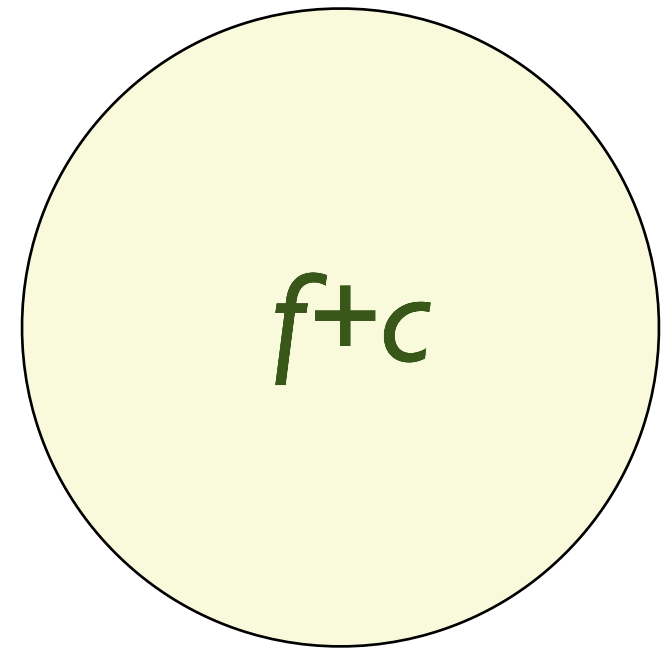
T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

Magnetic order and the heavy Fermi liquid in the Kondo lattice



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

Magnetic Metal:
f-electron moments
and
c-conduction electron
Fermi surface



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Heavy Fermi liquid
with "large" Fermi
surface of
hydridized *f* and
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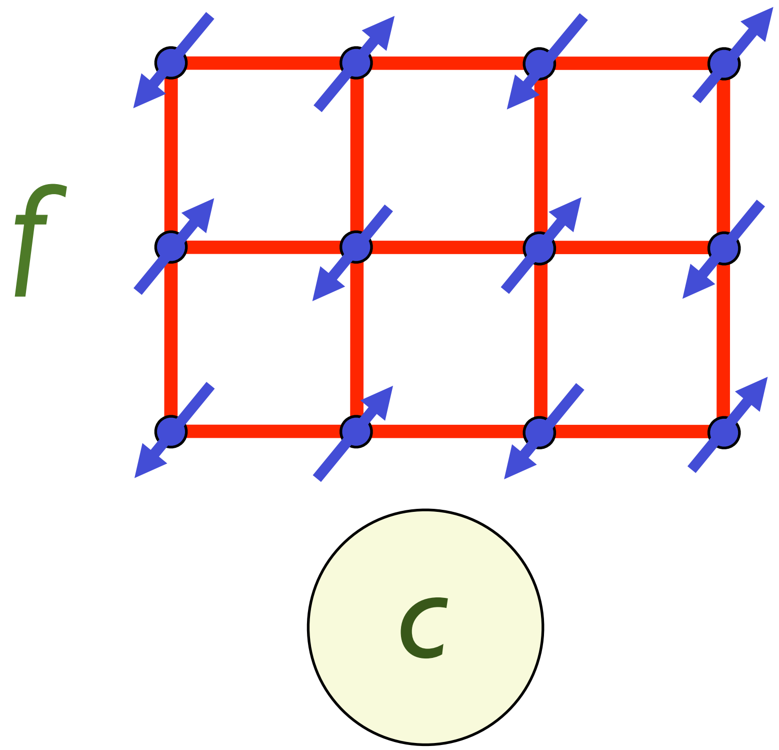
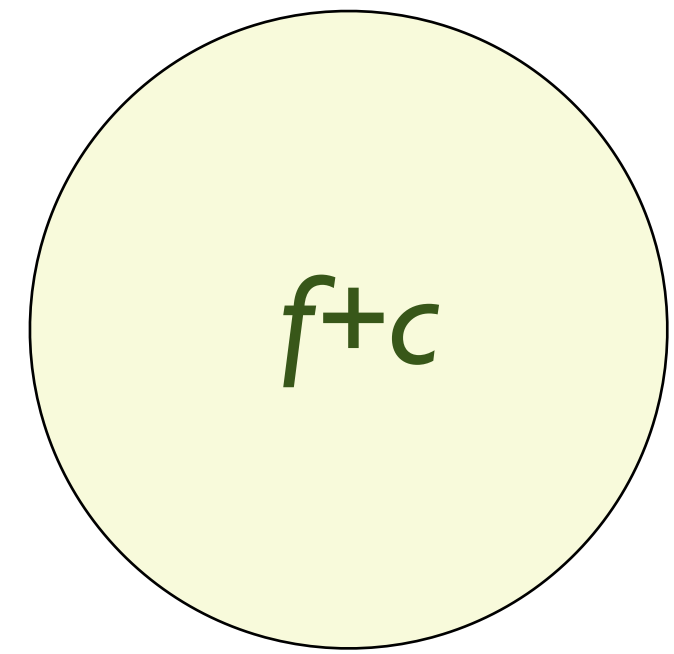
Separating onset of SDW order and the heavy Fermi liquid in the Kondo lattice





