Sign-problem-free Quantum Monte Carlo of the onset of antiferromagnetism in metals

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Matthias Punk

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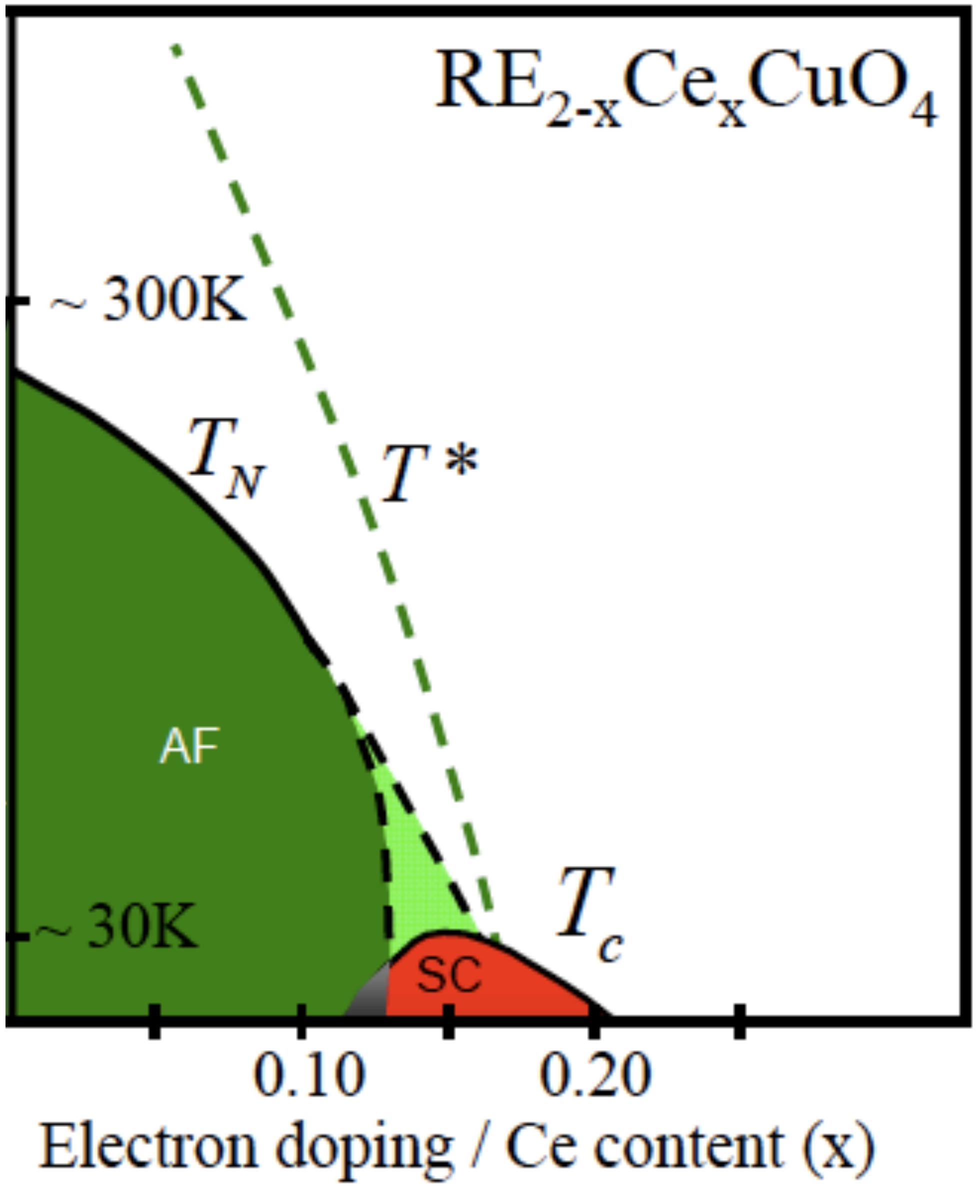
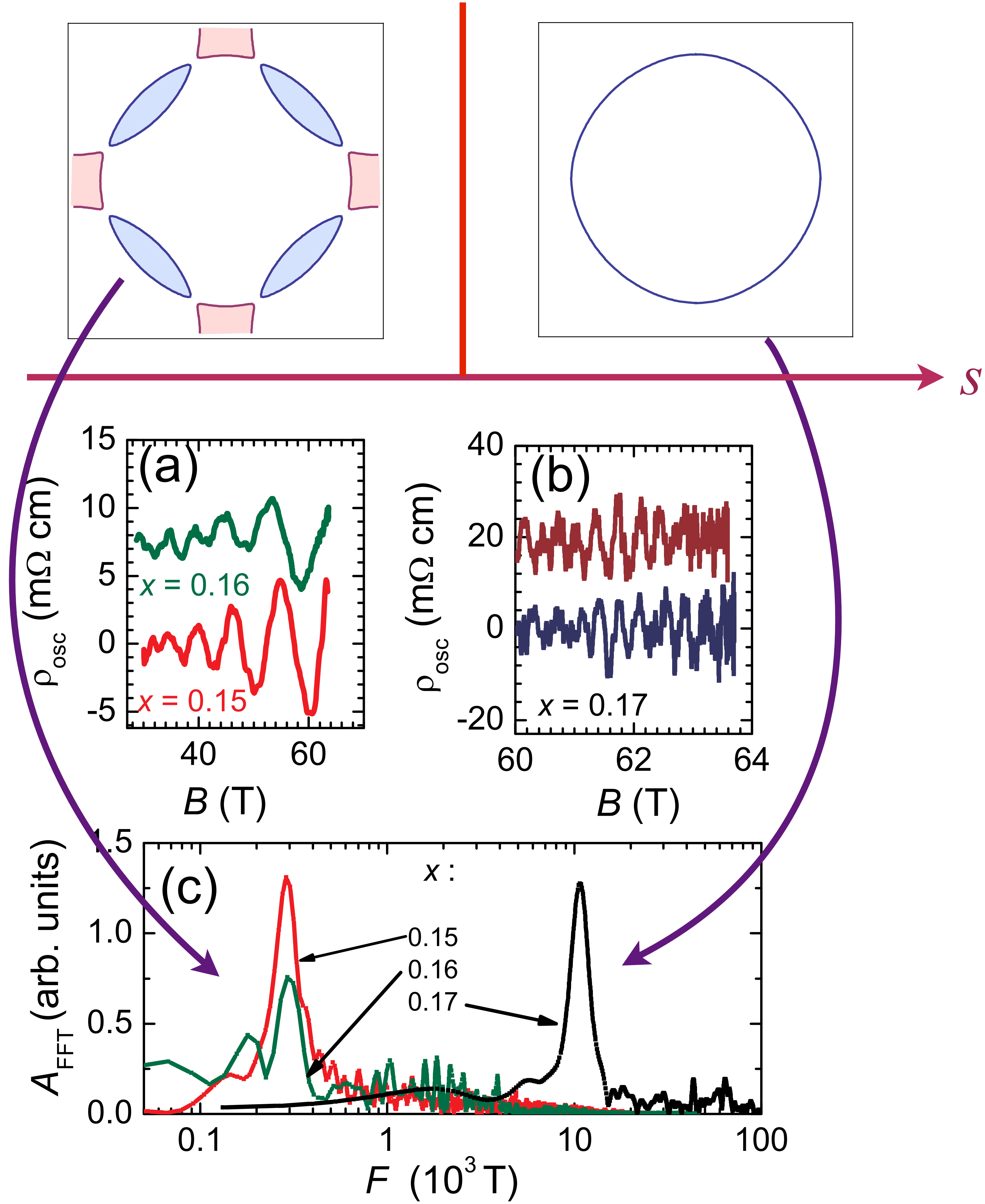
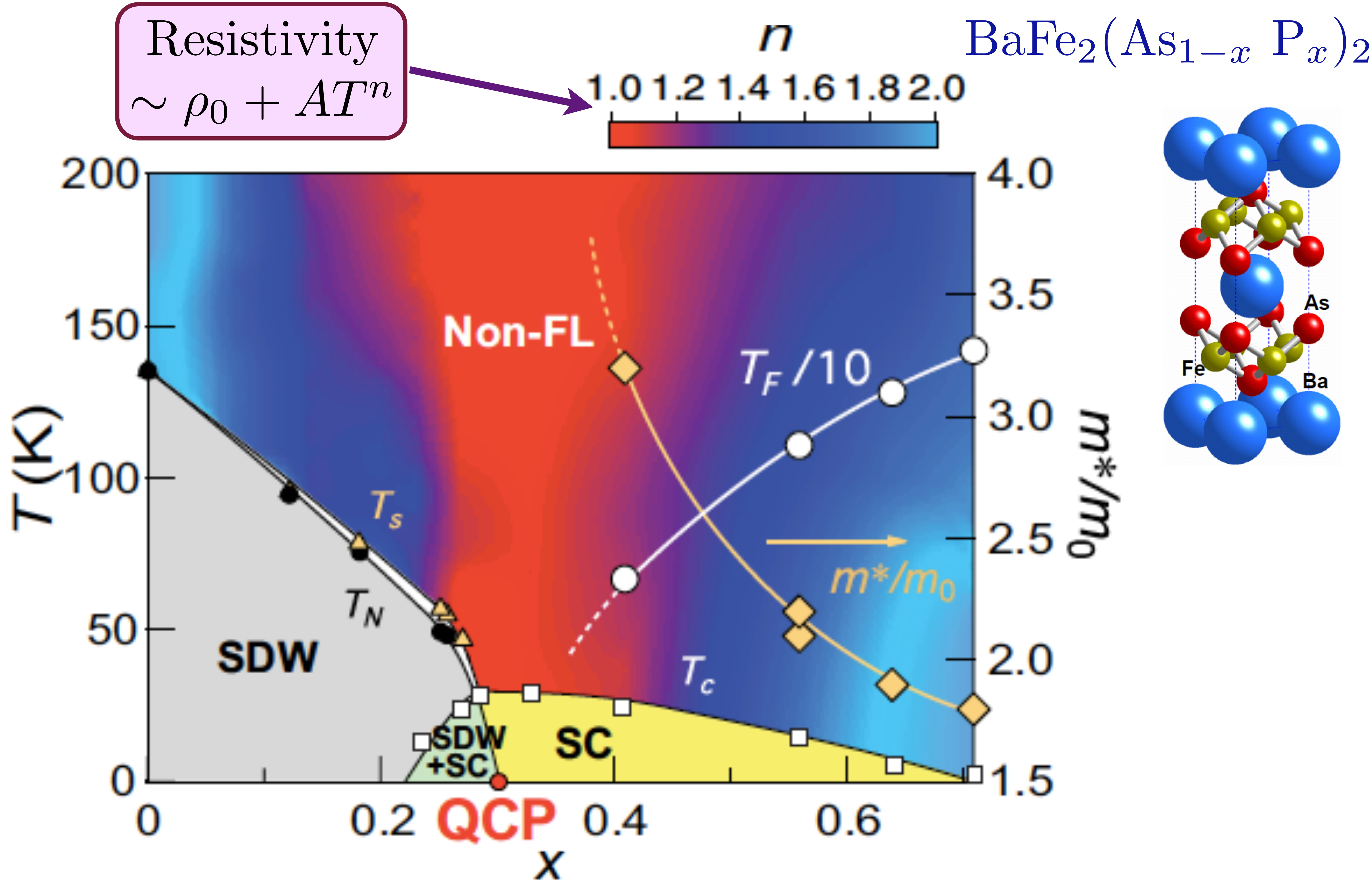




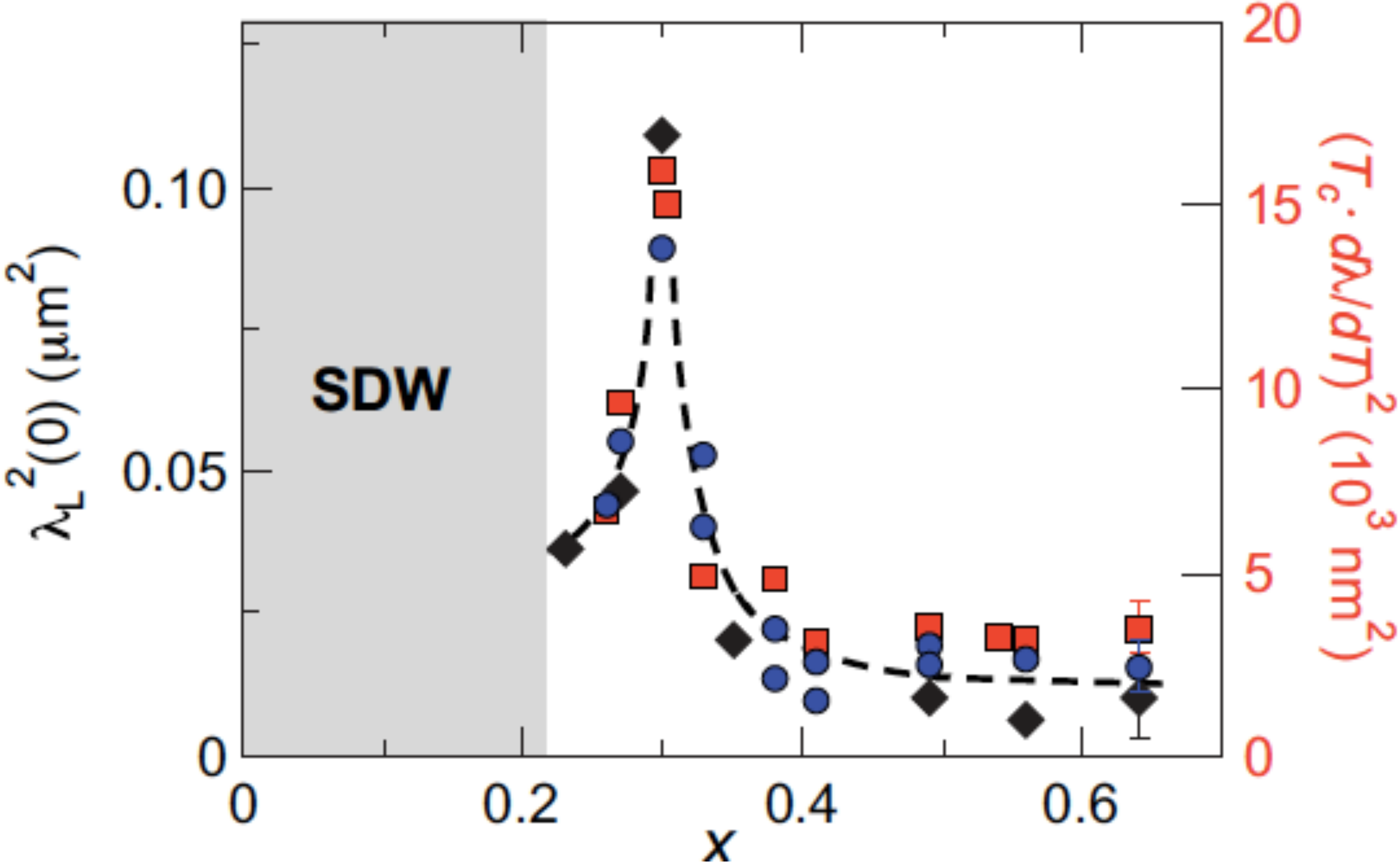
$Nd_{2-x}Ce_xCuO_4$

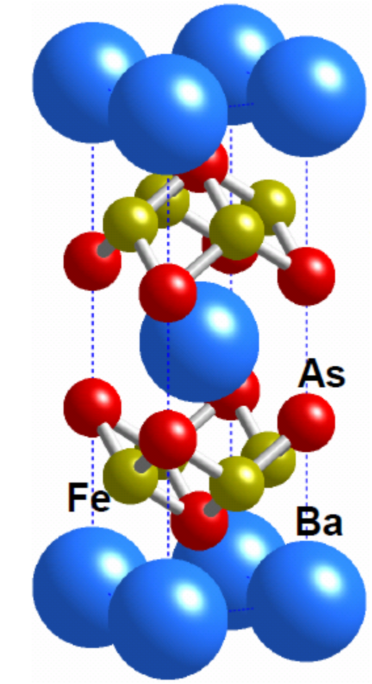
T. Helm, M.V. Kartsovnik,
M. Bartkowiak, N. Bittner,
M. Lambacher, A. Erb, J. Wosnitza,
and R. Gross,
Phys. Rev. Lett. **103**, 157002 (2009).



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).

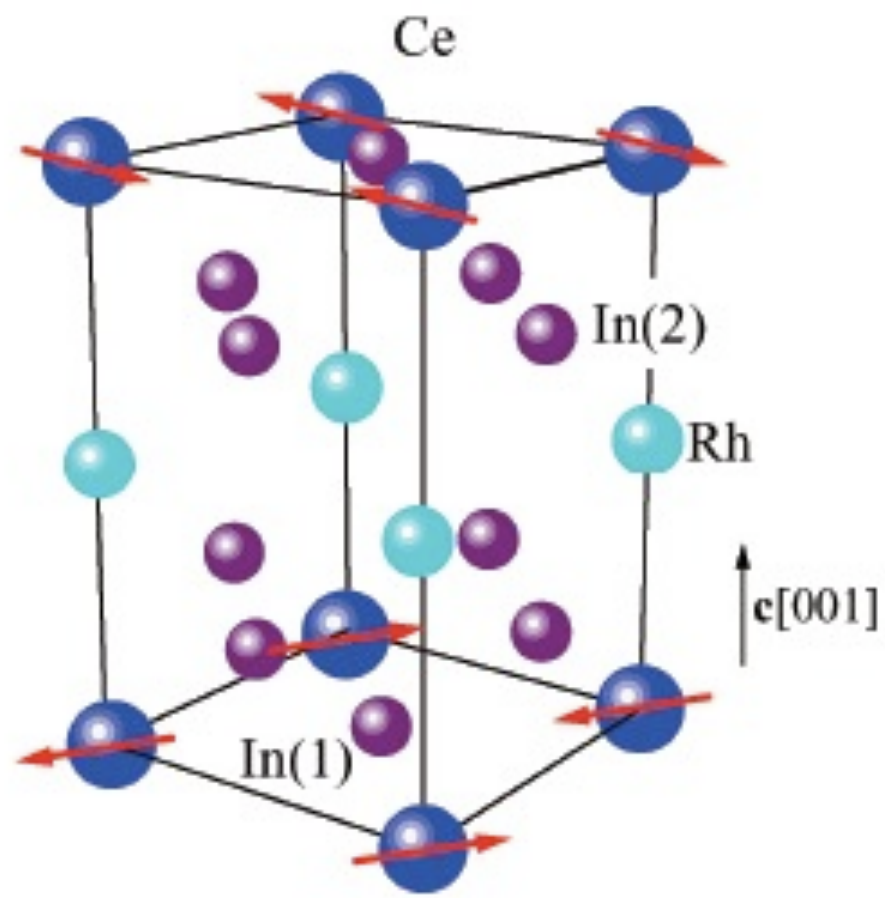
$BaFe_2(As_{1-x}\ P_x)_2$

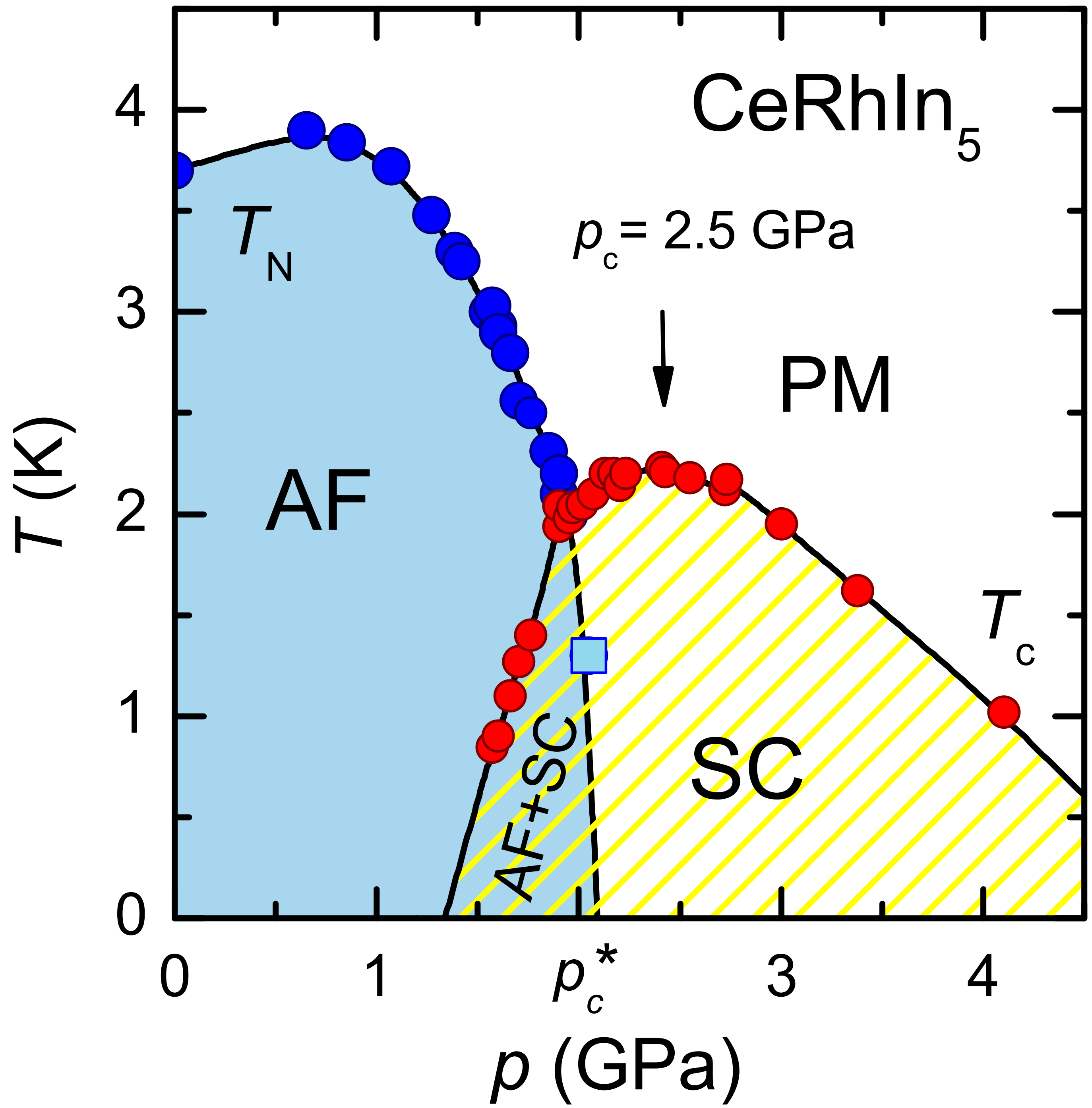




K. Hashimoto, K. Cho, T. Shibauchi, S. Kasahara, Y. Mizukami, R. Katsumata, Y. Tsuruhara, T. Terashima, H. Ikeda, M. A. Tanatar, H. Kitano, N. Salovich, R. W. Giannetta, P. Walmsley, A. Carrington, R. Prozorov, and Y. Matsuda, *Science* **336**, 1554 (2012).