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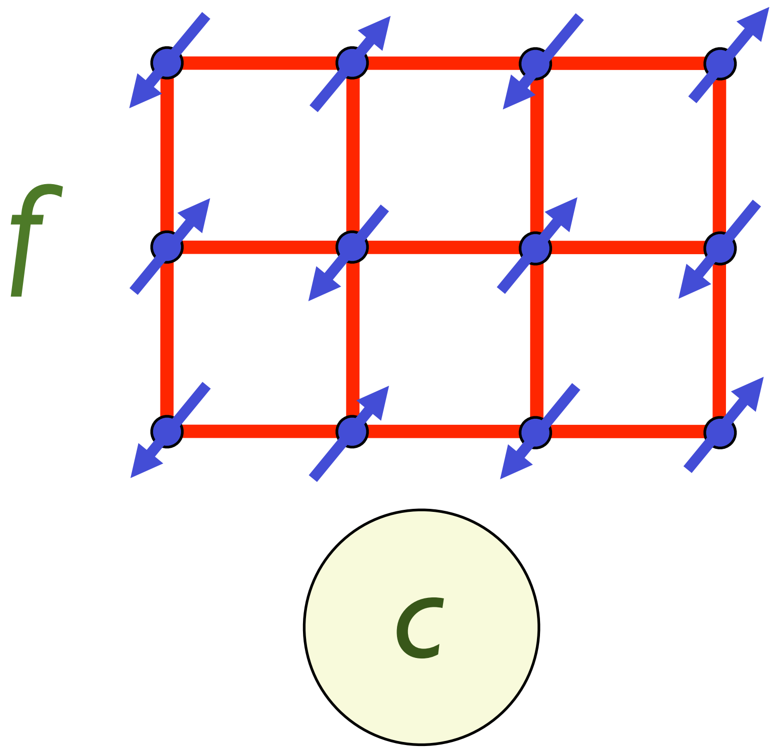

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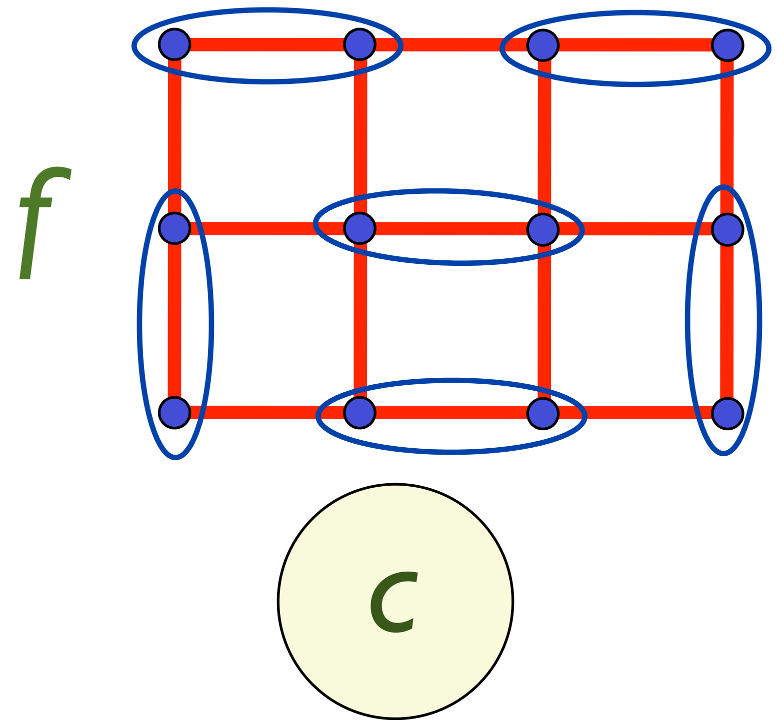
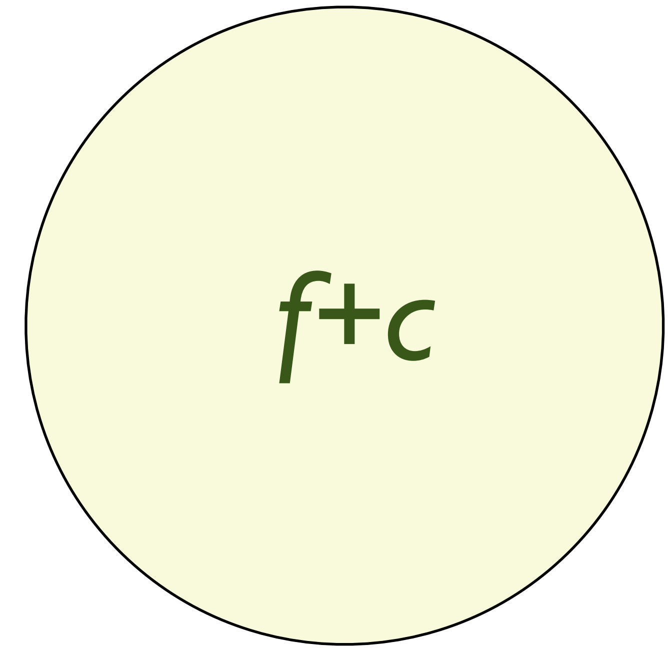


$\langle \vec{\varphi} \rangle = 0$

Conduction electron
Fermi surface
and
spin-liquid of
f-electrons



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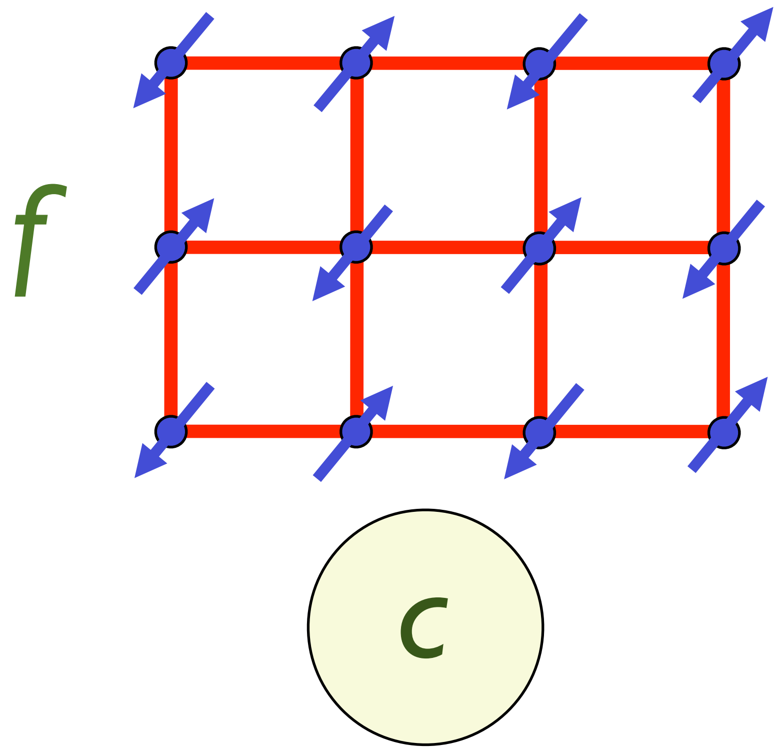