Lower T_c superconductivity in the heavy fermion compounds





G. Knebel, D. Aoki, and J. Flouquet, arXiv:0911.5223.
Tuson Park, F. Ronning, H. Q. Yuan, M. B. Salamon, R. Movshovich, J. L. Sarrao, and J. D. Thompson, *Nature* **440**, 65 (2006)

Outline

1. Weak coupling theory

2. Universal critical theory

3. Quantum Monte Carlo
   without the sign problem

4. Features of strong coupling

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1. Weak coupling theory

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The Hubbard Model

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

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

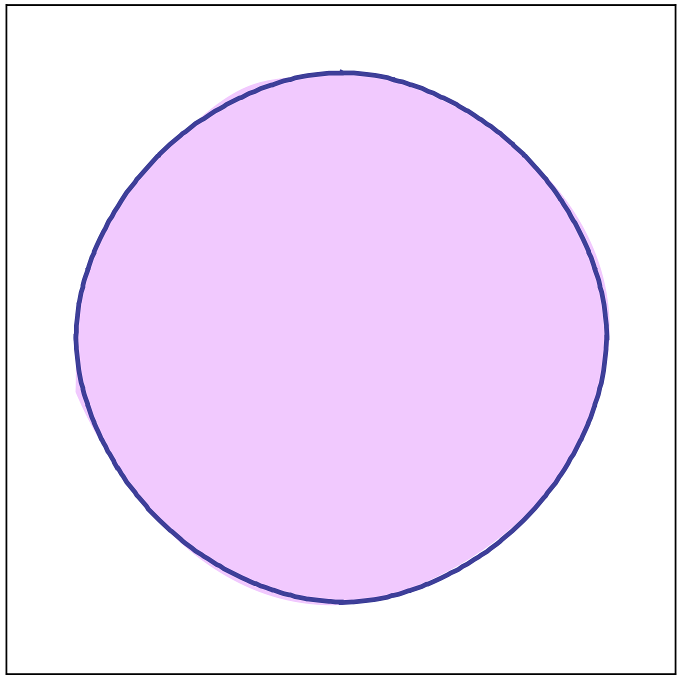
Spin index $\alpha = \uparrow, \downarrow$

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

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

Fermi surface+antiferromagnetism

Metal with "large"
Fermi surface



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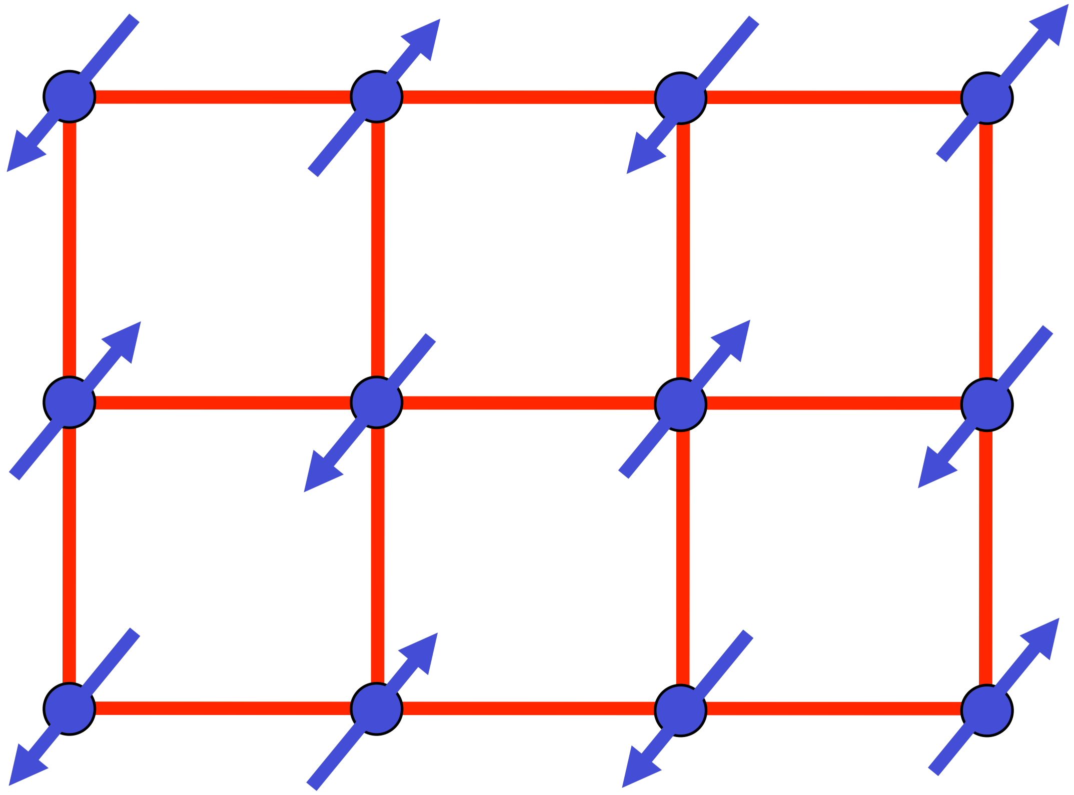


The electron spin polarization obeys

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

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

The Hubbard Model

Decouple *U* term by a Hubbard-Stratanovich transformation

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

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

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

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

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

The Hubbard Model

Decouple *U* term by a Hubbard-Stratanovich transformation

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

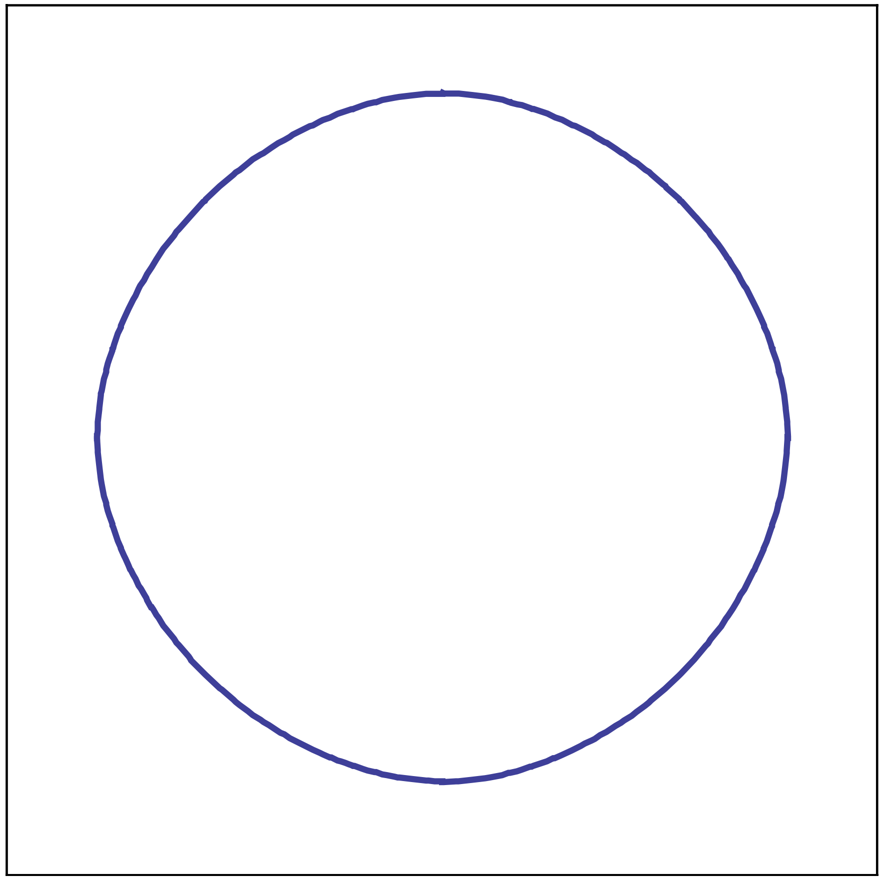
$$\mathcal{L}_c = c_a^\dagger \varepsilon(-i\boldsymbol{\nabla}) c_a$$

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

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

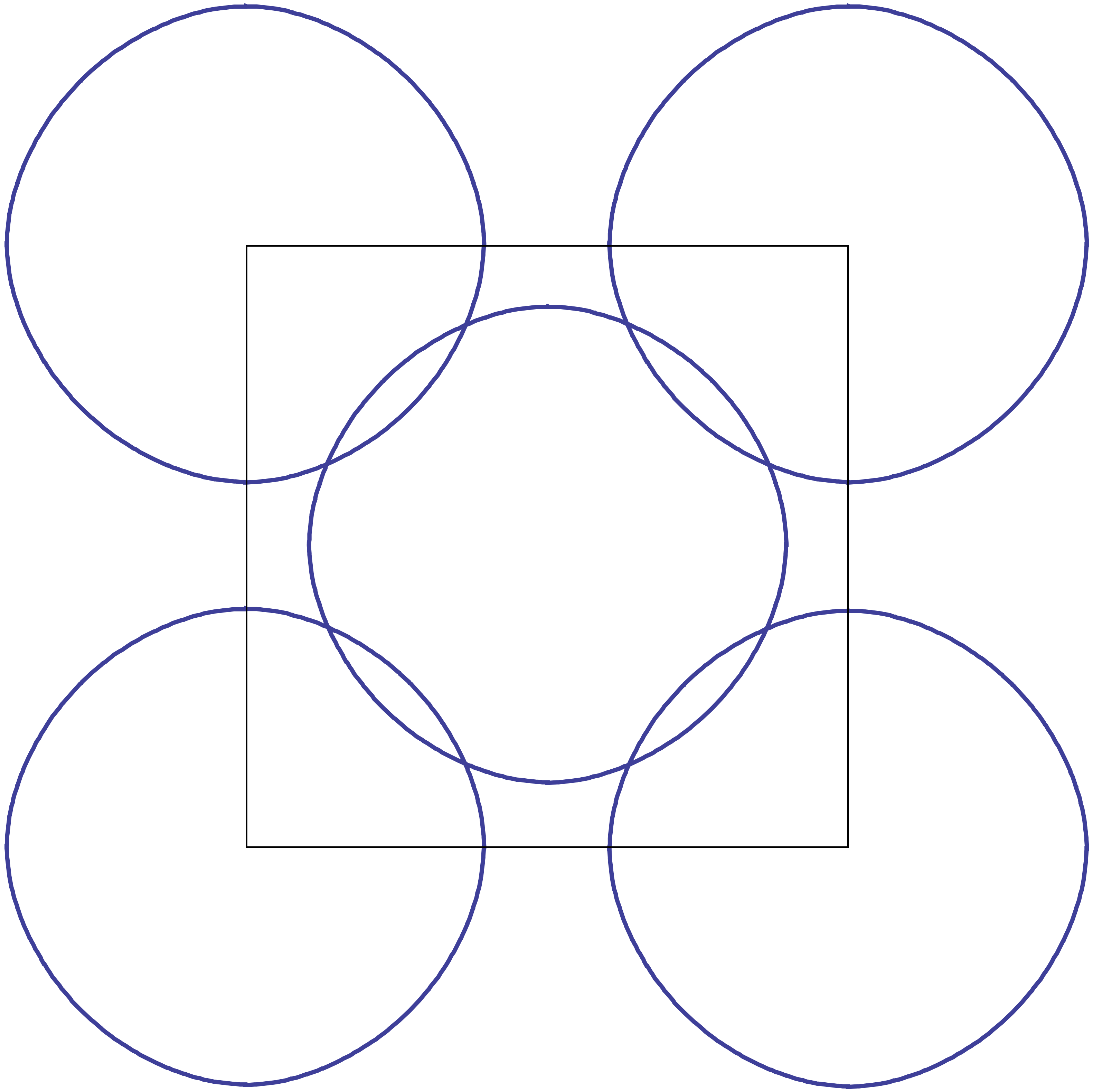
Hertz, Moriya, Millis: integrate out fermions, and focus on effective theory of damped excitations of the order parameter φ_α. Method <u>*fails*</u> in $d = 2$.

Fermi surface+antiferromagnetism



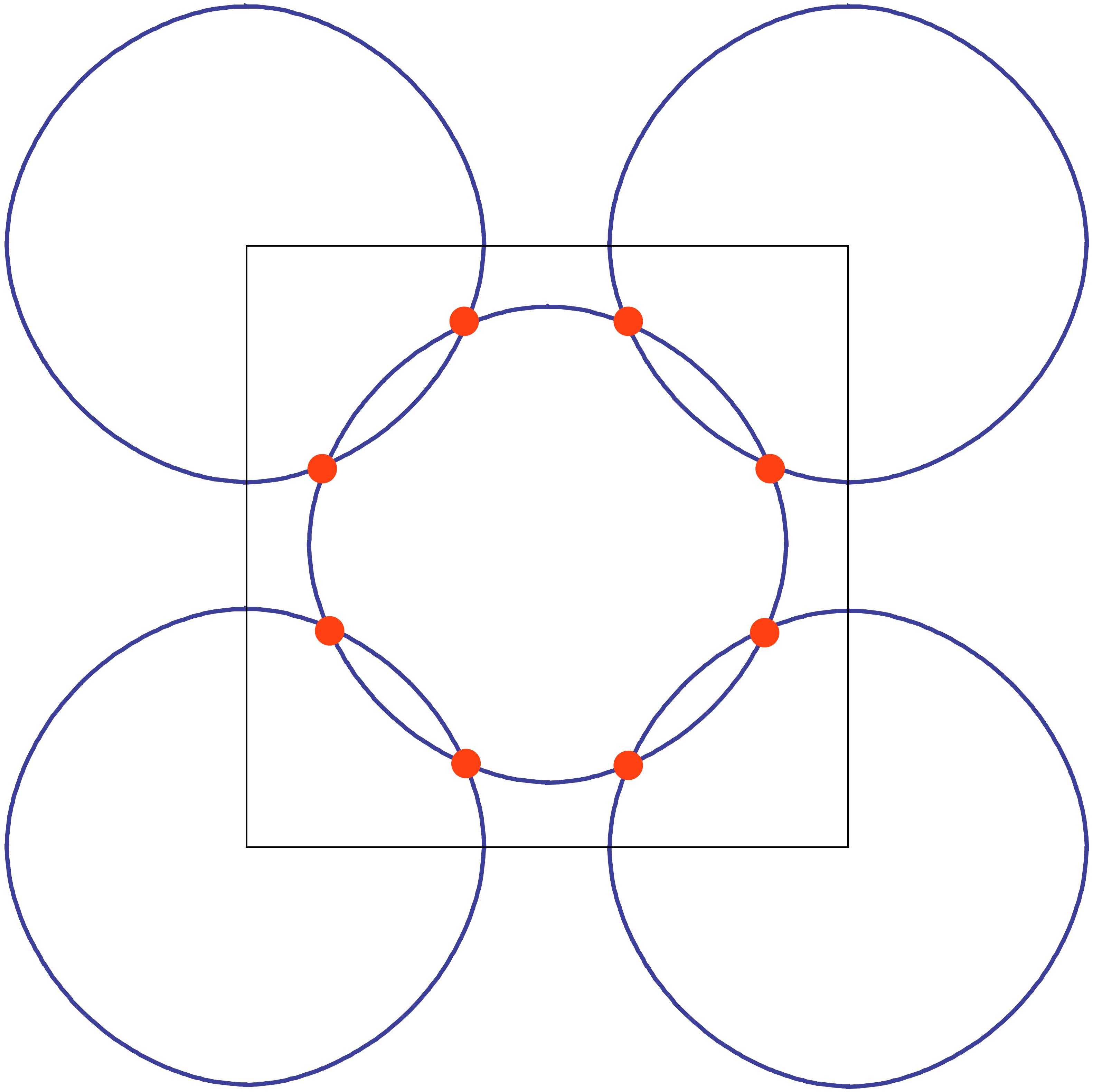
Metal with "large" Fermi surface

Fermi surface+antiferromagnetism



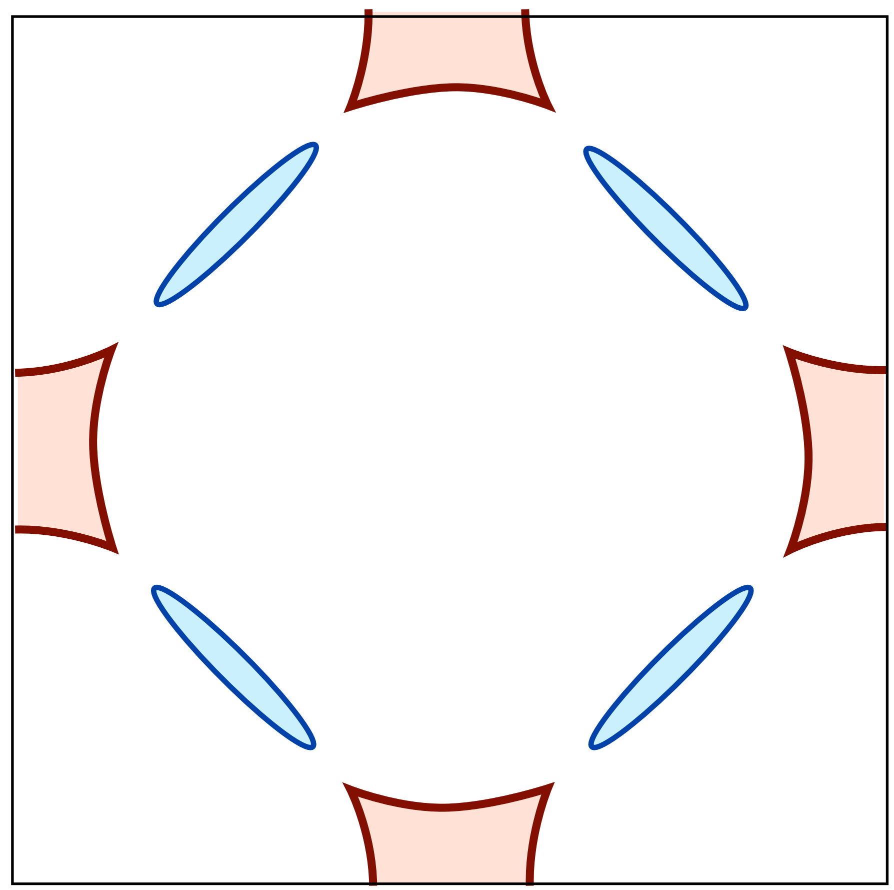
Fermi surfaces translated by $\mathbf{K} = (\pi, \pi)$.

Fermi surface+antiferromagnetism



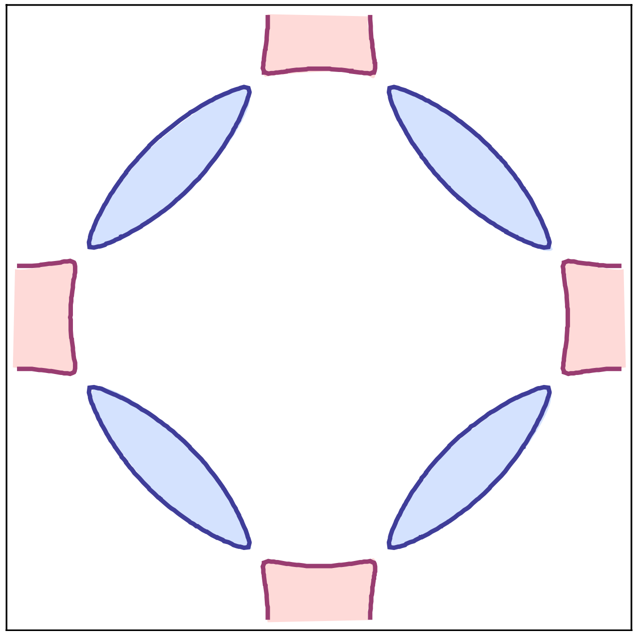
"Hot" spots

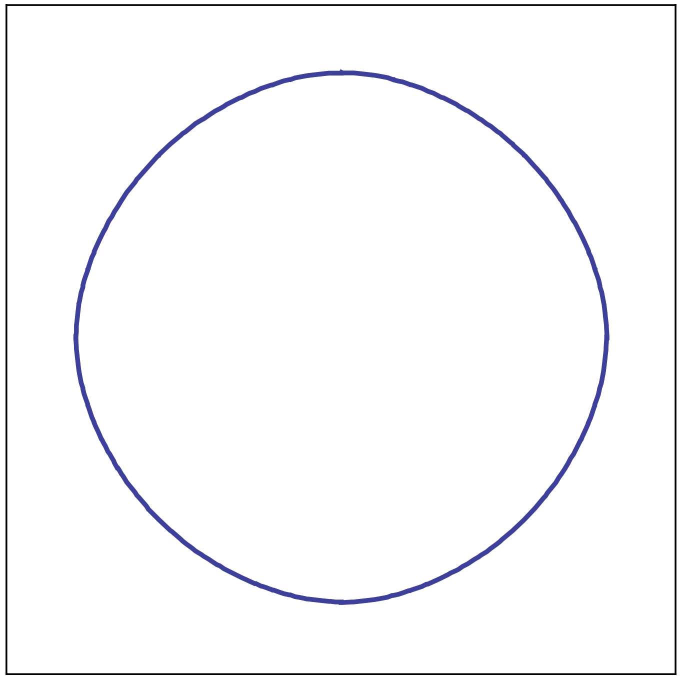
Fermi surface+antiferromagnetism



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

Fermi surface+antiferromagnetism





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

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

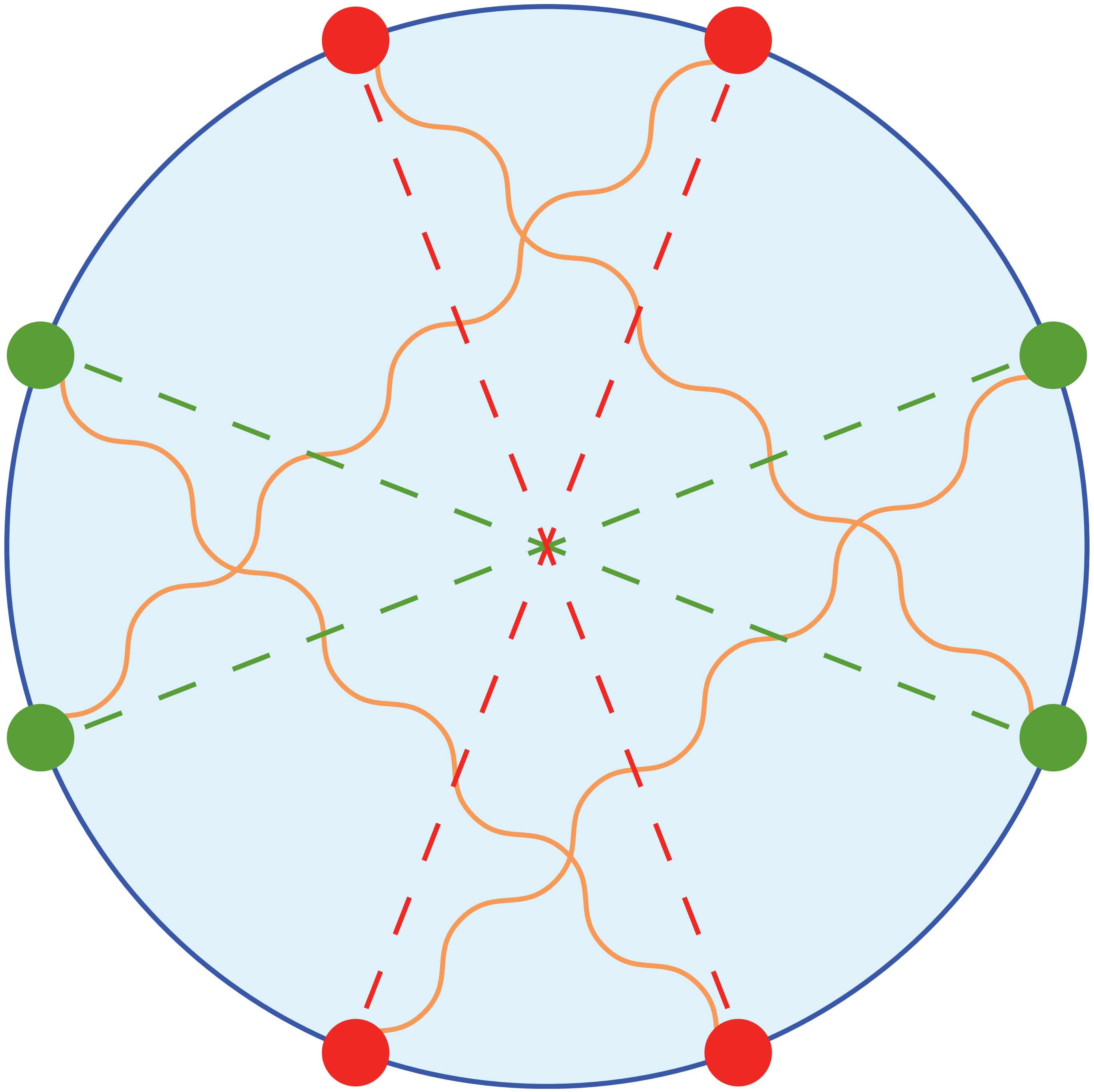
Metal with electron and hole pockets

Metal with "large" Fermi surface

Increasing interaction

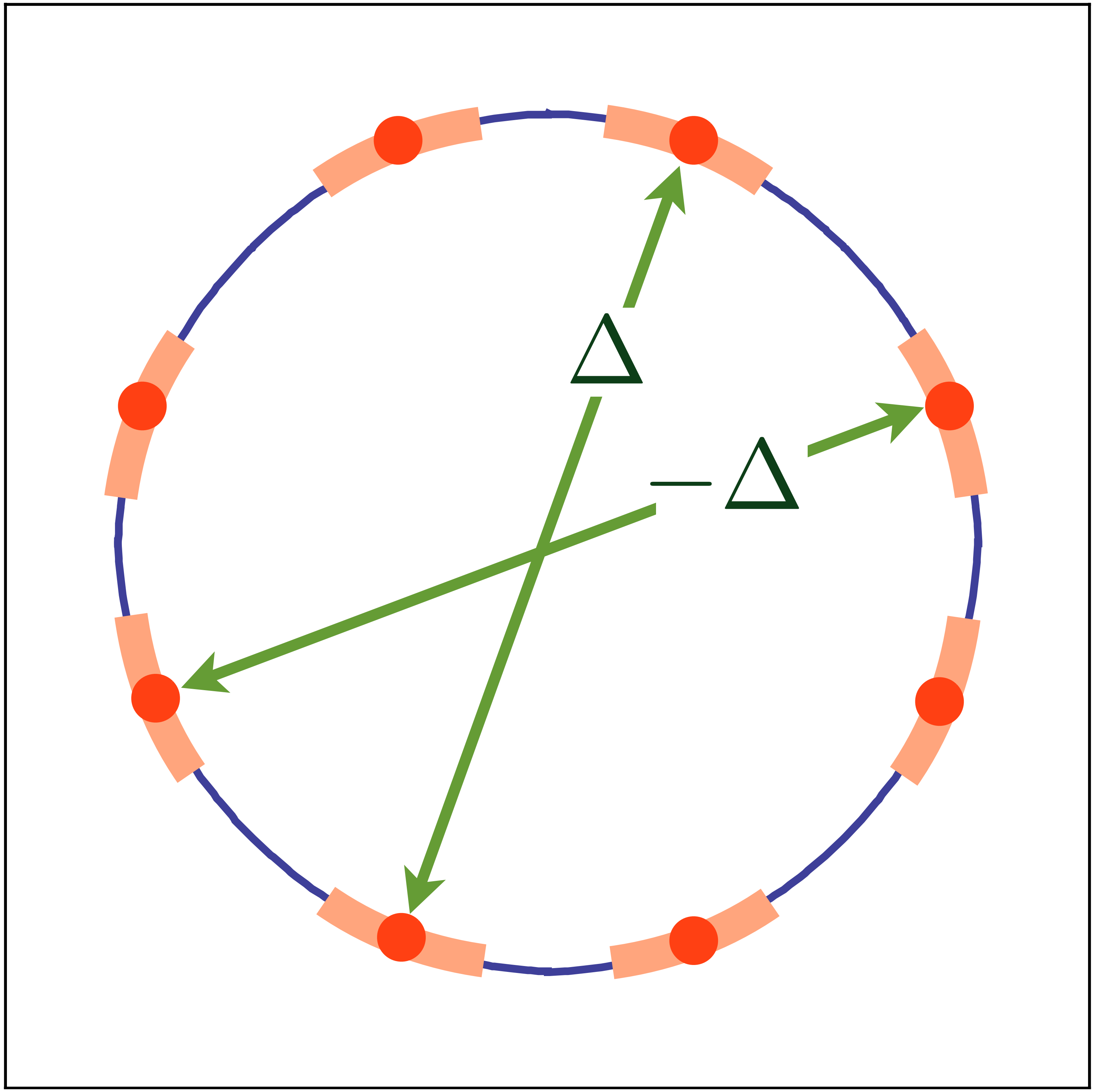
S. Sachdev, A.V. Chubukov, and A. Sokol, *Phys. Rev. B* **51**, 14874 (1995).
A.V. Chubukov and D. K. Morr, *Physics Reports* **288**, 355 (1997).

Pairing "glue" from antiferromagnetic fluctuations



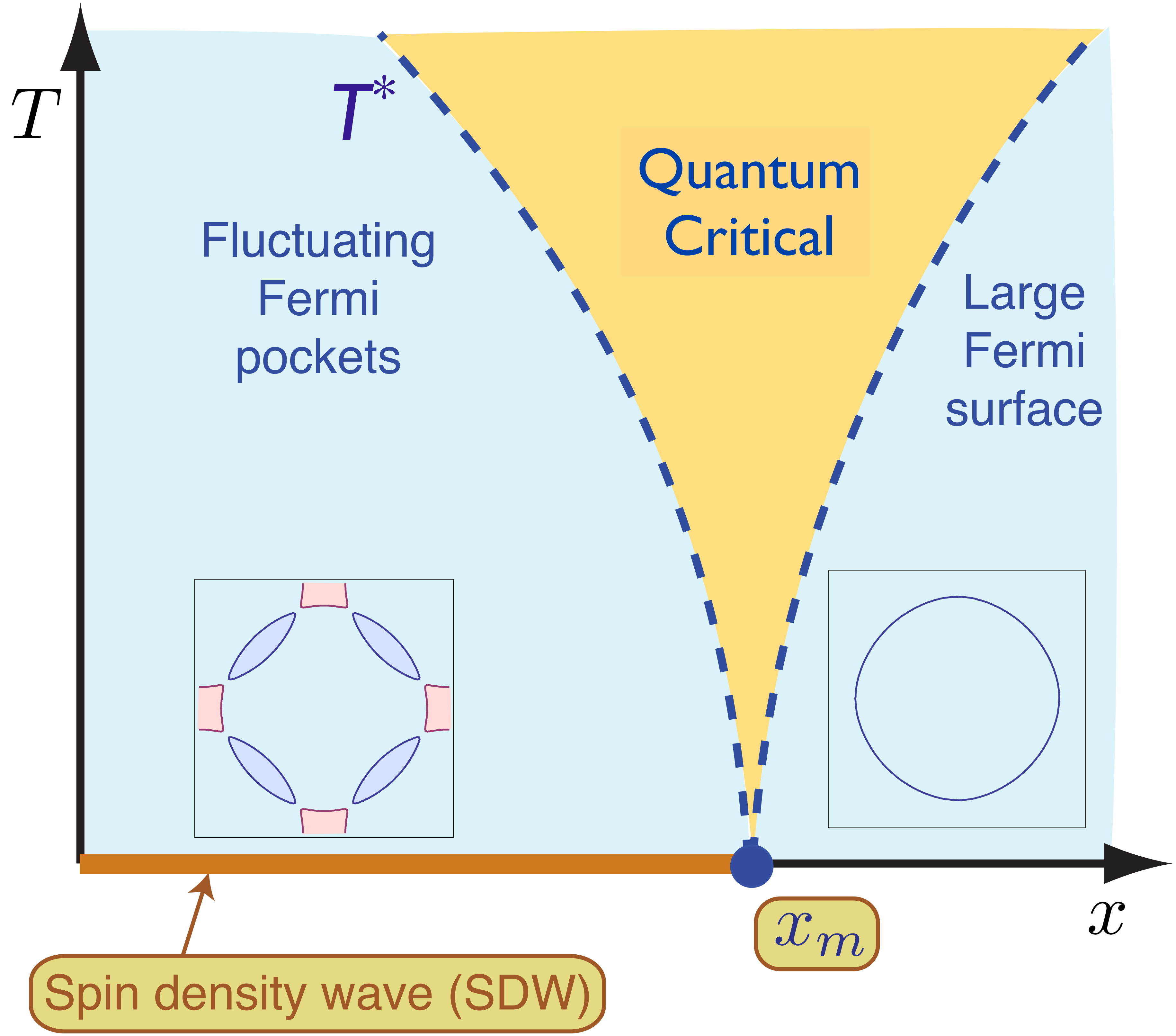
V. J. Emery, *J. Phys. (Paris) Colloq.* **44**, C3-977 (1983)
D.J. Scalapino, E. Loh, and J.E. Hirsch, *Phys. Rev. B* **34**, 8190 (1986)
K. Miyake, S. Schmitt-Rink, and C. M. Varma, *Phys. Rev. B* **34**, 6554 (1986)
S. Raghu, S.A. Kivelson, and D.J. Scalapino, *Phys. Rev. B* **81**, 224505 (2010)

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



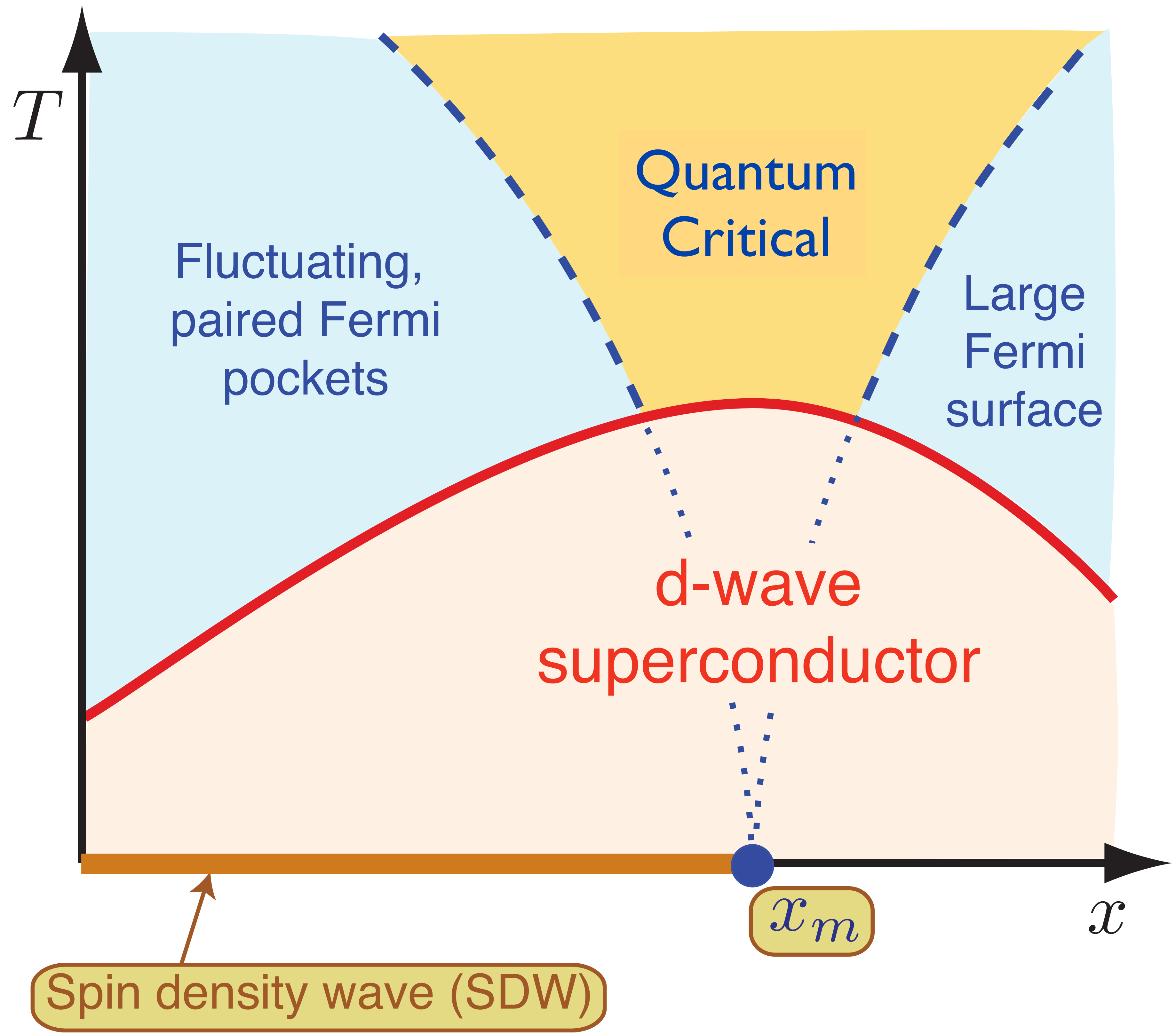
Unconventional pairing at *and near* hot spots

Fermi surface+antiferromagnetism



Underlying SDW ordering quantum critical point in **metal** at $x = x_m$

Fermi surface+antiferromagnetism



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

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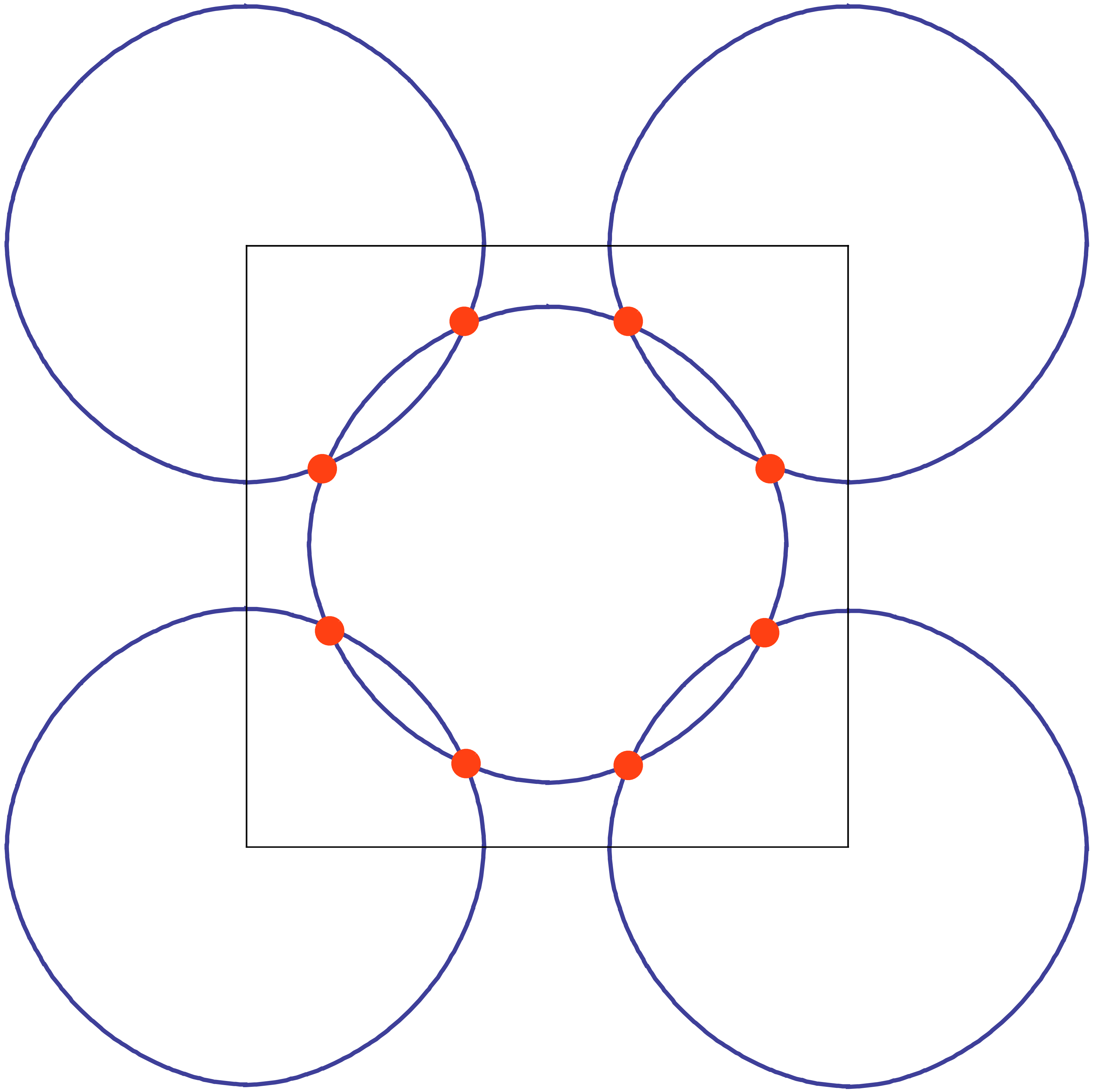
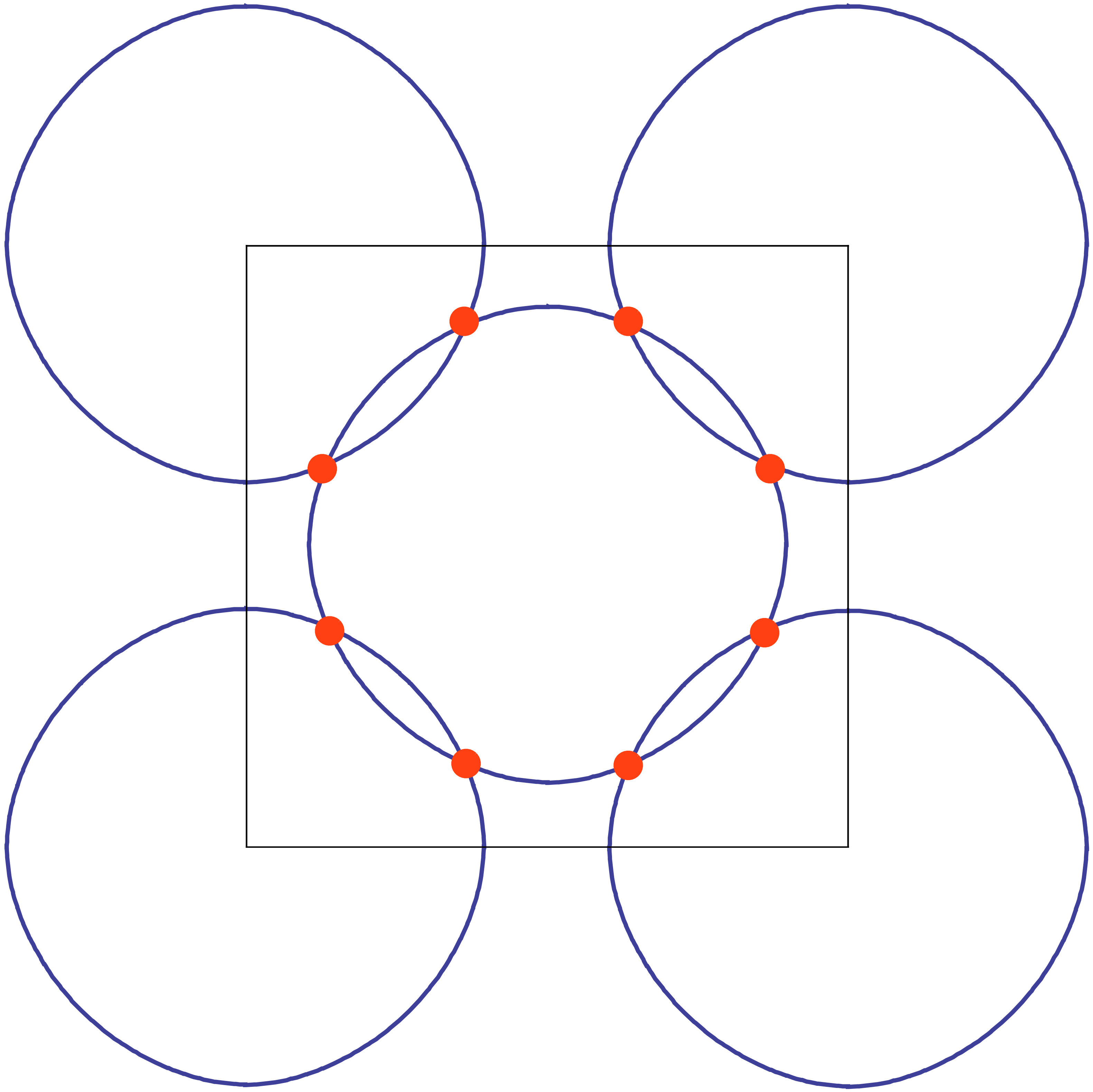
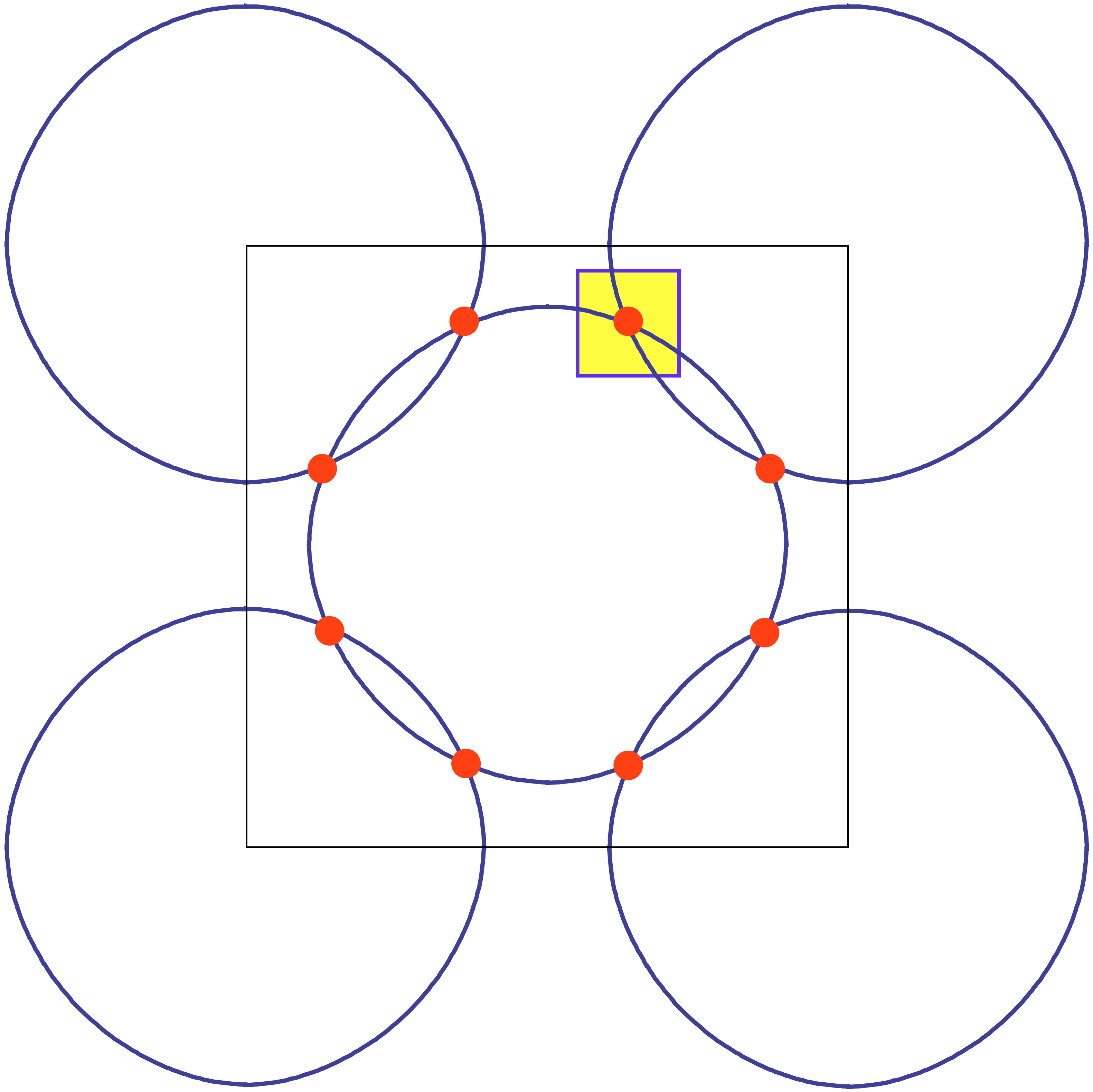