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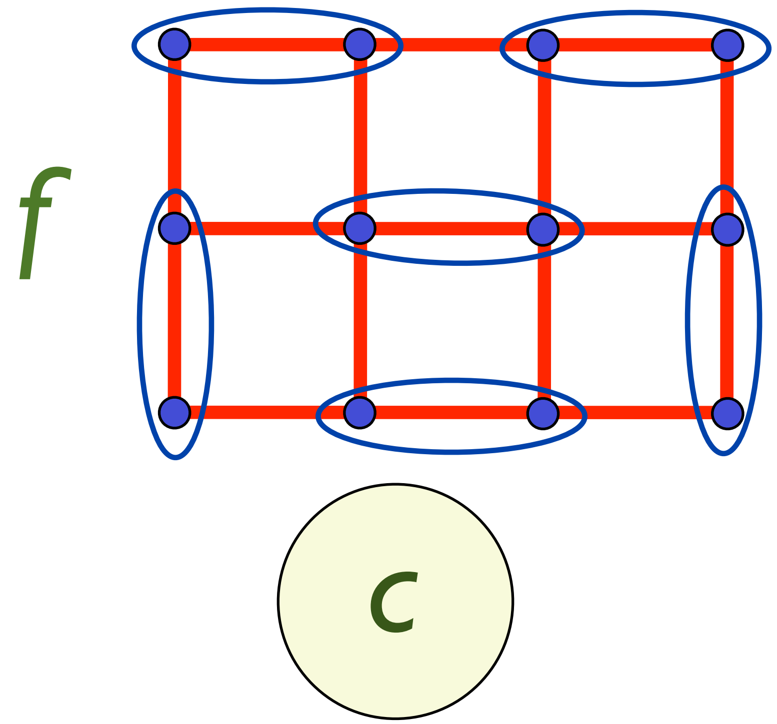

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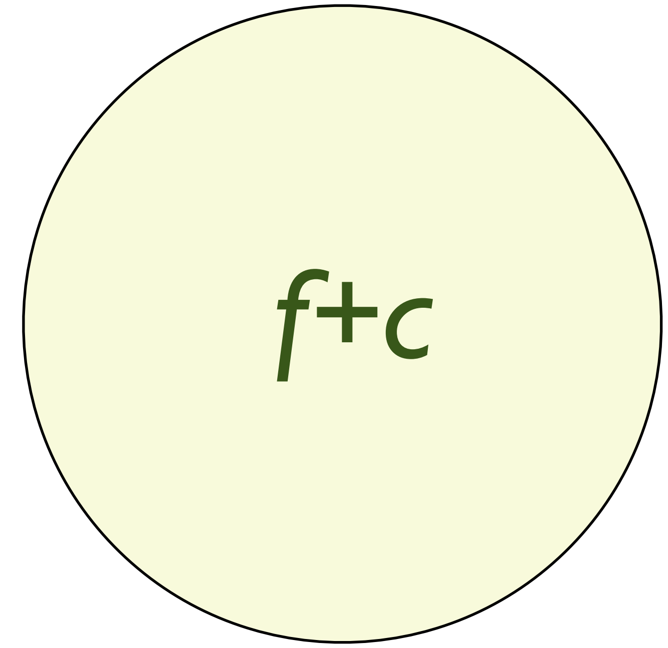