“Hot” spots

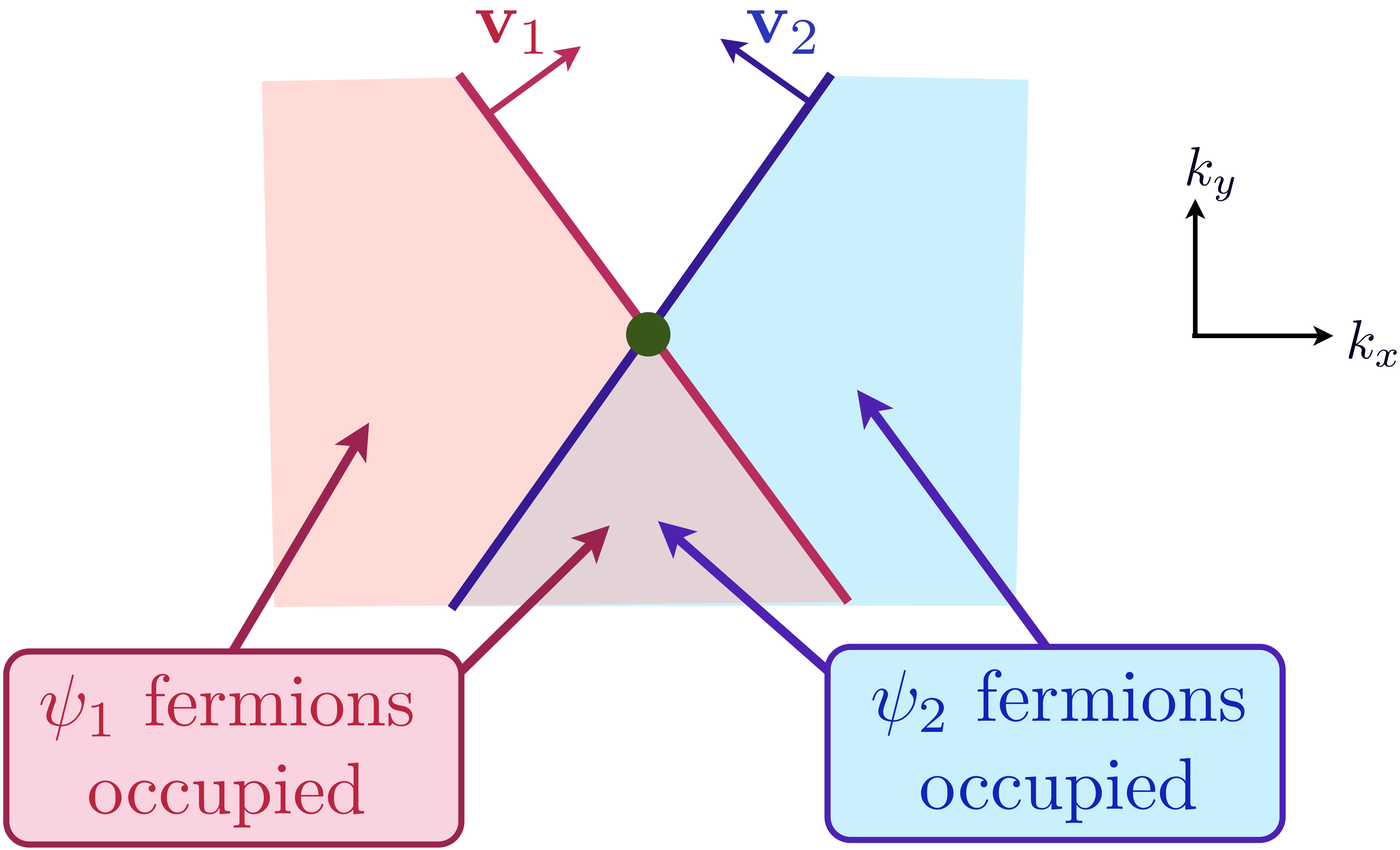


Low energy theory for critical point near hot spots



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



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

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

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

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

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

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

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

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

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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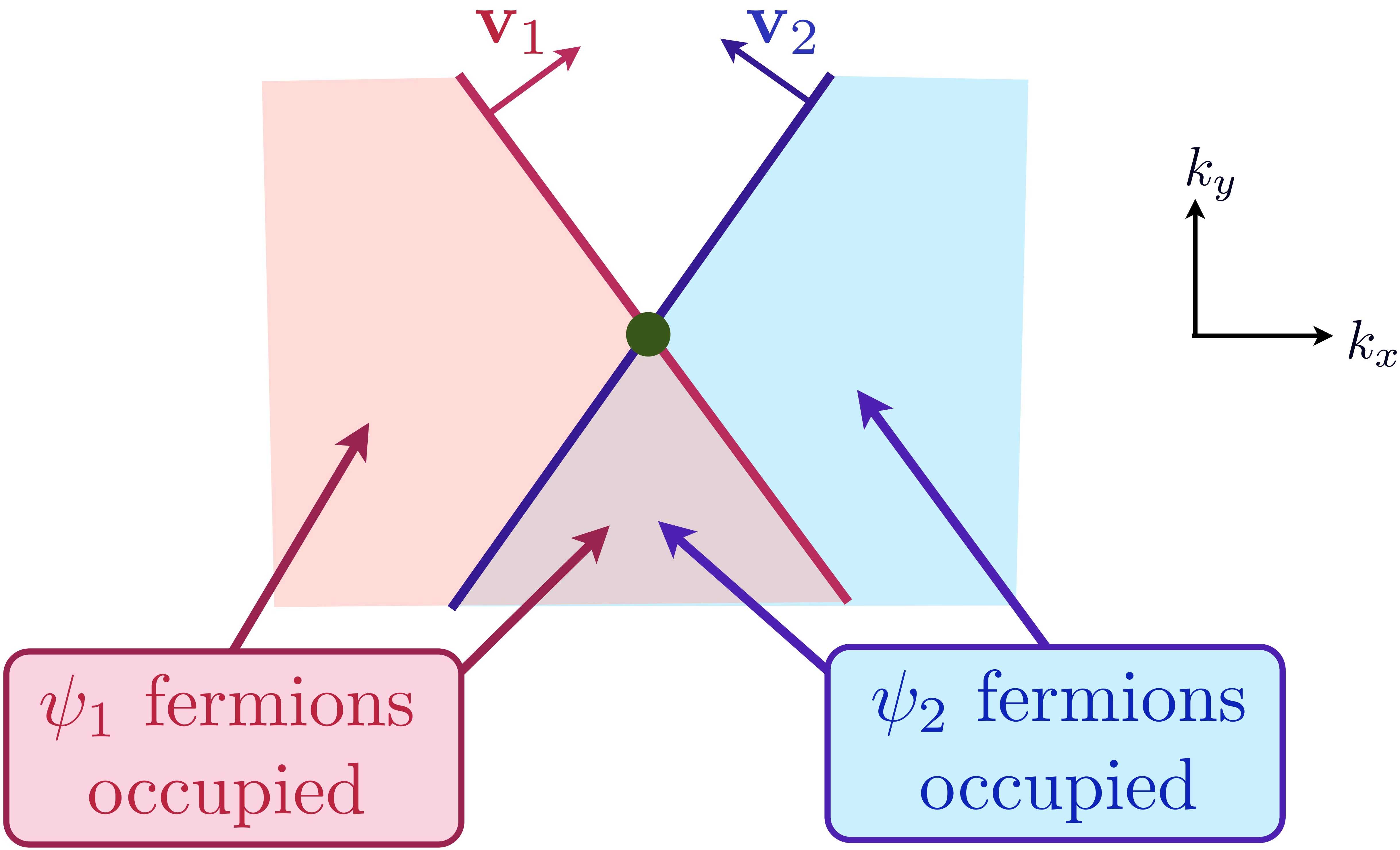
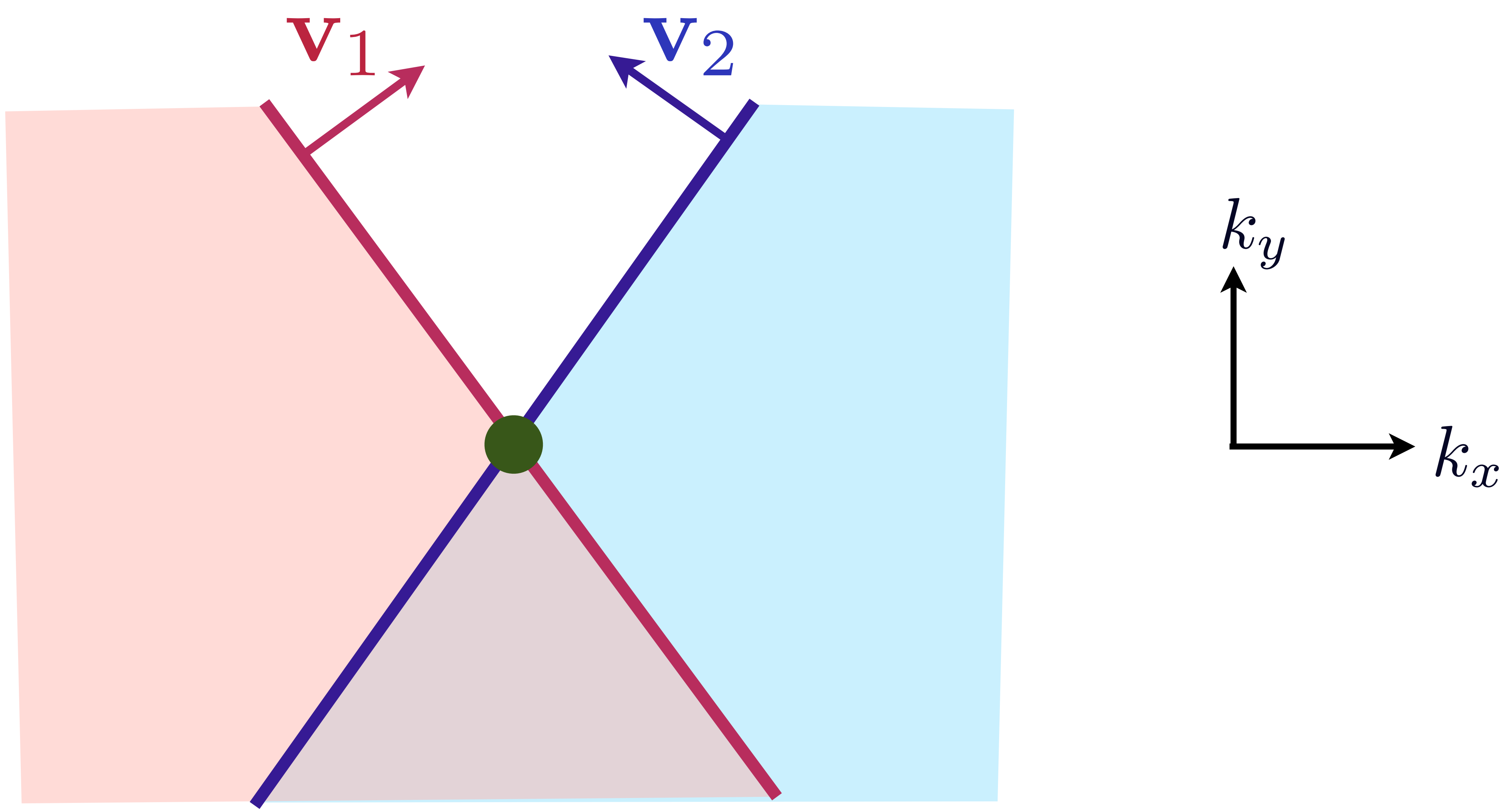
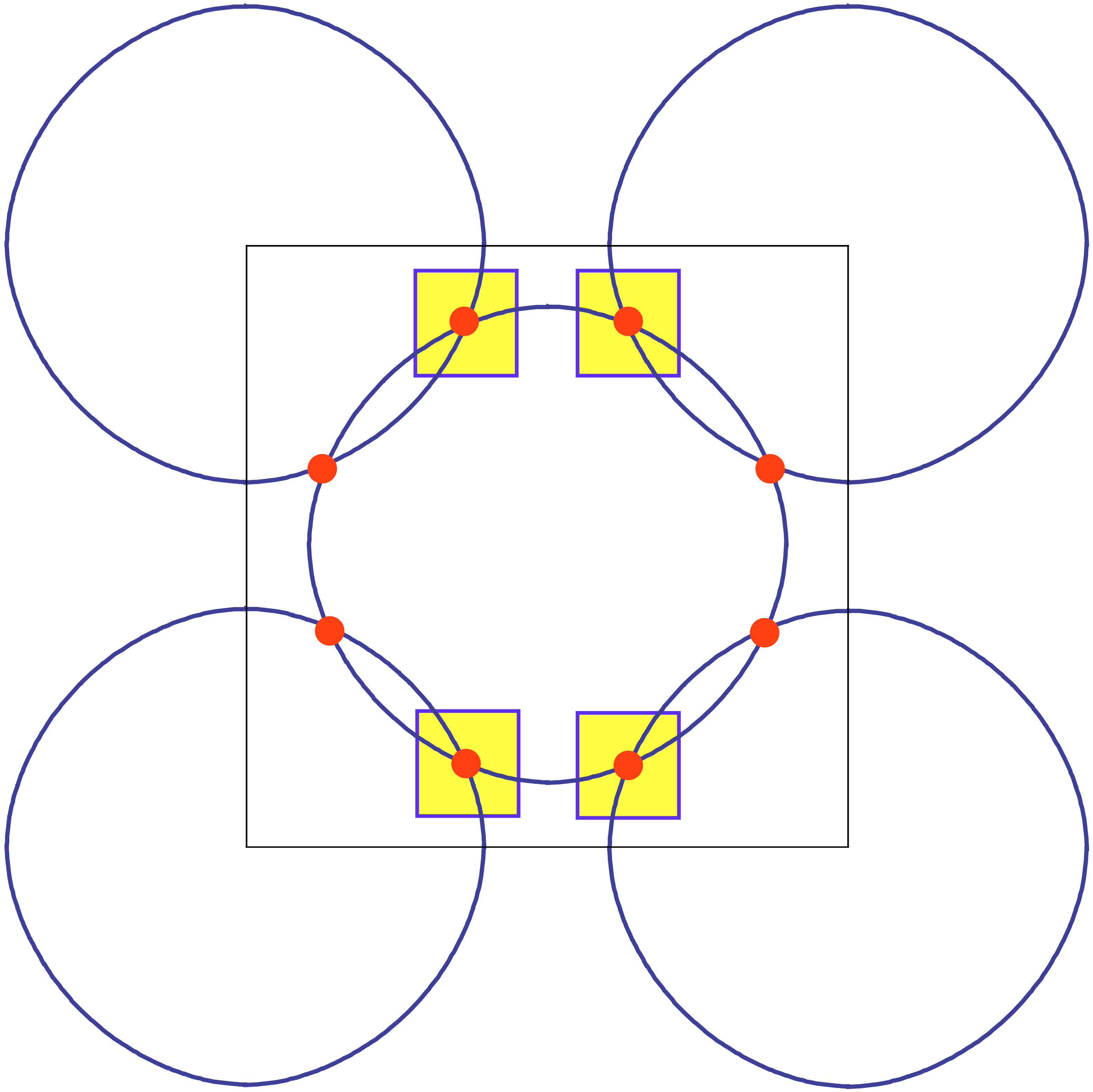


Theory has fermions $\psi_{1,2}$ (with Fermi velocities $\mathbf{v}_{1,2}$) and boson order parameter $\vec{\varphi}$, interacting with coupling λ

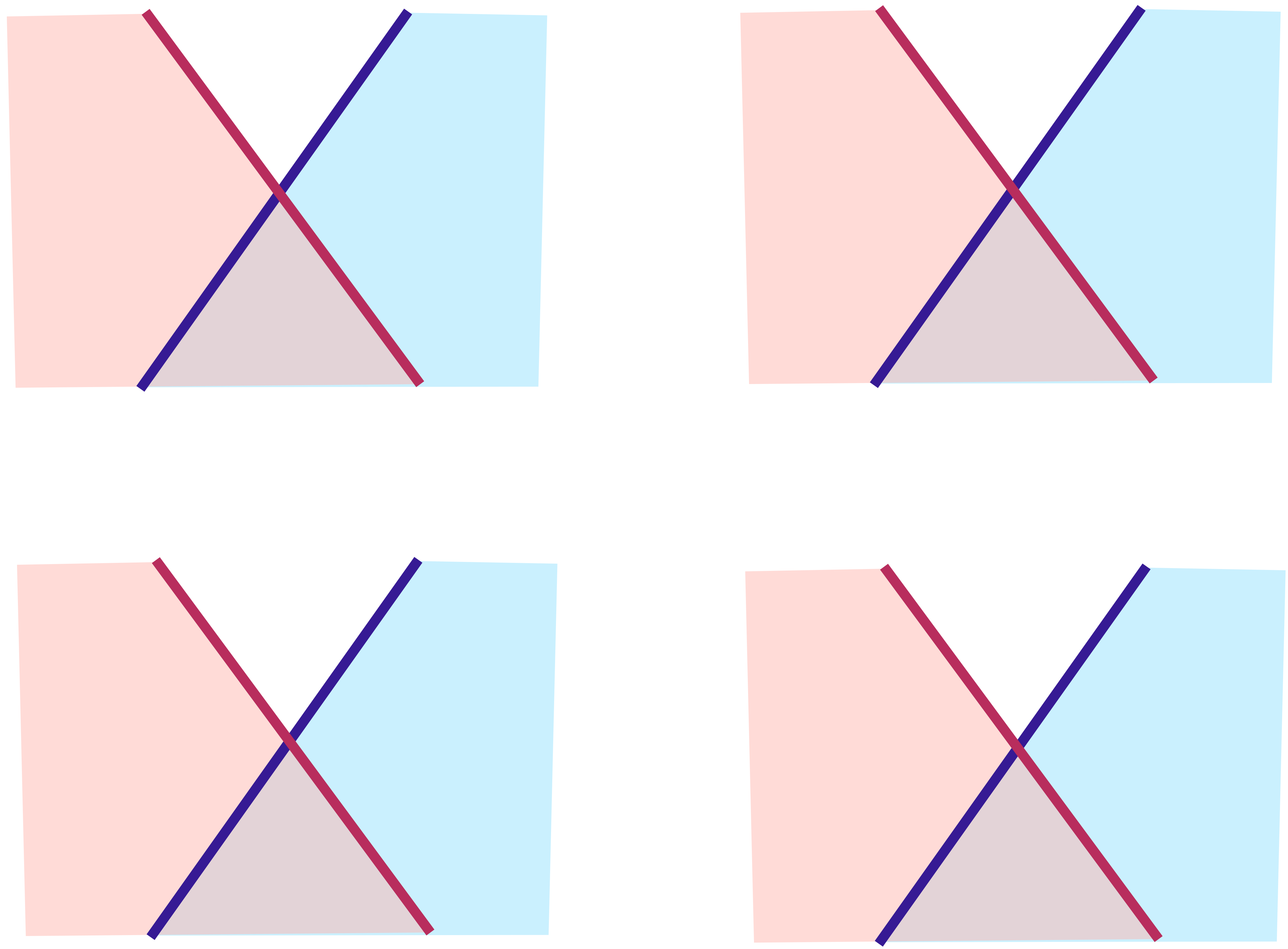


To faithfully realize low energy theory in quantum Monte Carlo, we need a UV completion in which Fermi lines don't end and all weights are positive.

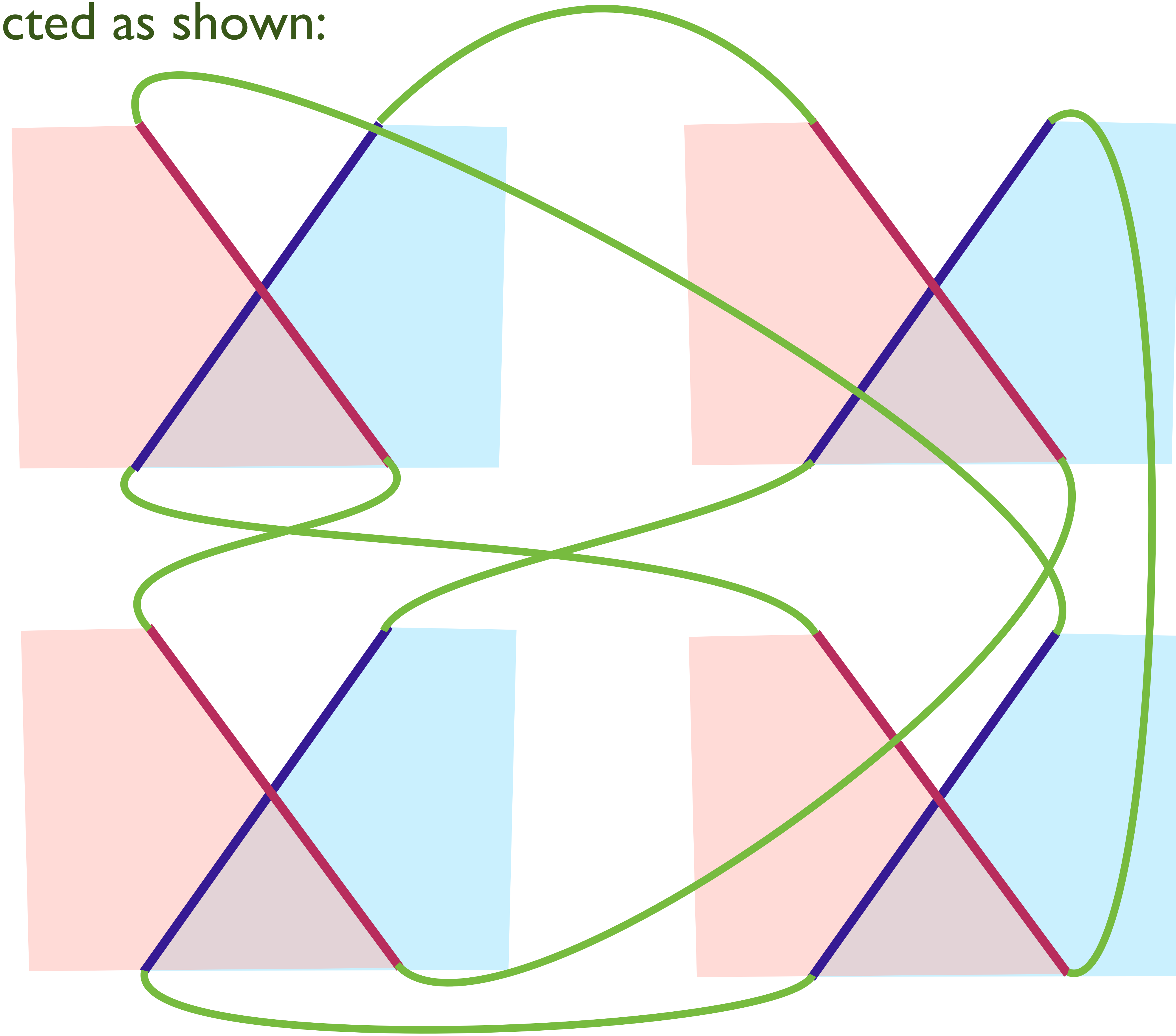


Low energy theory for critical point near hot spots

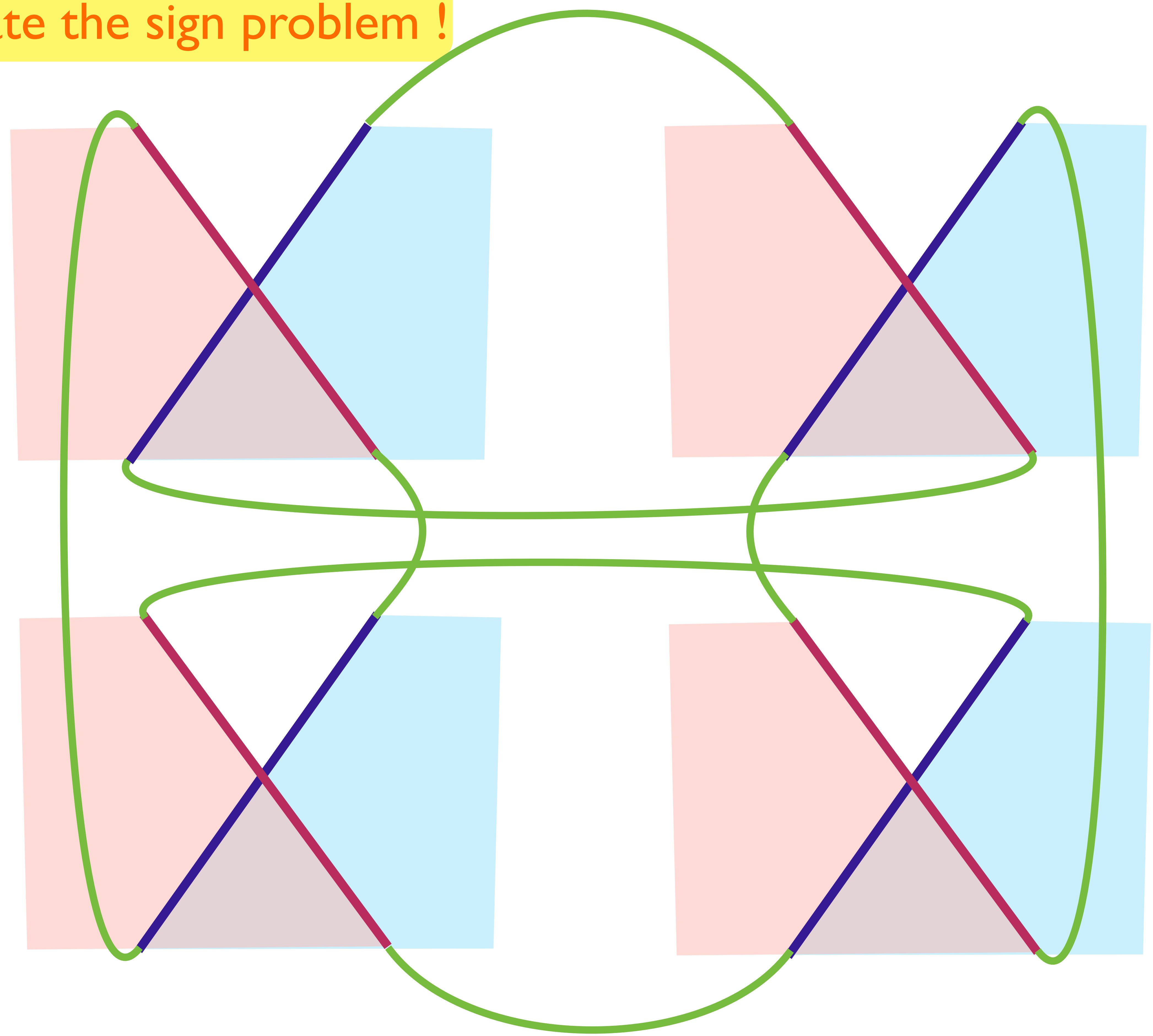
We have 4 copies of the hot spot theory......



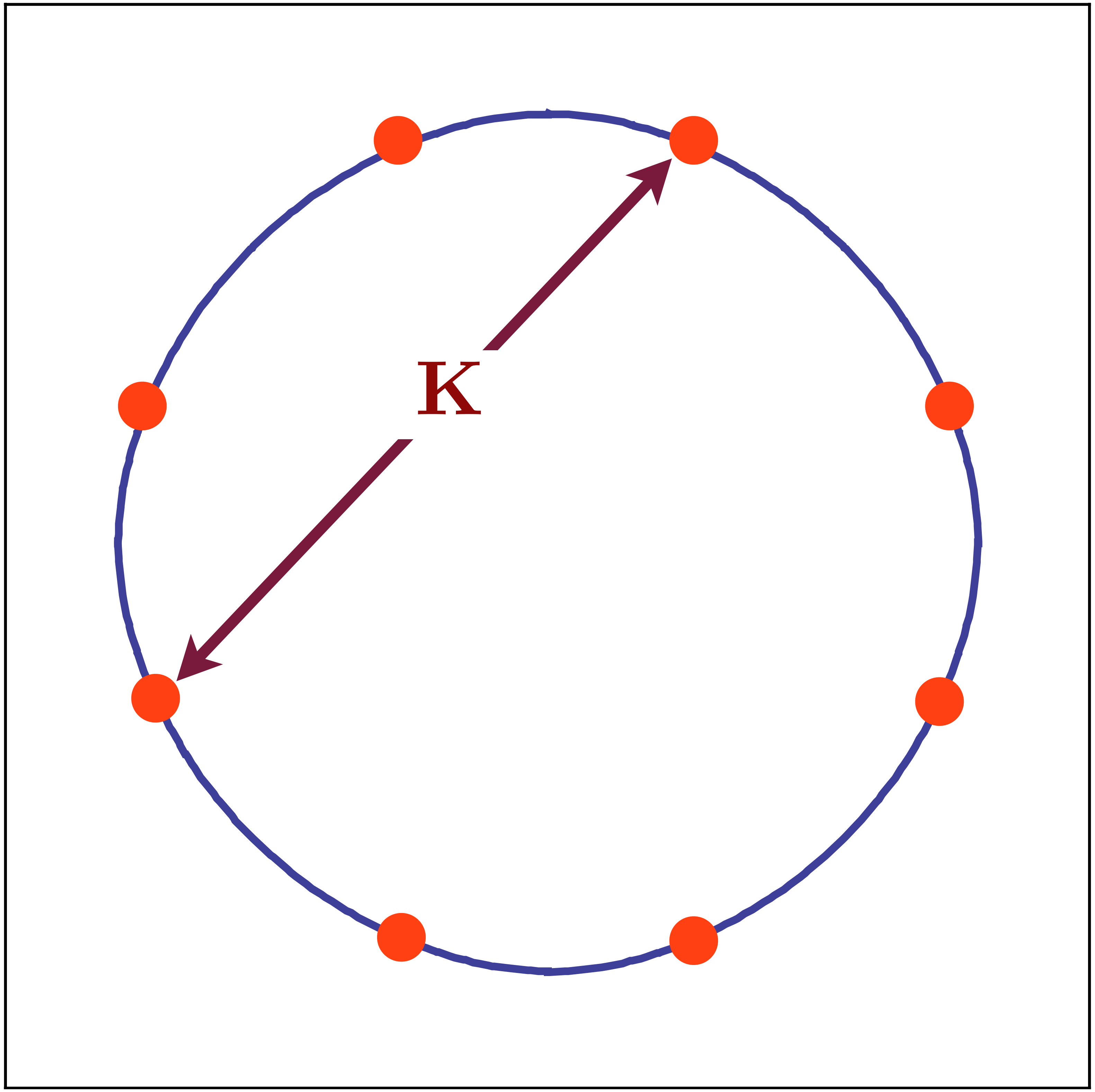
and their Fermi lines are connected as shown:



Reconnect Fermi lines and eliminate the sign problem !