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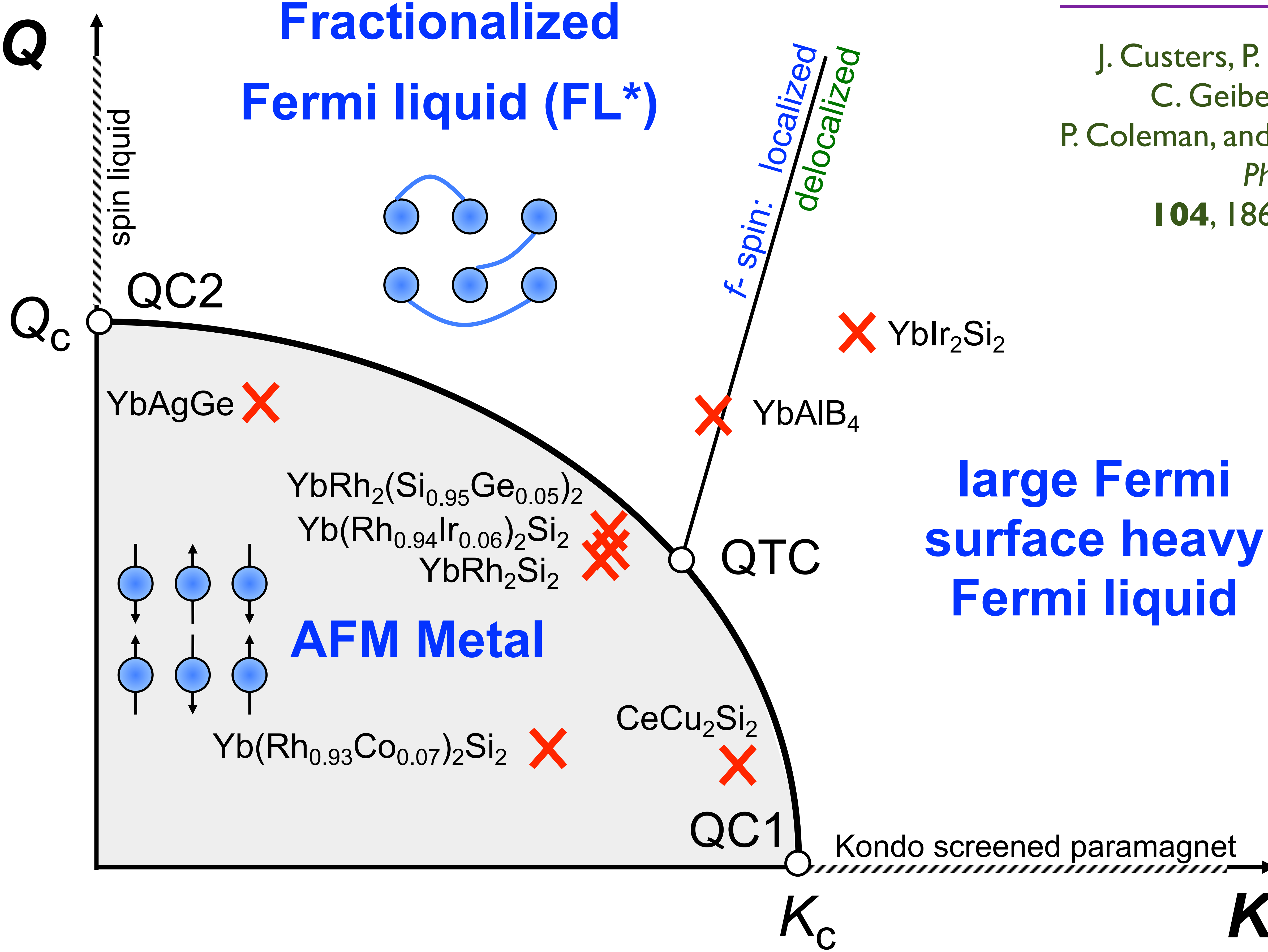
Heavy Fermi liquid with "large" Fermi surface of hydridized *f* and *c*-conduction electrons

T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

Experimental perpective on same phase diagrams of Kondo lattice

J. Custers, P. Gegenwart, C. Geibel, F. Steglich, P. Coleman, and S. Paschen, *Phys. Rev. Lett.* **104**, 186402 (2010)



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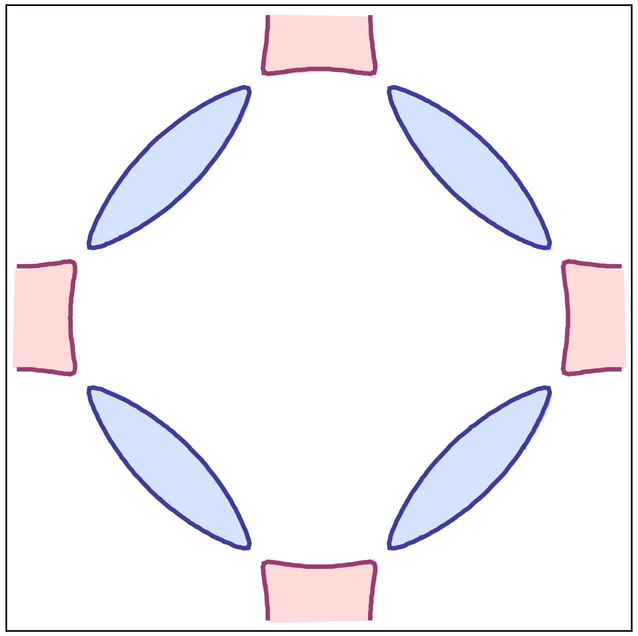

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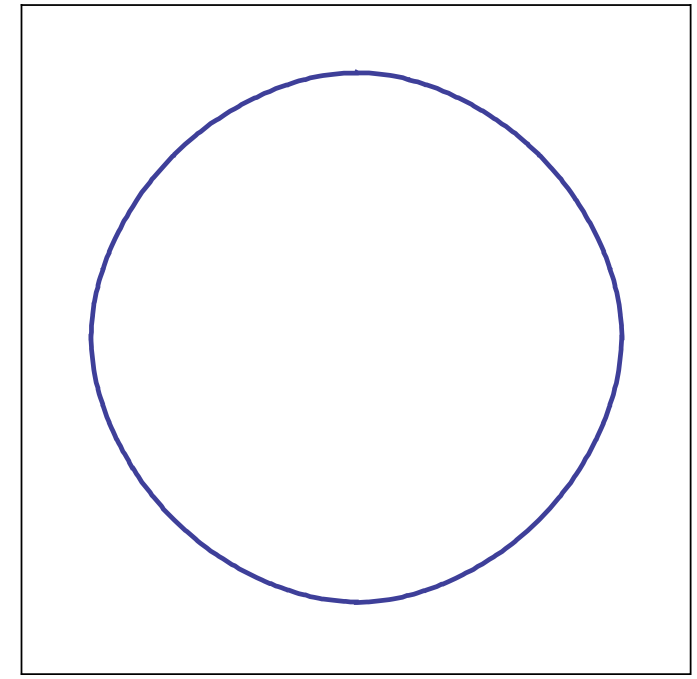