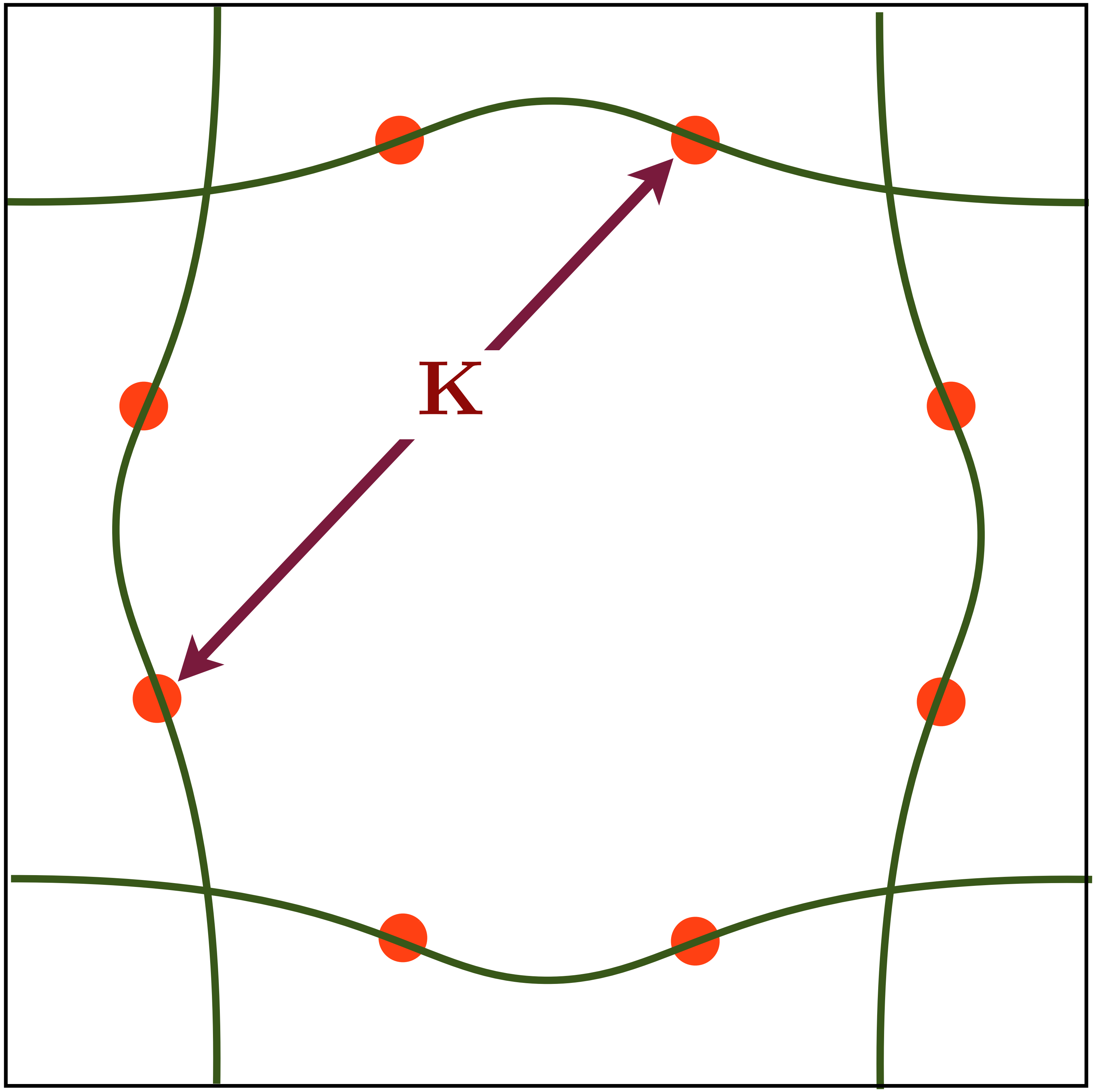


QMC for the onset of antiferromagnetism



Hot spots in a single band model

QMC for the onset of antiferromagnetism

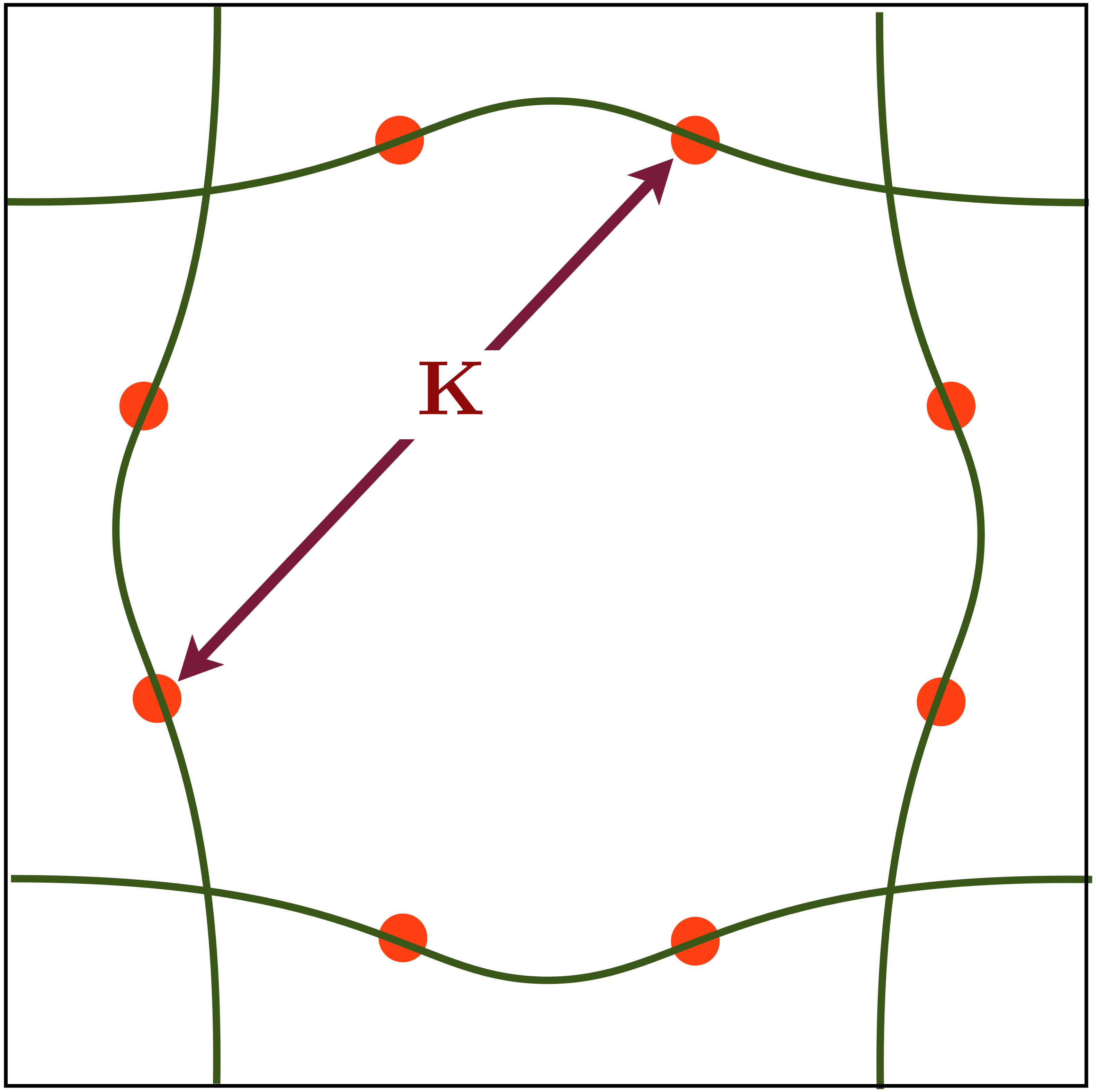


Hot spots in a two band model

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 antiferromagnetism.



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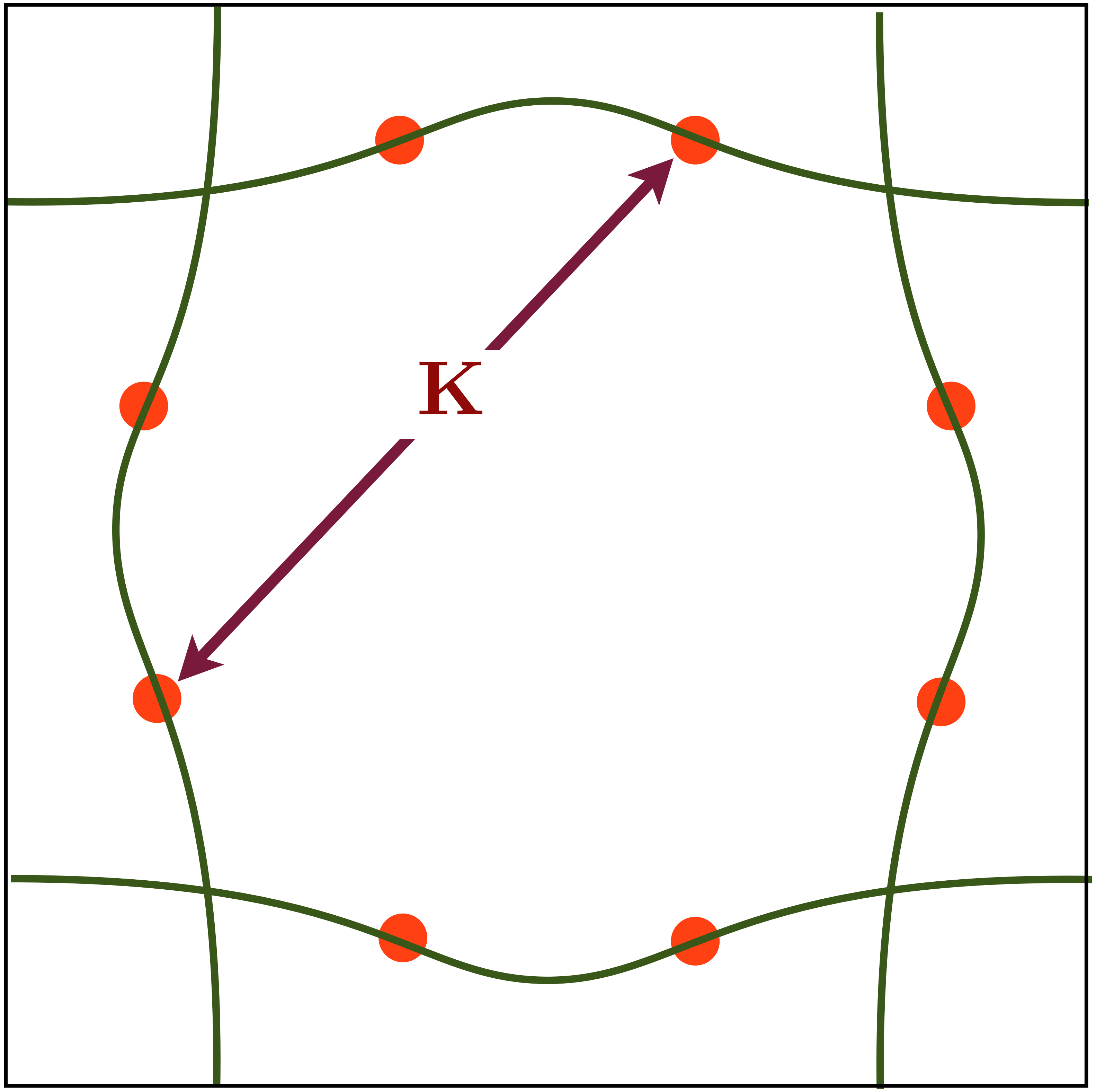
QMC for the onset of antiferromagnetism



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E. Berg,
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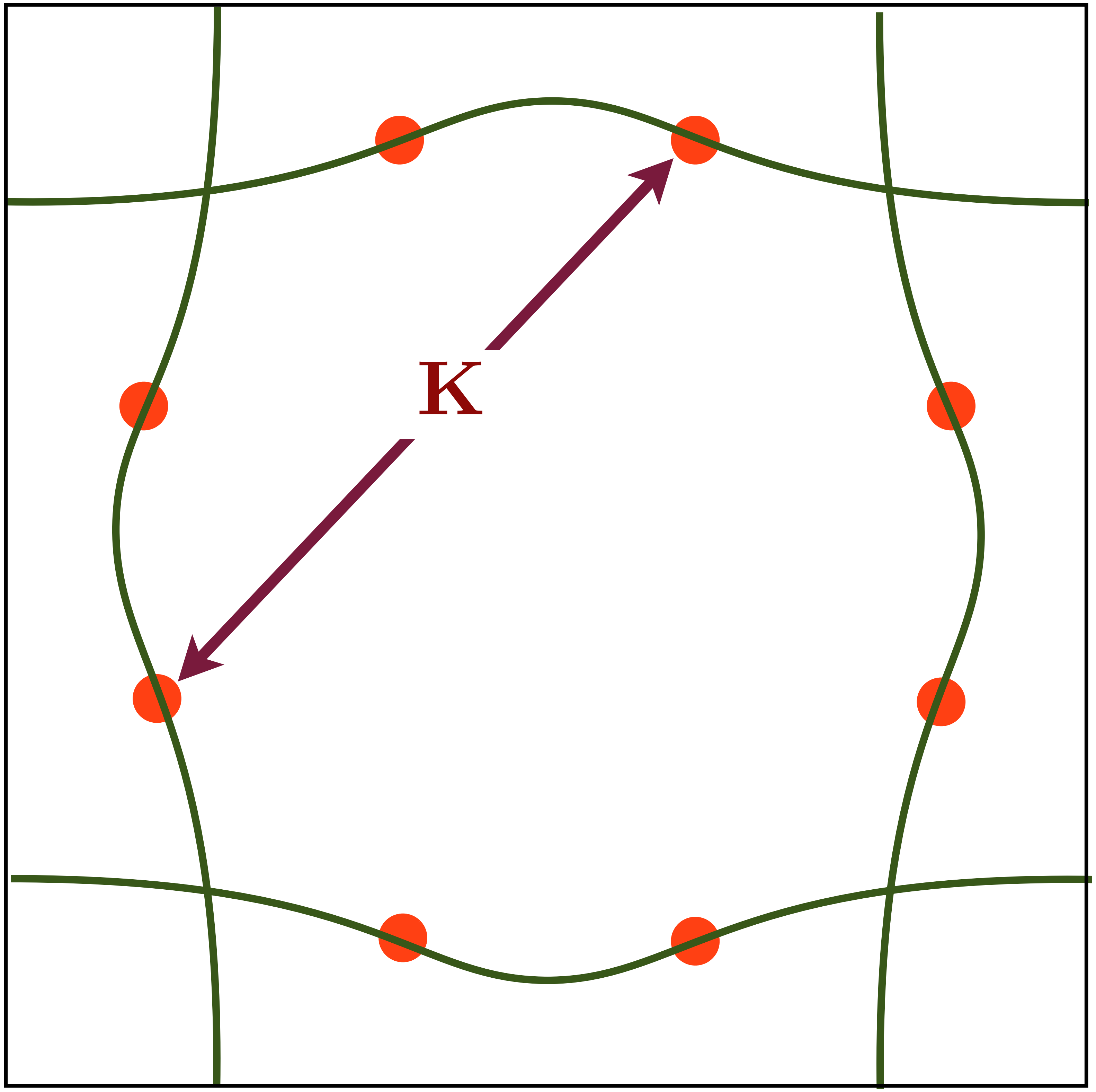
QMC for the onset of antiferromagnetism

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



Hot spots in a two band model

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QMC for the onset of antiferromagnetism

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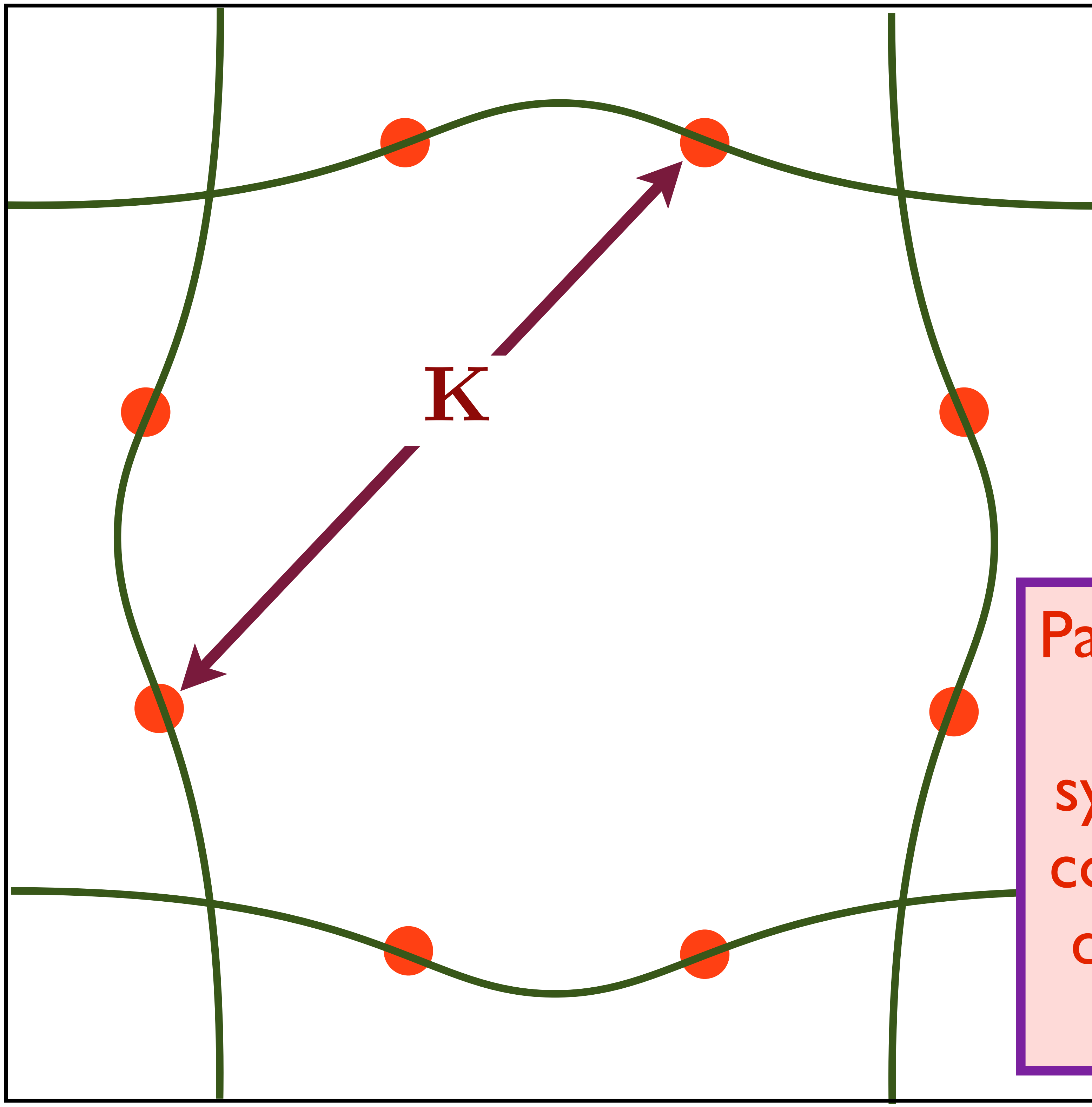

Hot spots in a two band model

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 $\vec{\varphi}$.

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

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

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

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

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

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

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 $\vec{\varphi}$.

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

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

No sign problem !

QMC for the onset of antiferromagnetism

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

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

Tuesday, October 9, 12

QMC for the onset of antiferromagnetism

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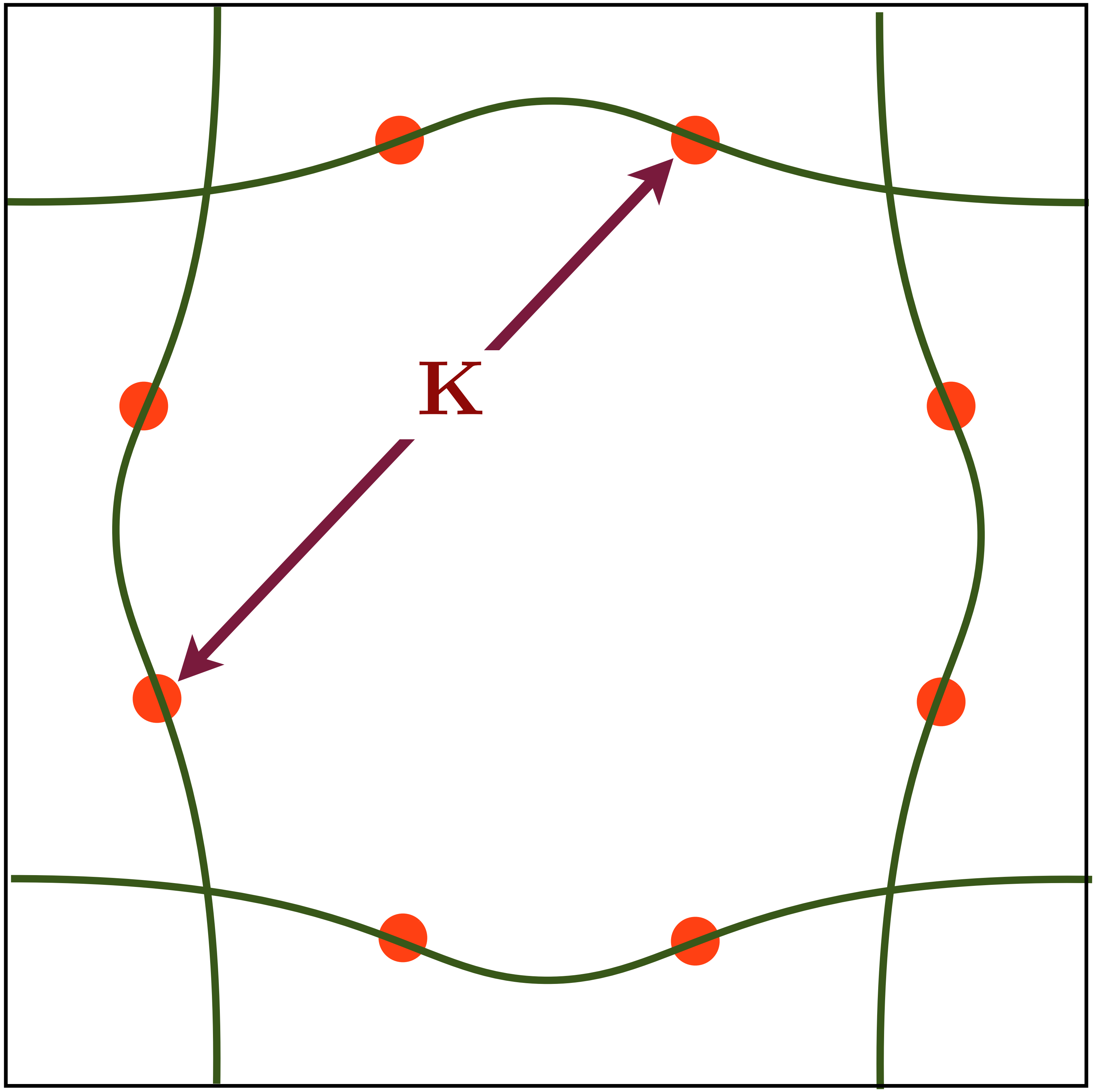
E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

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

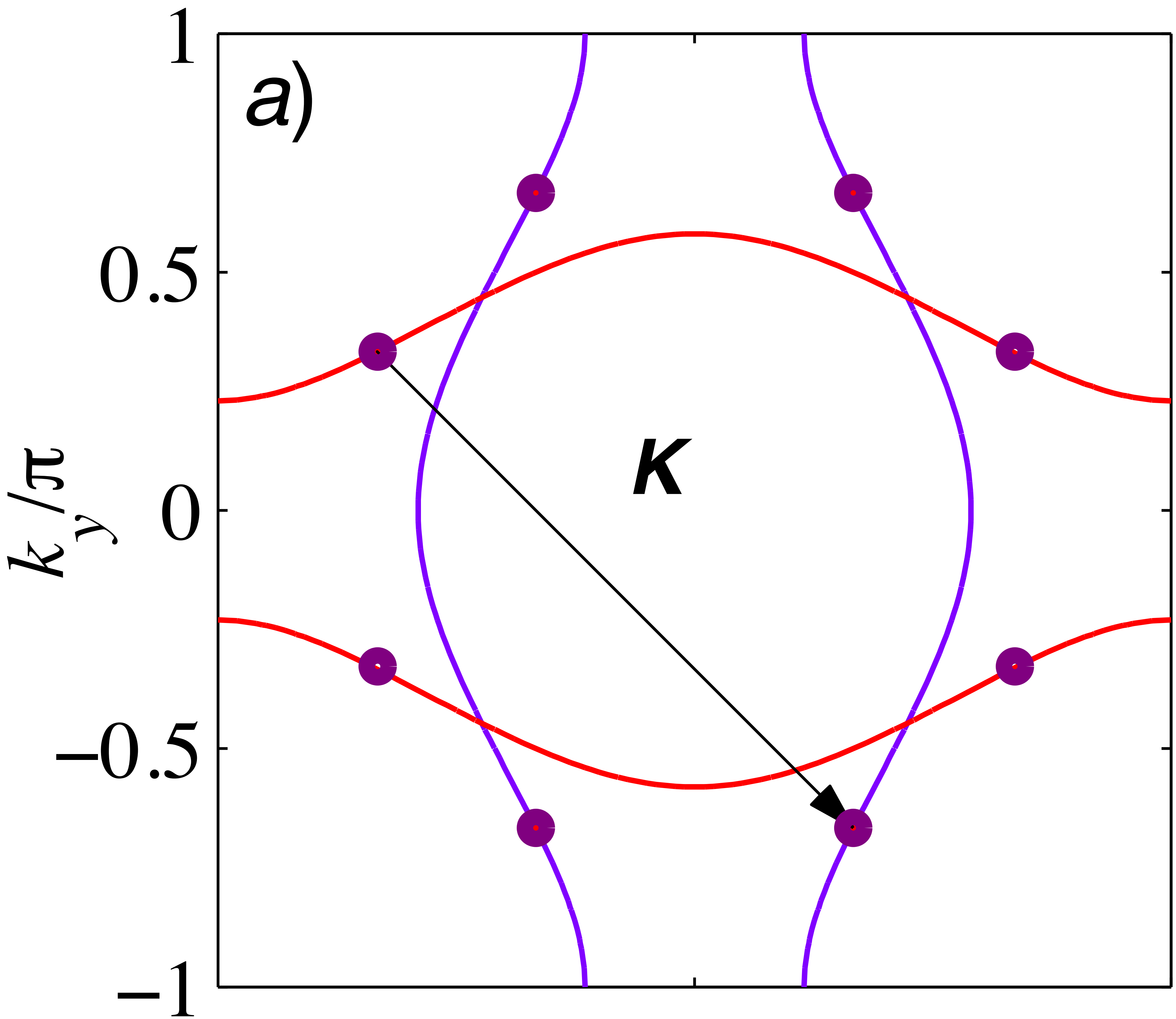
QMC for the onset of antiferromagnetism



Hot spots in a two band model

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

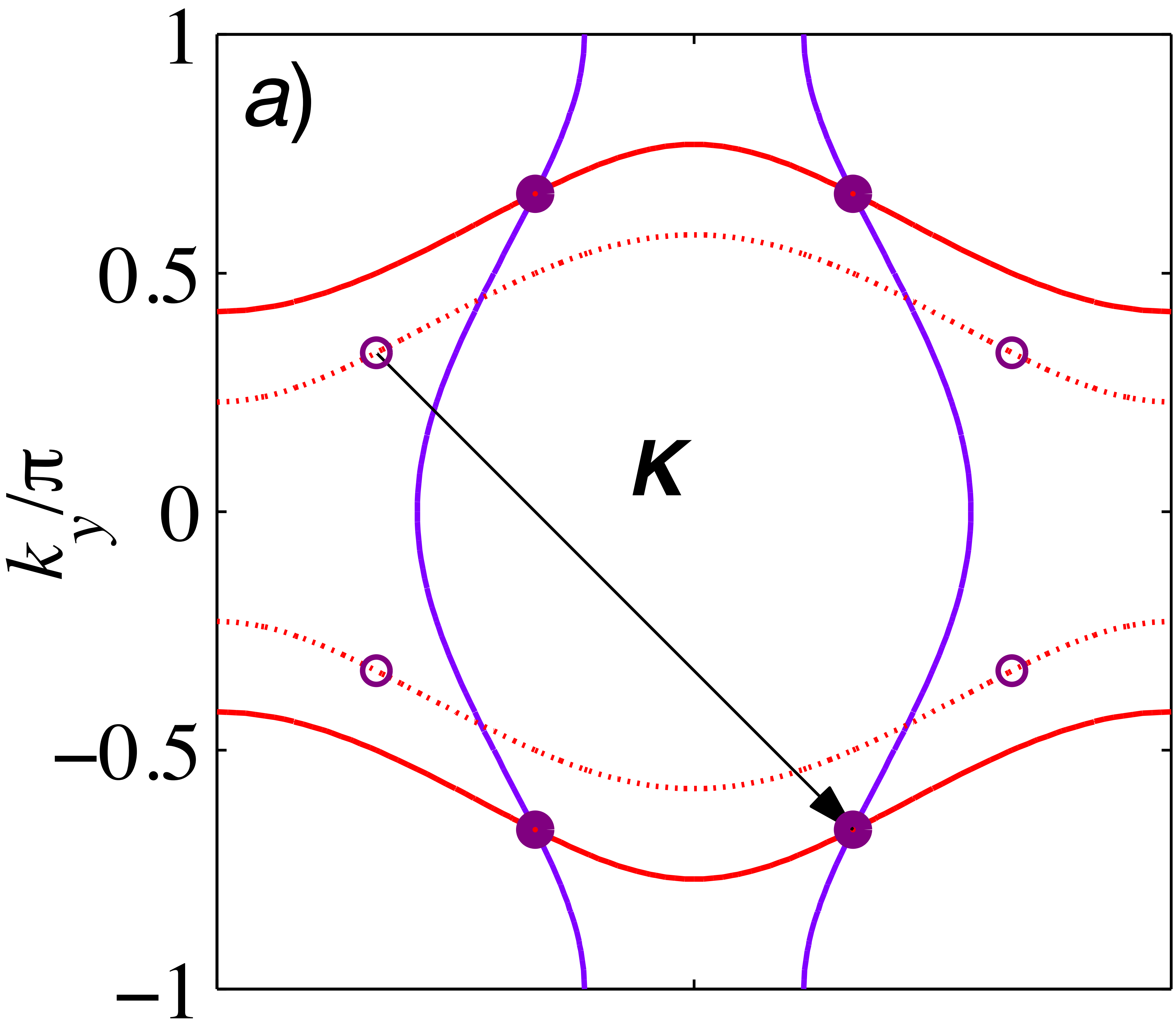
QMC for the onset of antiferromagnetism



Center Brillouin zone at $(\pi,\pi,)$

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

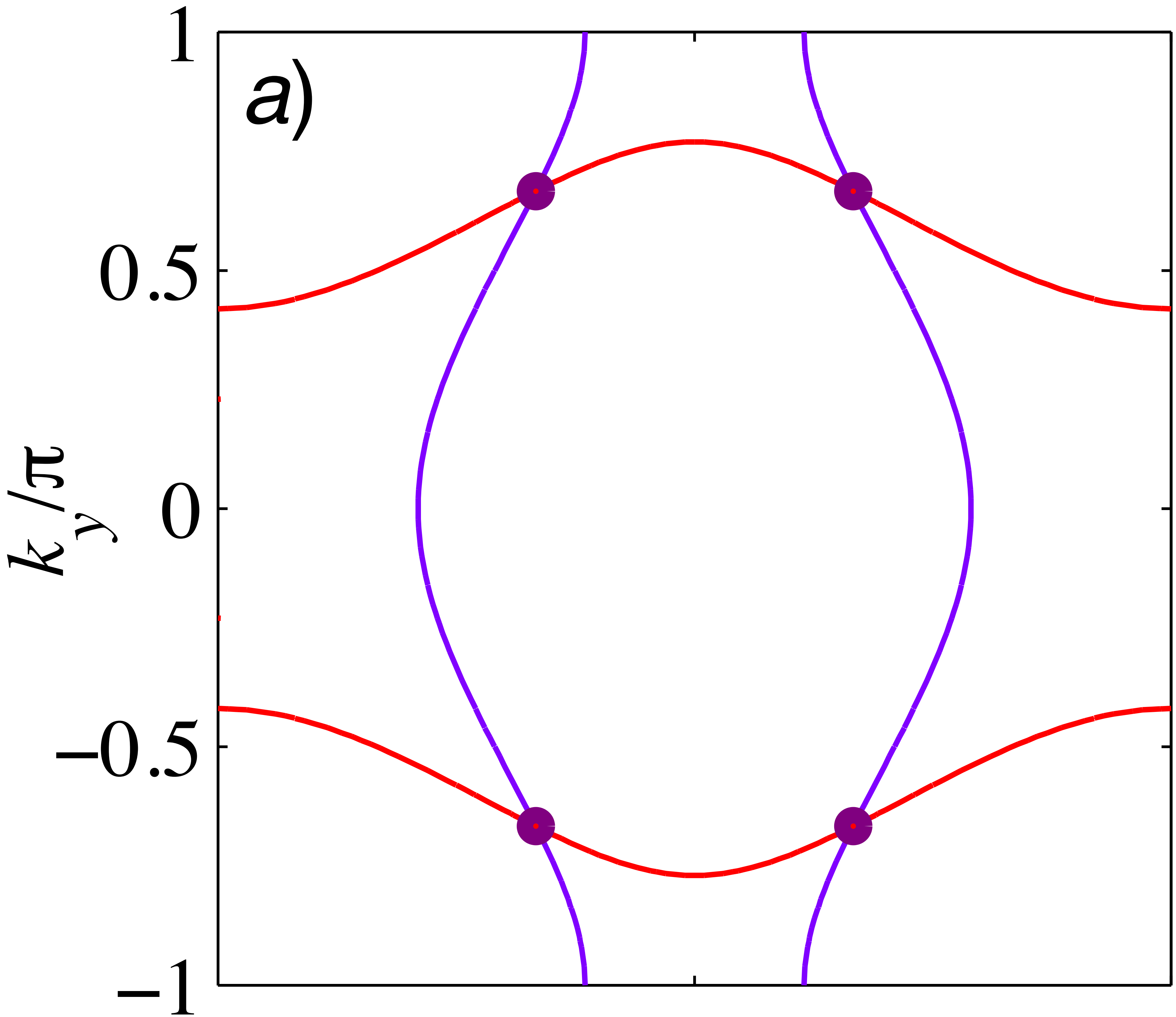
QMC for the onset of antiferromagnetism



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

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

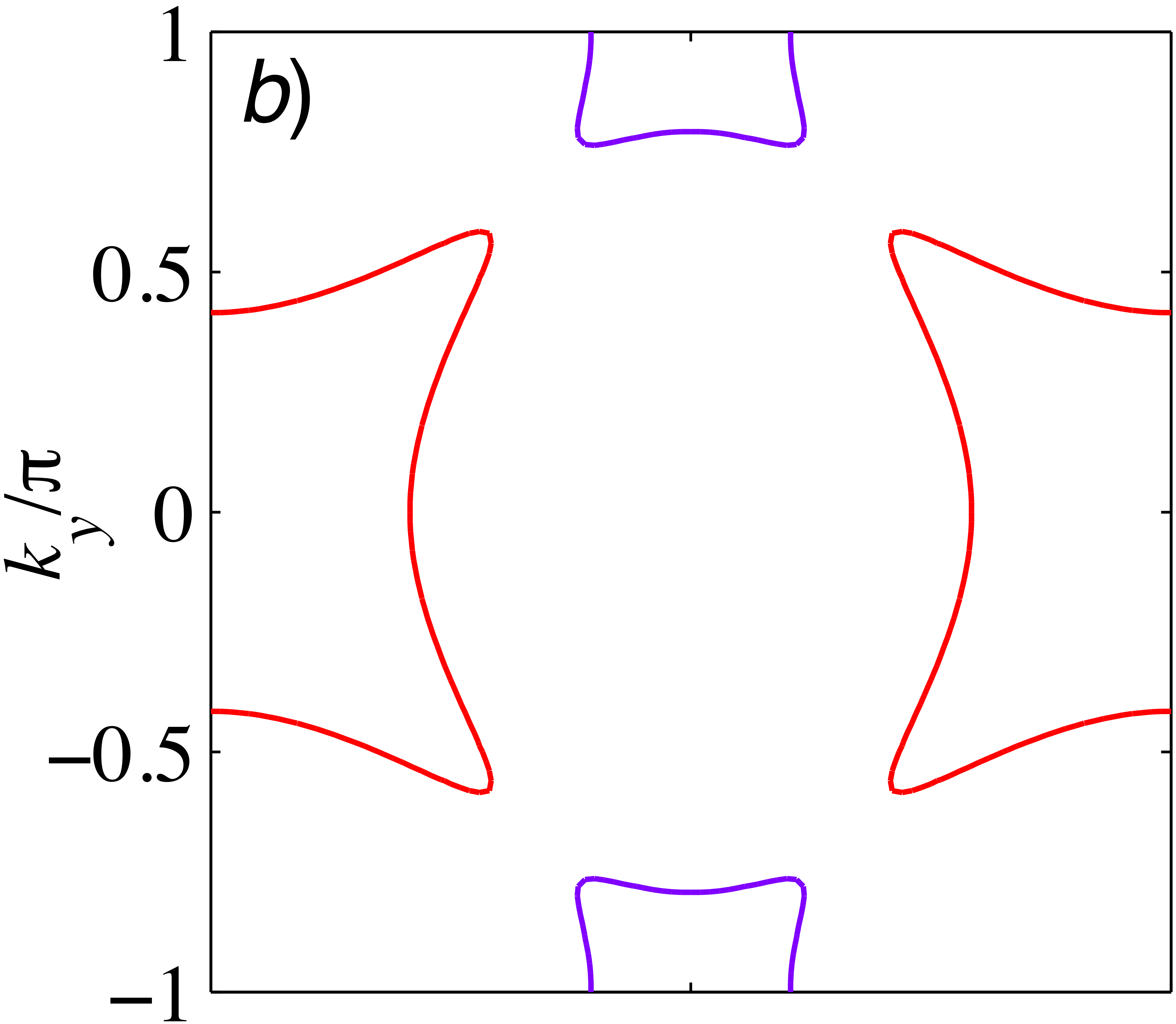
QMC for the onset of antiferromagnetism



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

Now hot spots are at Fermi surface intersections

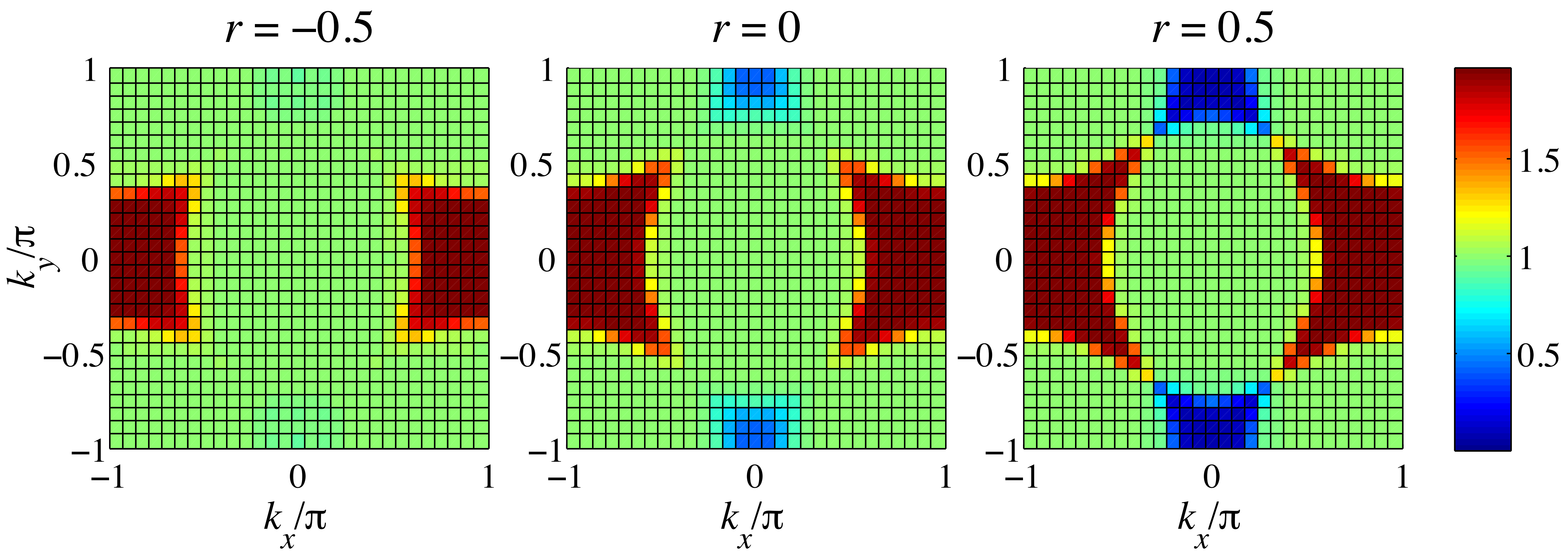
QMC for the onset of antiferromagnetism



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

Expected Fermi surfaces in the AFM ordered phase

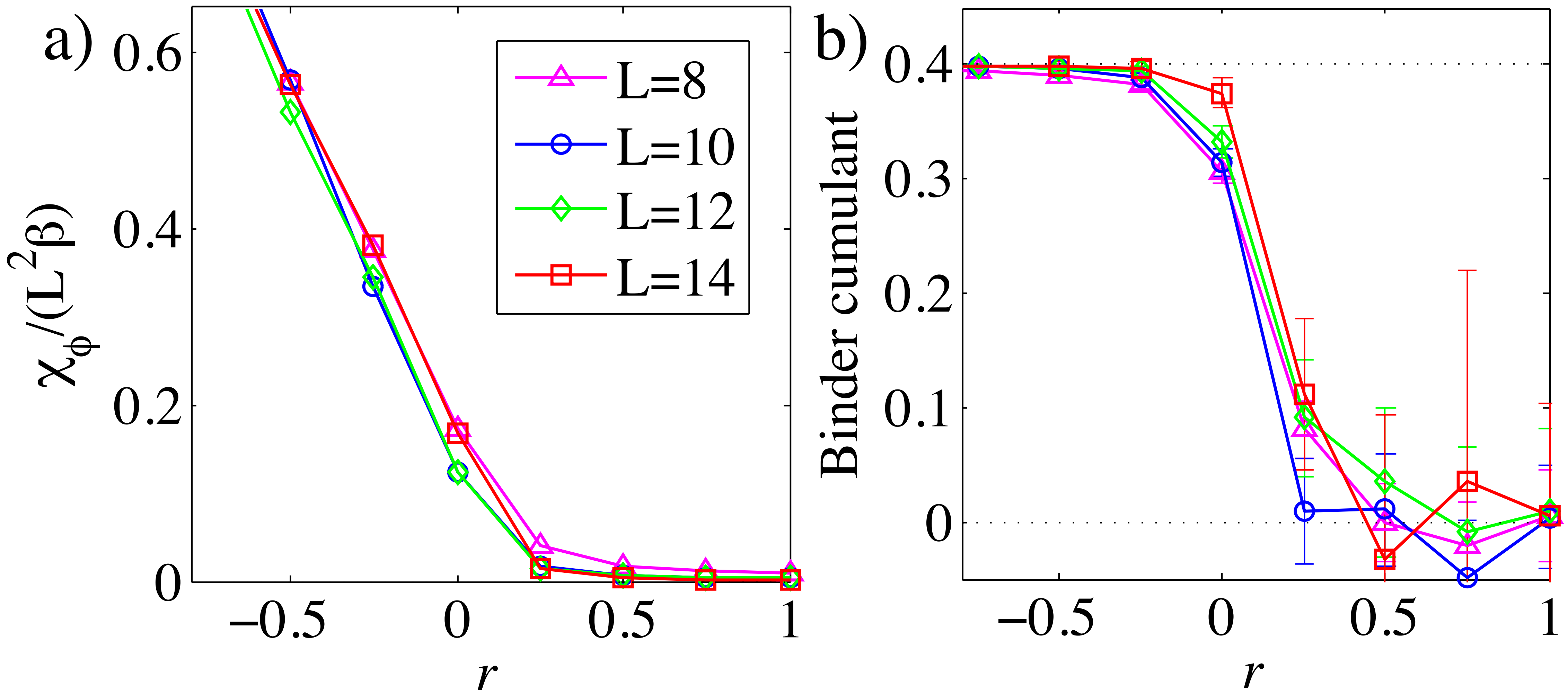
QMC for the onset of antiferromagnetism



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

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

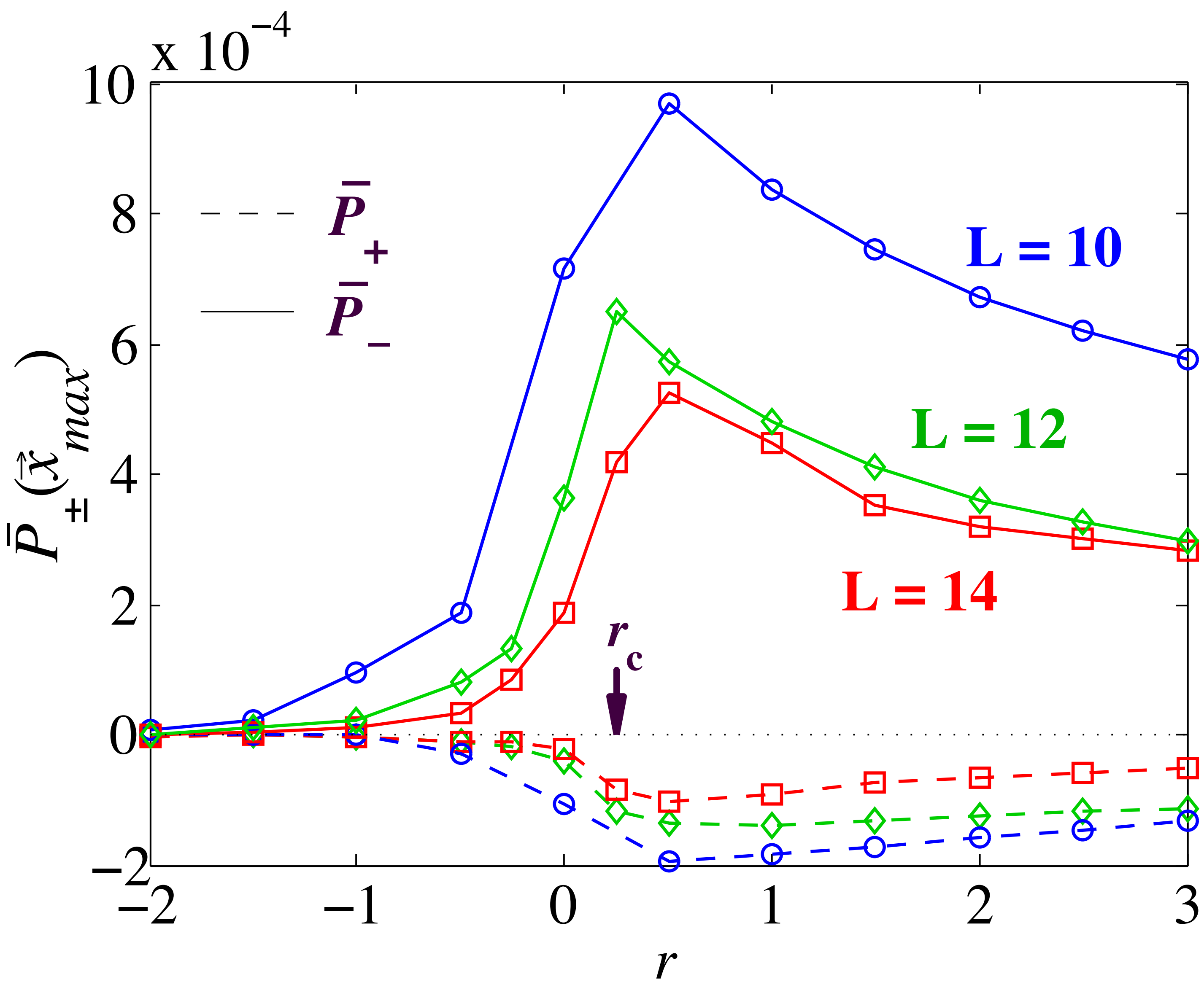
QMC for the onset of antiferromagnetism



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

Outline

1. Weak coupling theory

2. Universal critical theory

3. Quantum Monte Carlo
   without the sign problem

4. Features of strong coupling

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4. Features of strong coupling

Features of strong coupling

- Shift in QCP due to superconductivity: "backbending" of SDW order.