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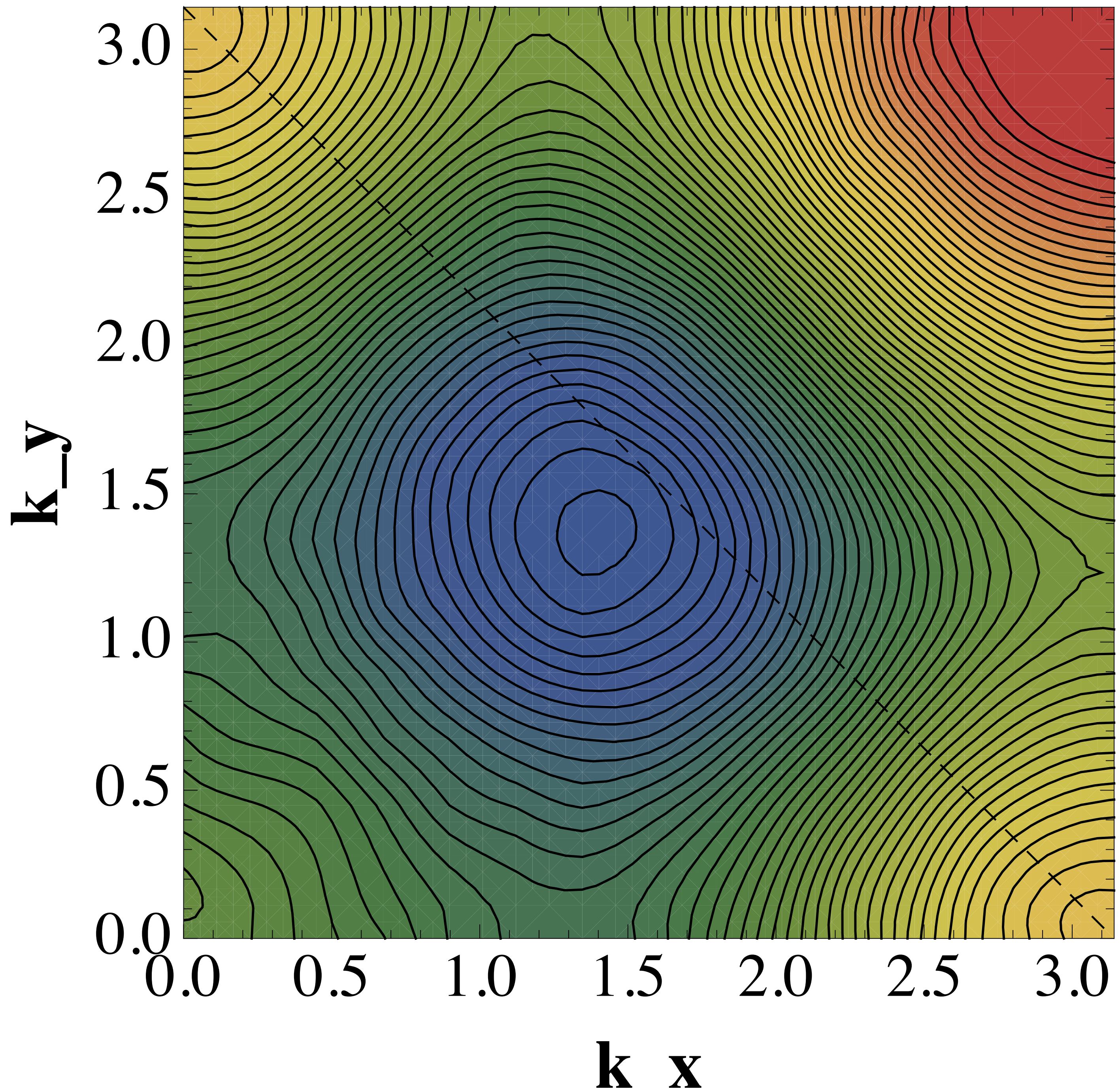

Hole pocket of a $\mathbb{Z}_2$-FL* phase in a *single*-band t-J model

M. Punk and S. Sachdev, *Phys. Rev. B* **85**, 195123 (2012)

Characteristics of FL* phase

- Fermi surface volume does not count all electrons.

T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

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T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

Characteristics of FL* phase

- Fermi surface volume does not count all electrons.

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- These topological excitations are needed to account for the deficit in the Fermi surface volume, in M. Oshikawa's proof of the Luttinger theorem.

T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

Conclusions

Solved sign-problem for generic universal theory for the onset of antiferromagnetism in two-dimensional metals.
Good prospects for studying non-Fermi liquid physics at non-zero temperature

Conclusions

Pseudo-gap phase of hole-doped cuprates as a "fractionalized Fermi liquid": Hole pockets which violate the Luttinger theorem, in a phase with "topological" excitations.