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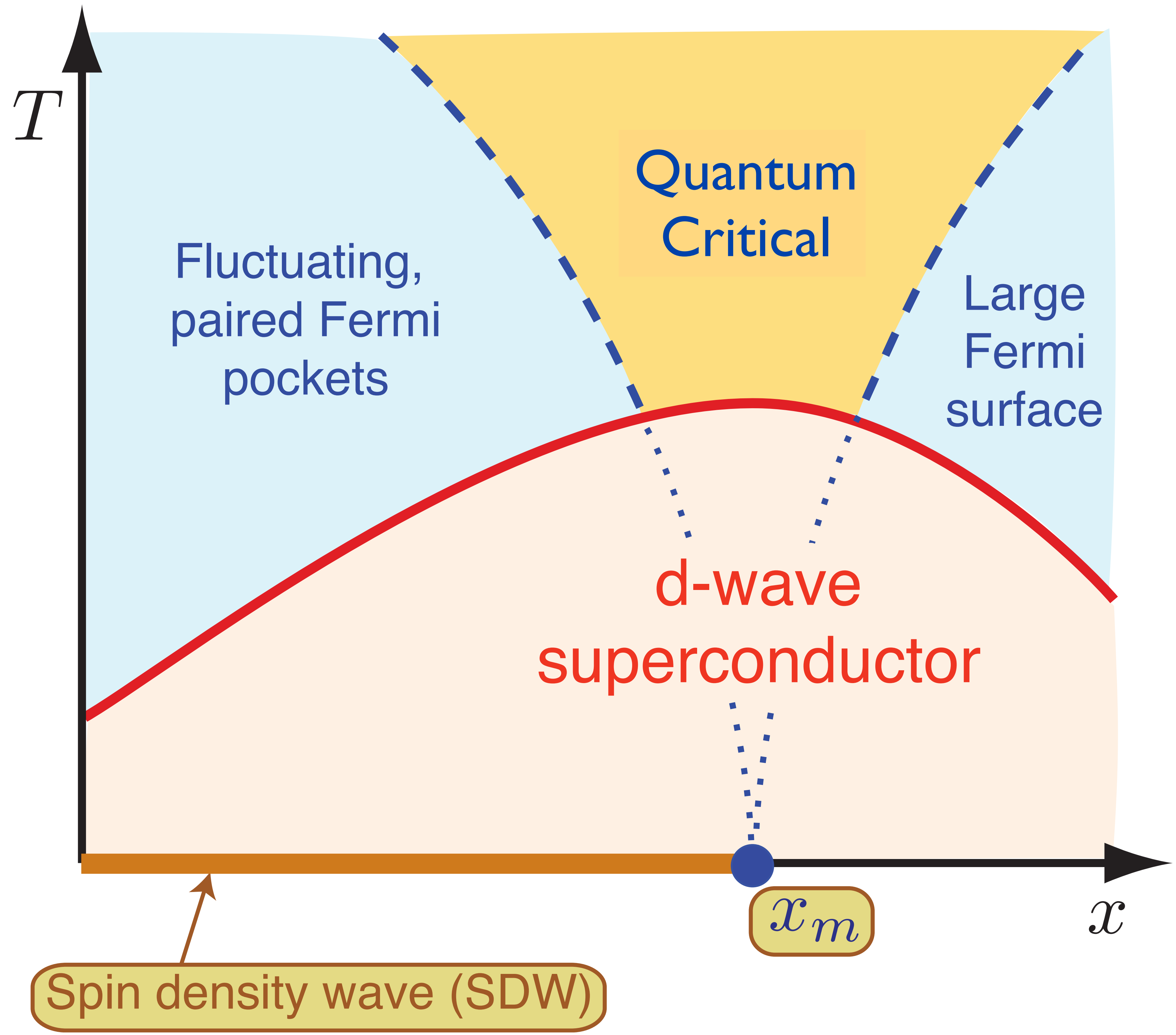
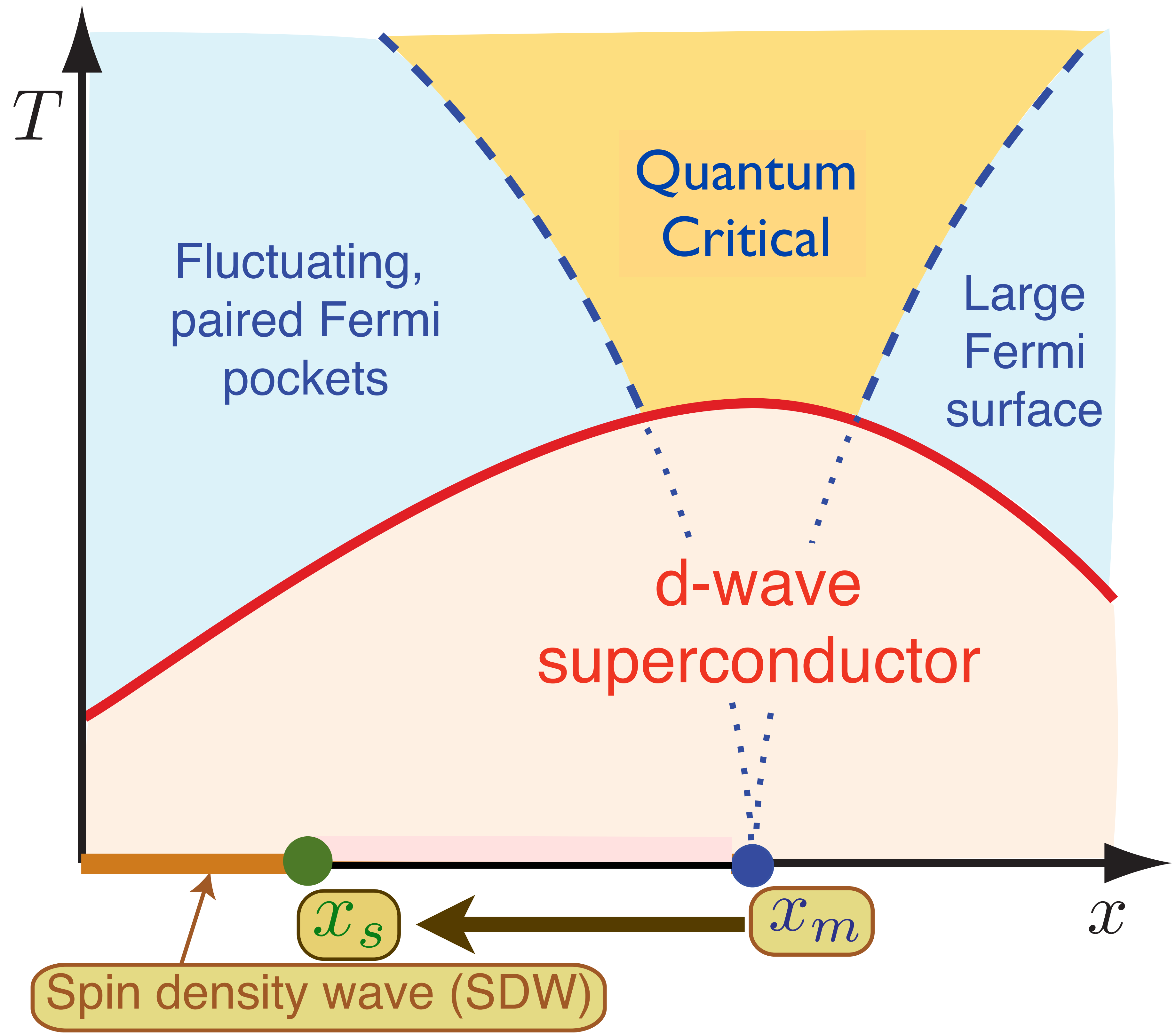


QCP for the onset of SDW order is actually within a superconductor

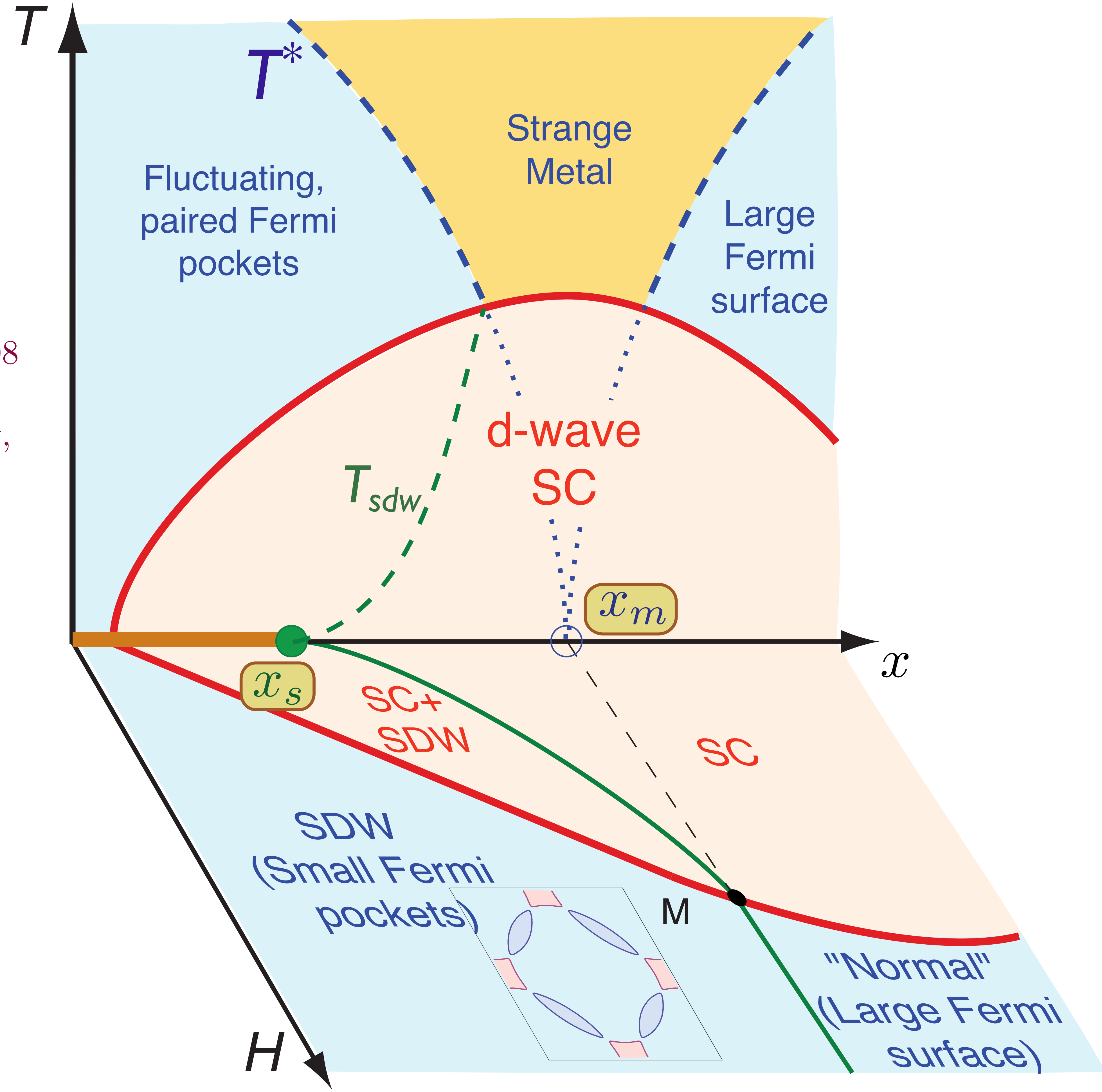


Competition between SDW order and superconductivity moves the actual quantum critical point to $x = x_s < x_m$.

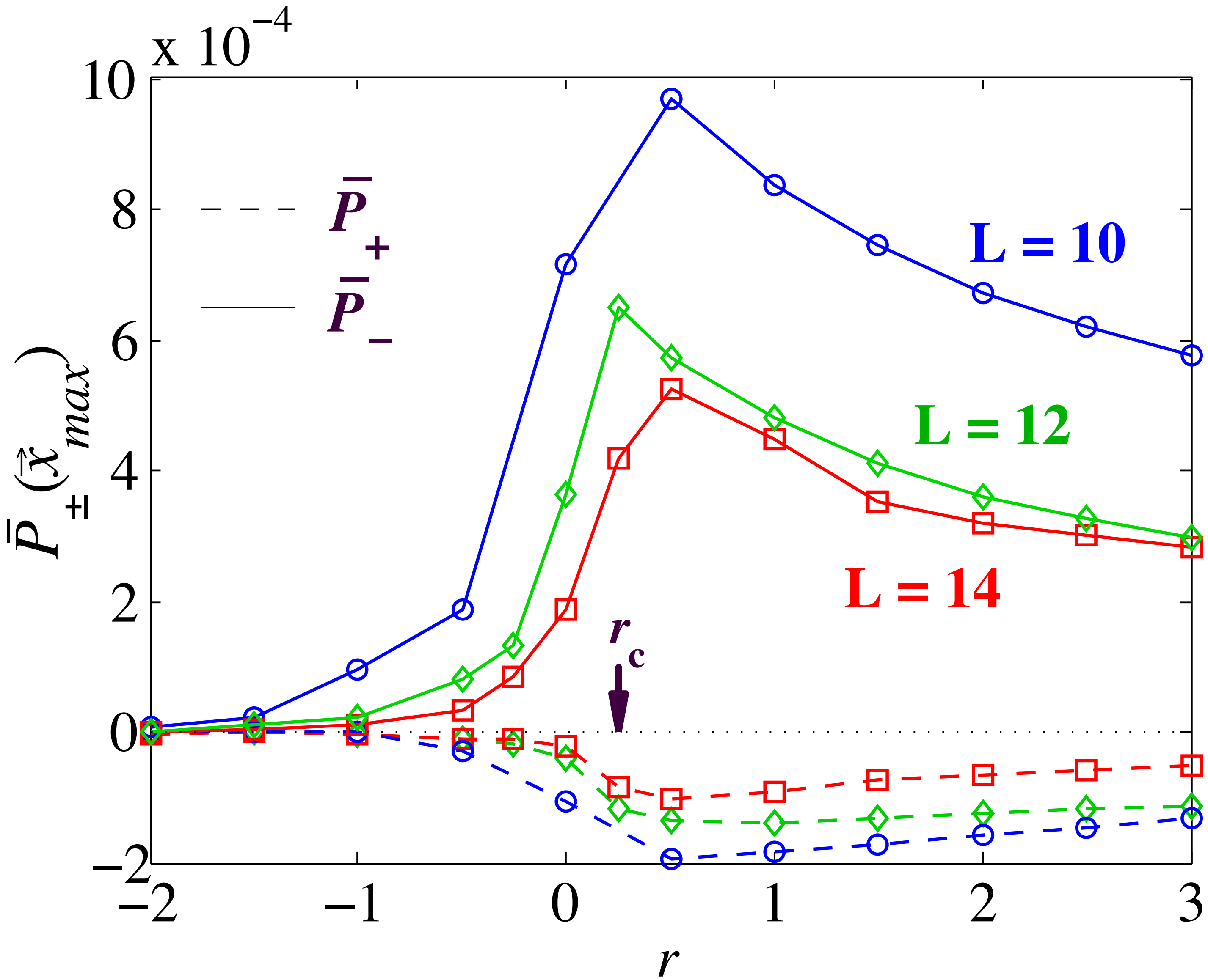
E. Demler, S. Sachdev and Y. Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

S. Sachdev, arXiv:0907.0008

E. G. Moon and S. Sachdev, *Phy. Rev. B* **80**, 035117 (2009)



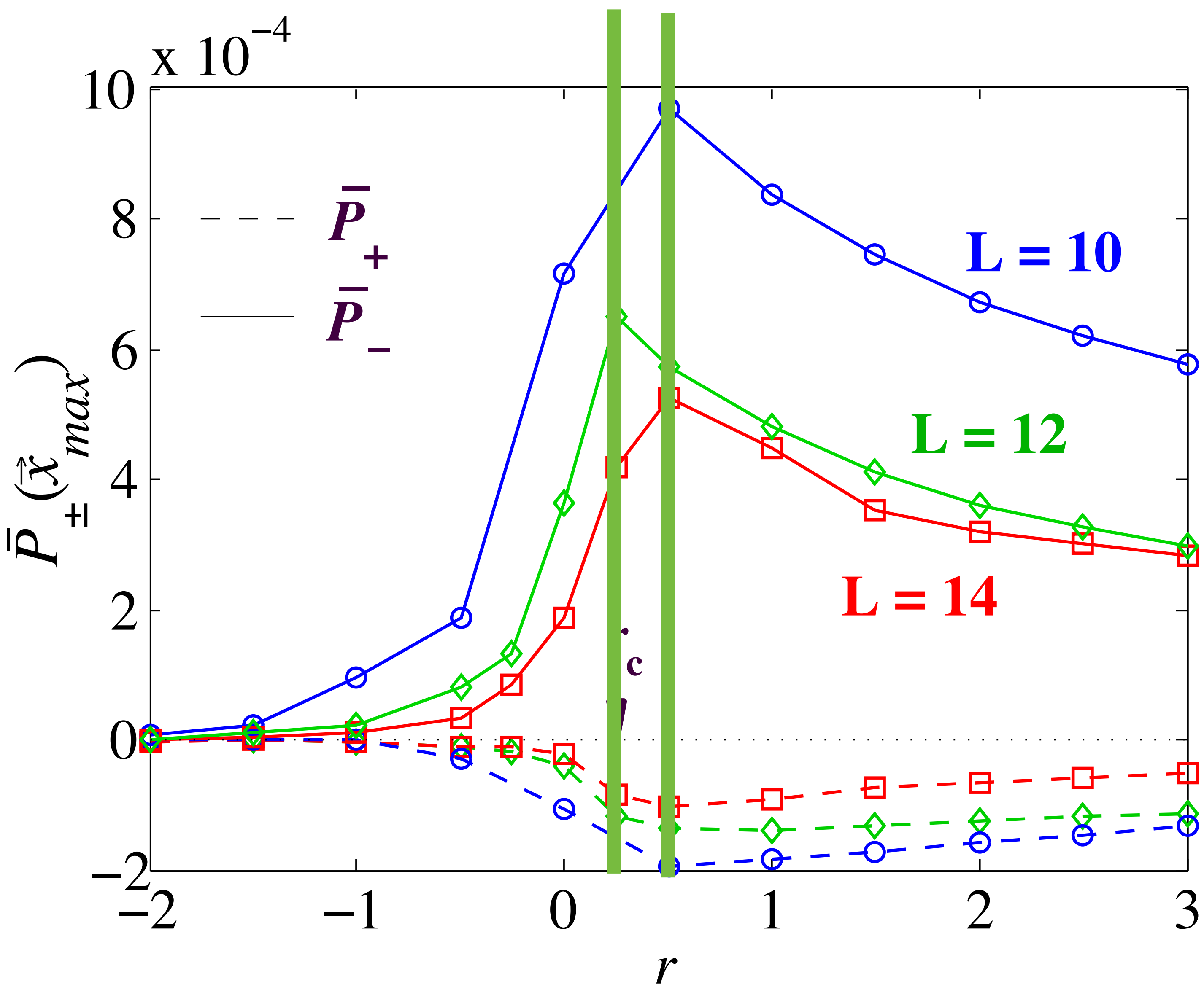
QMC for the onset of antiferromagnetism



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

Features of strong coupling

- Shift in QCP due to superconductivity: "backbending" of SDW order.
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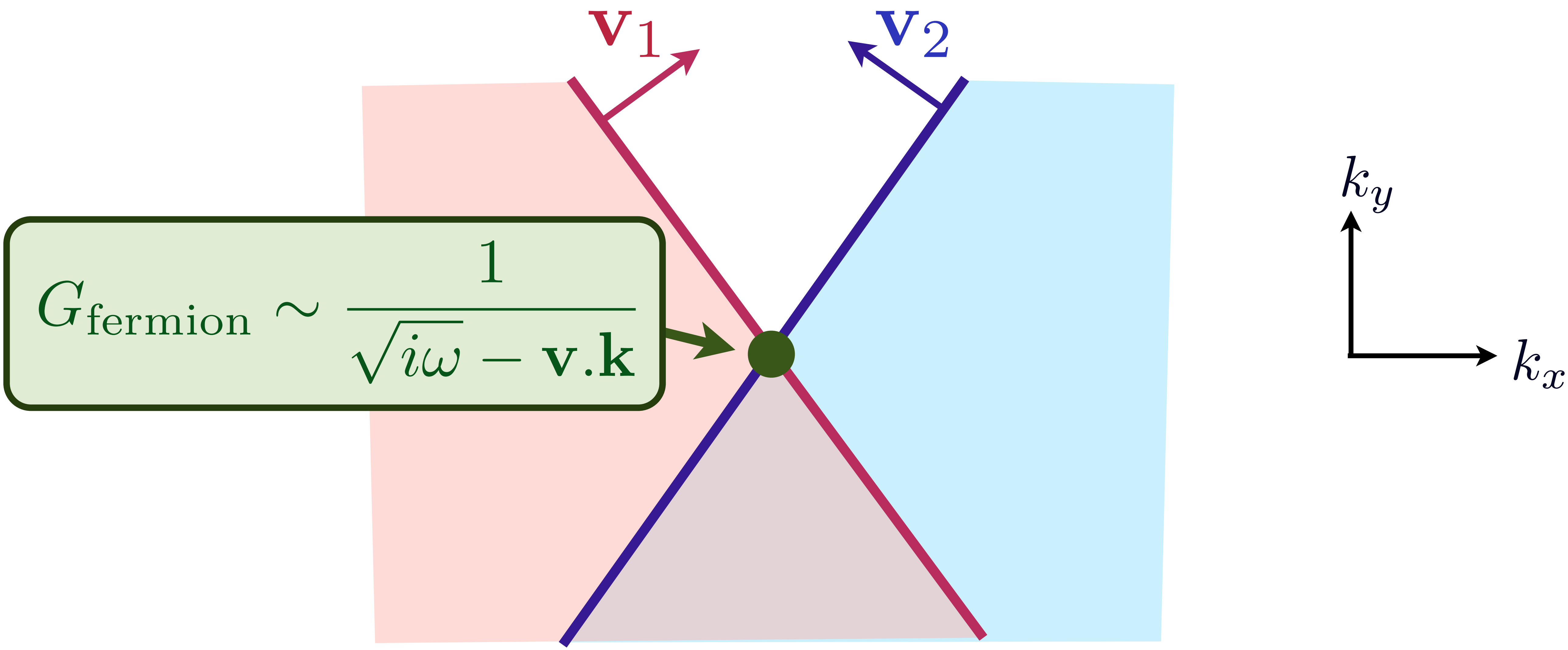
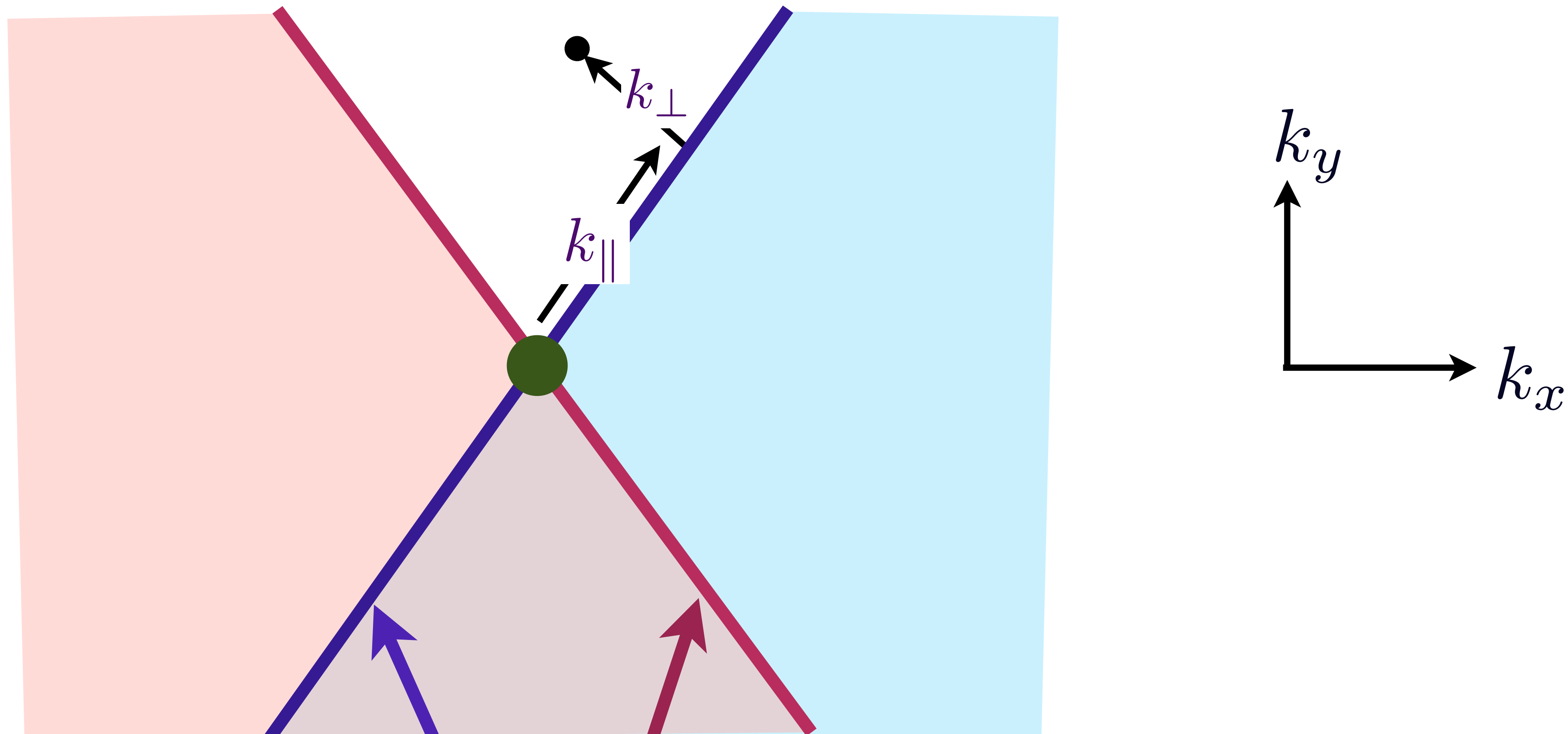
Two loop results: Non-Fermi liquid spectrum at hot spots

$$G_{\text{fermion}} \sim \frac{1}{\sqrt{i\omega} - \mathbf{v}.\mathbf{k}}$$



A. J. Millis, *Phys. Rev. B* **45**, 13047 (1992)
Ar. Abanov and A.V. Chubukov, *Phys. Rev. Lett.* **93**, 255702 (2004)

Two loop results: Quasiparticle weight vanishes upon approaching hot spots



$$G_{\text{fermion}} = \frac{Z(k_\parallel)}{\omega - v_F(k_\parallel)k_\perp}, \quad Z(k_\parallel) \sim v_F(k_\parallel) \sim k_\parallel$$

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

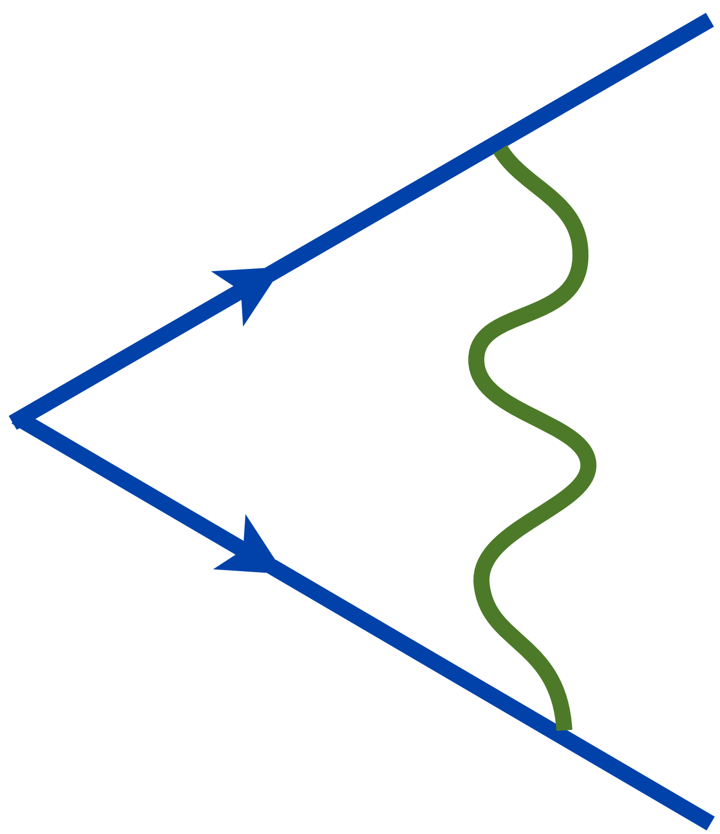
Pairing by SDW fluctuation exchange

Weak-coupling theory

Fermi energy

$$1 + \lambda^2 \rho(E_F) \log\left(\frac{E_F}{\omega}\right)$$

Density of states at Fermi energy



Pairing by SDW fluctuation exchange

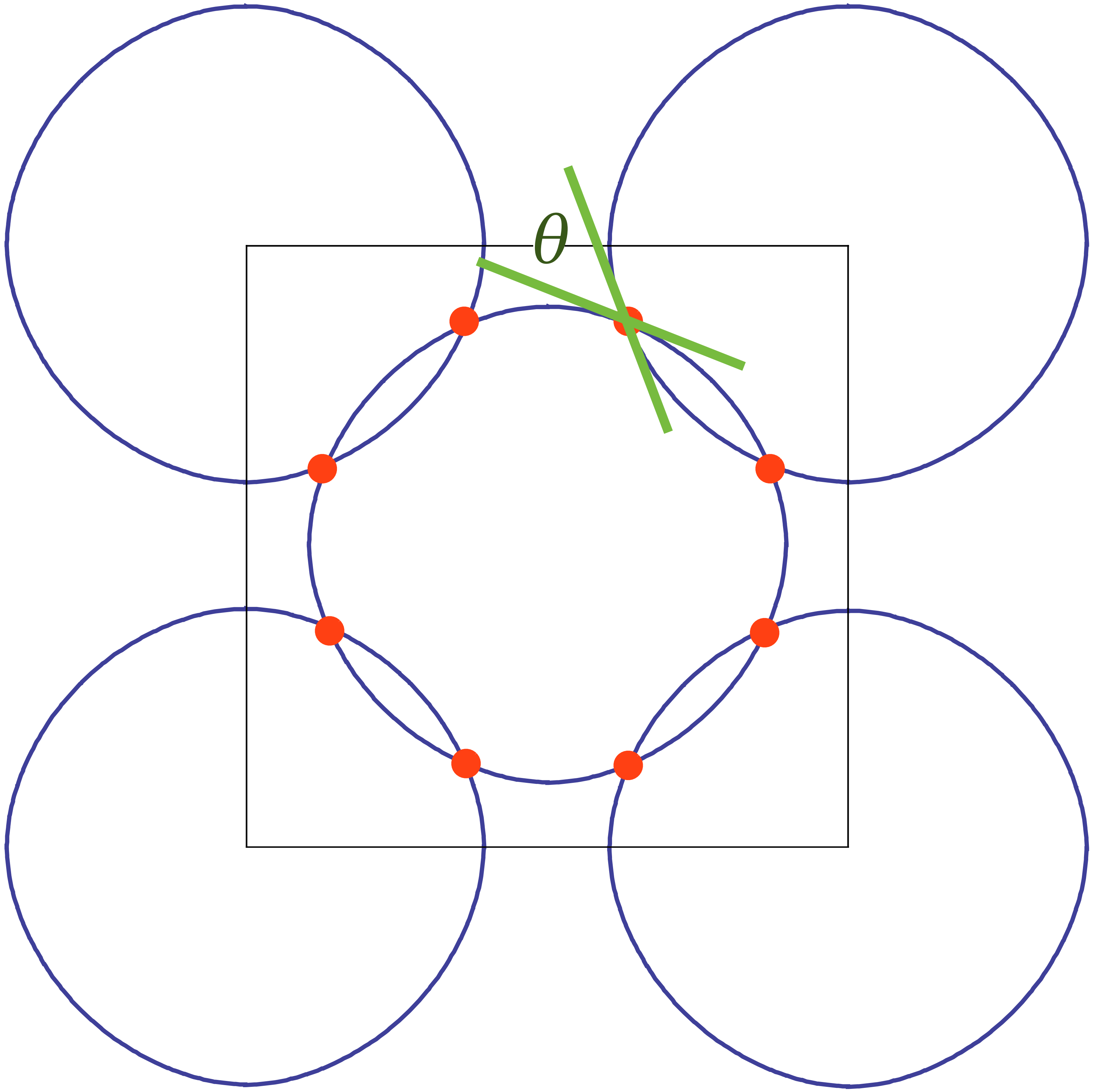
Antiferromagnetic critical point

Fermi energy

$$1 + \frac{\sin\theta}{2\pi}\log^2\left(\frac{E_F}{\omega}\right)$$

θ is the angle between Fermi lines.
Independent of interaction strength
U in 2 dimensions.

(see also Ar. Abanov, A.V. Chubukov, and A. M. Finkel'stein, *Europhys. Lett.* **54**, 488 (2001))
M. A. Metlitski and S. Sachdev, *Phys. Rev. B* **82**, 075128 (2010)


θ

Pairing by SDW fluctuation exchange

Antiferromagnetic critical point

$$1 + \frac{\sin\theta}{2\pi} \log^2 \left(\frac{E_F}{\omega} \right)$$

- **Universal** $\log^2$ singularity arises from Fermi lines; singularity *at* hot spots is weaker.
- Interference between BCS and quantum-critical logs.
- Momentum dependence of self-energy is crucial.
- Not suppressed by $1/N$ factor in $1/N$ expansion.

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

Features of strong coupling

- Shift in QCP due to superconductivity: "backbending" of SDW order.
- Pairing instability is $(\log)^2$ with universal co-efficient.
- Leading subdominant instability is bond-modulated charge order.
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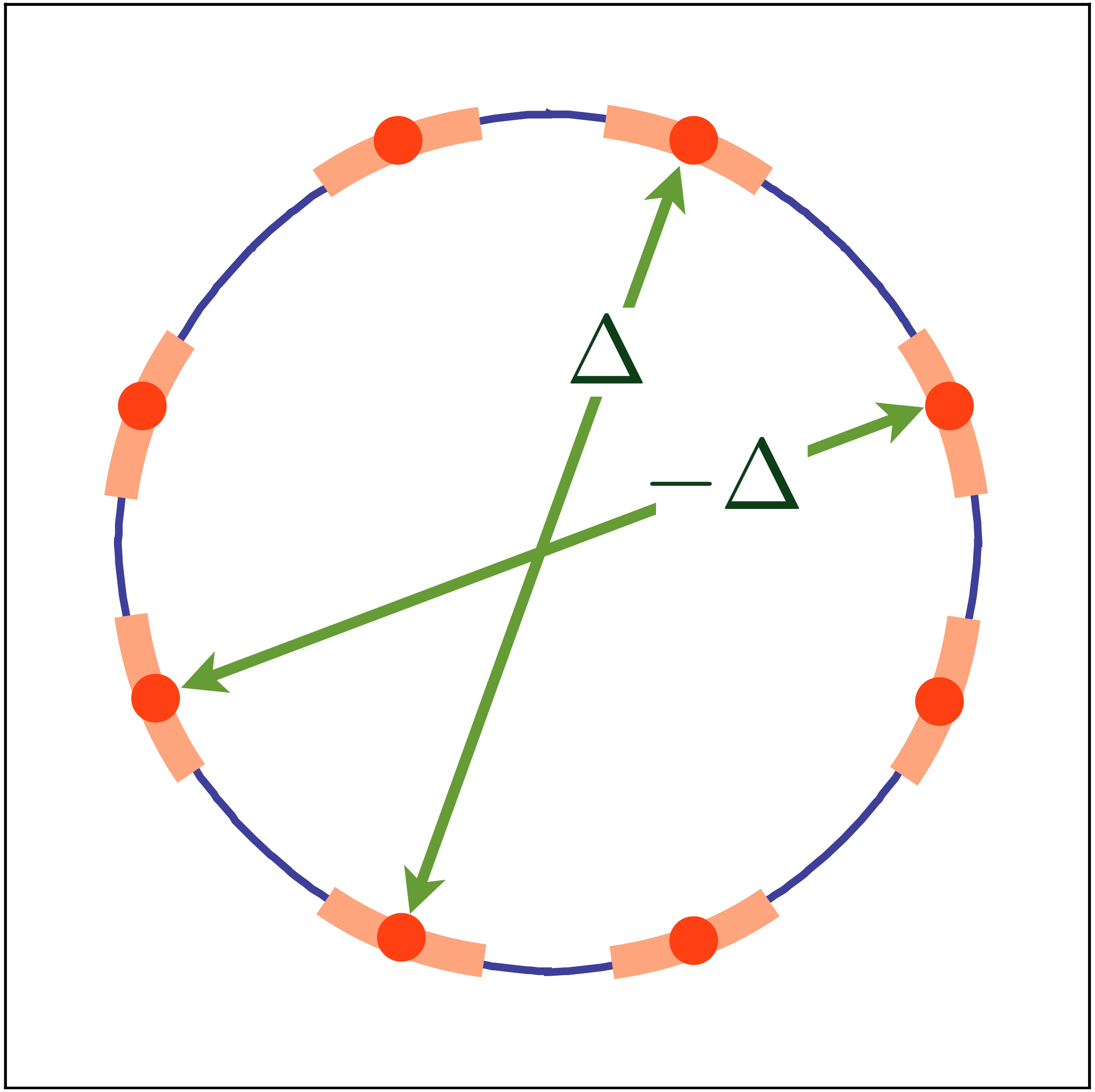
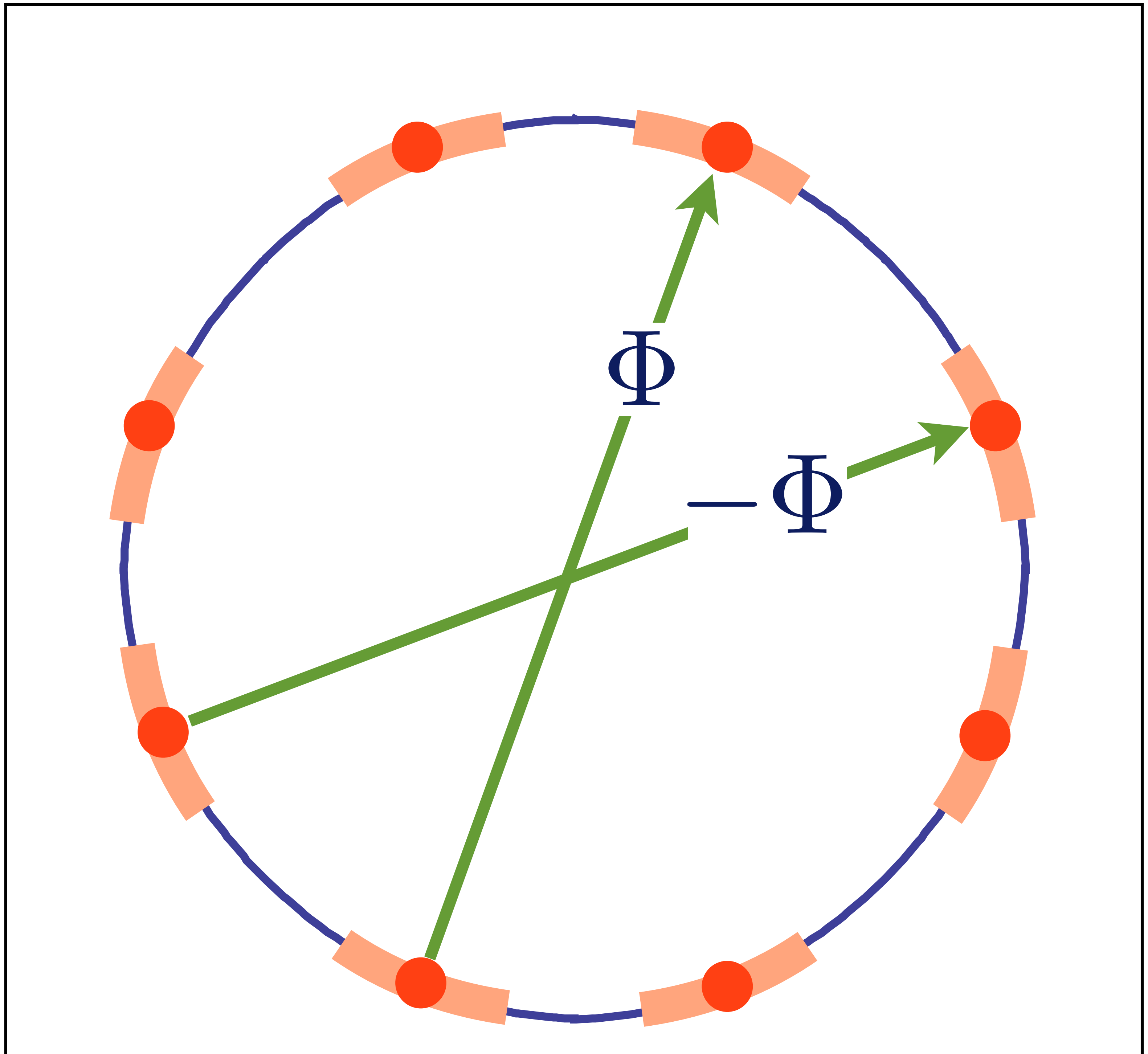
$$\left\langle c^\dagger_{\mathbf{k}\alpha} c^\dagger_{-\mathbf{k}\beta} \right\rangle = \varepsilon_{\alpha\beta} \Delta(\cos k_x - \cos k_y)$$



Log-squared instability to d-wave pairing

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

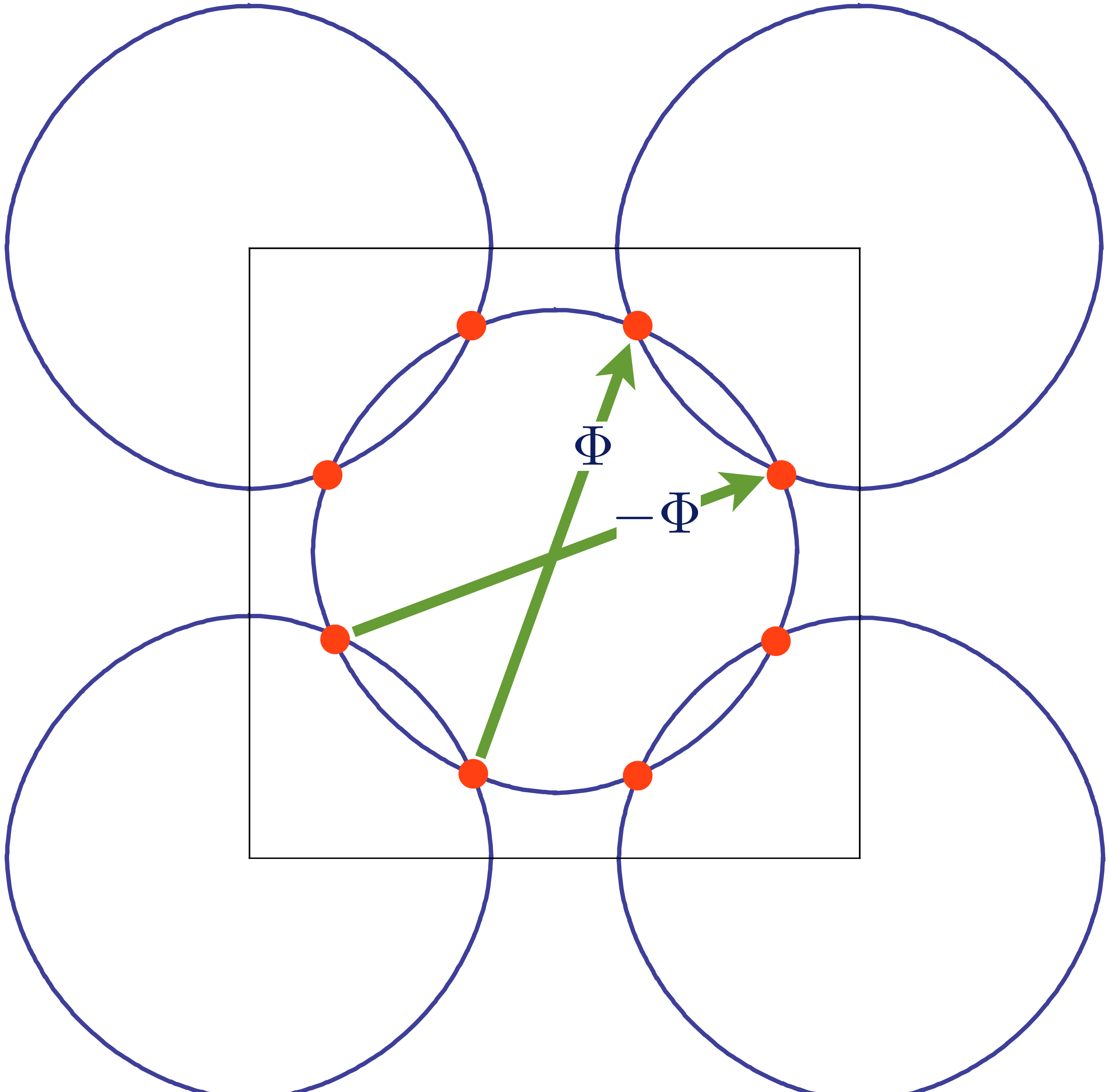


$\mathbf{Q}$ is '$2k_F$' wavevector

Similar log-squared instability in particle-hole channel to bond-modulated charge order

Bond-modulated charge order

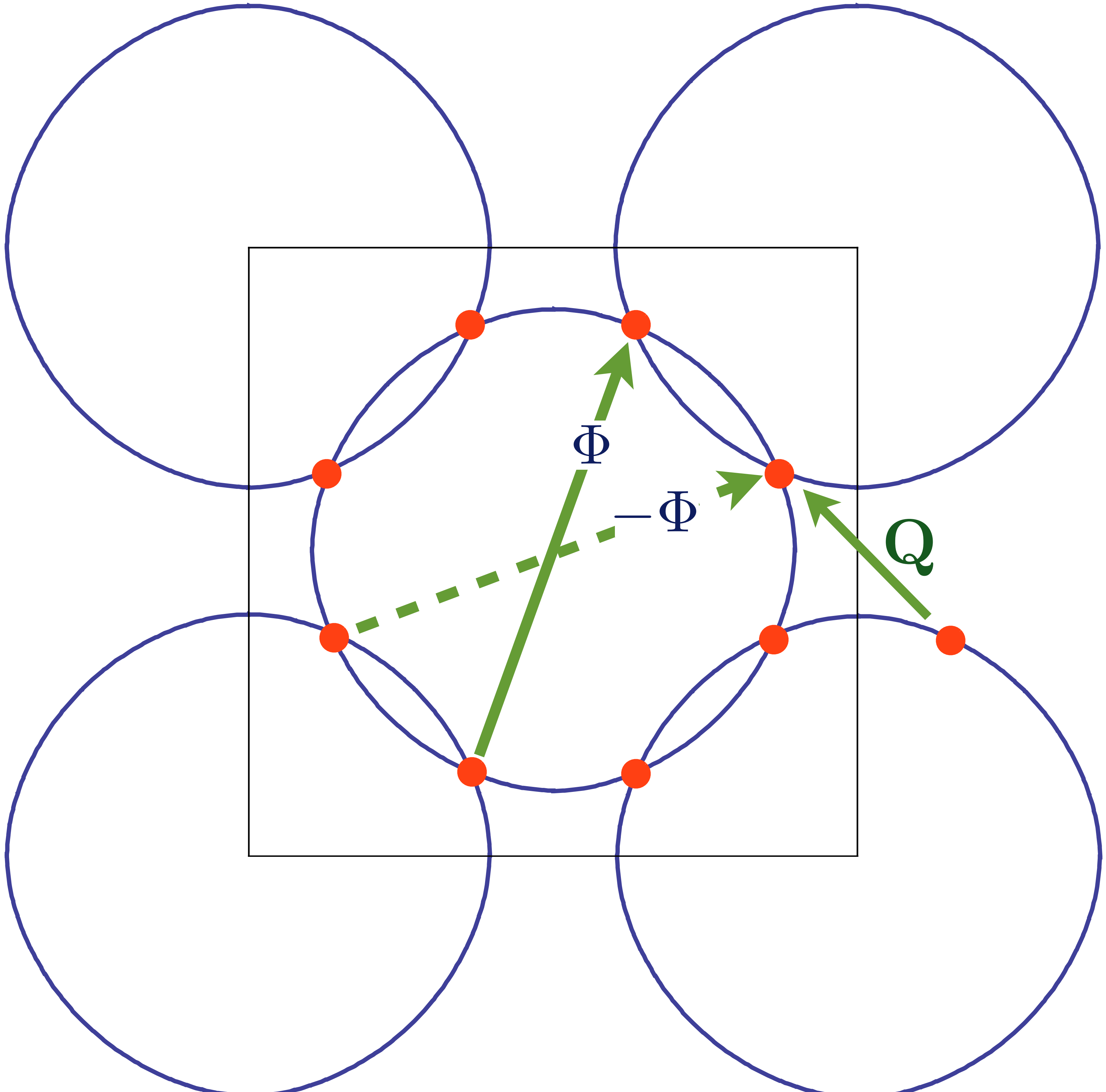
M.A. Metlitski and S. Sachdev,
Phys. Rev. B **82**, 075128 (2010)



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

Bond-modulated charge order

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



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M. A. Metlitski and S. Sachdev,
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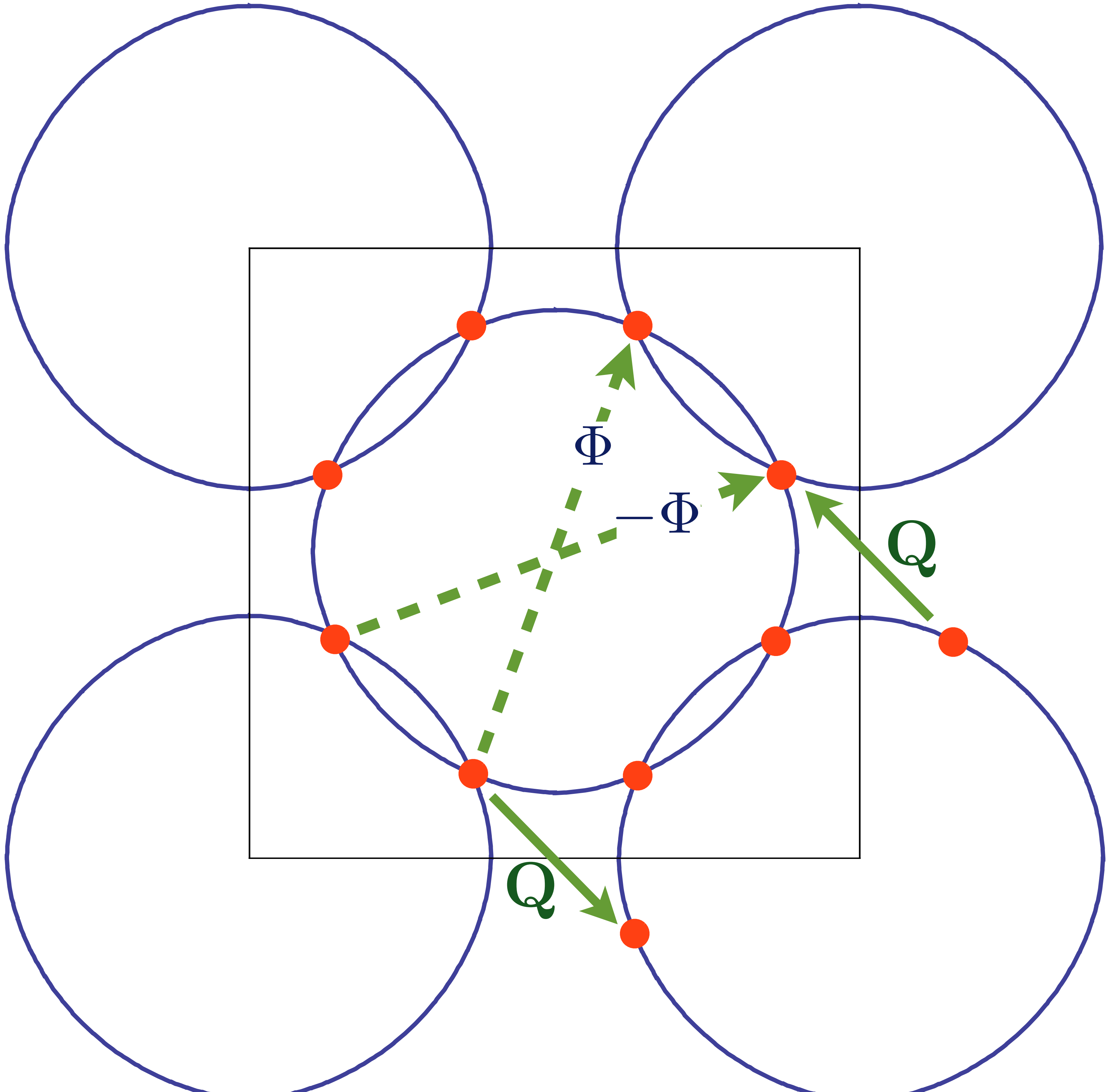

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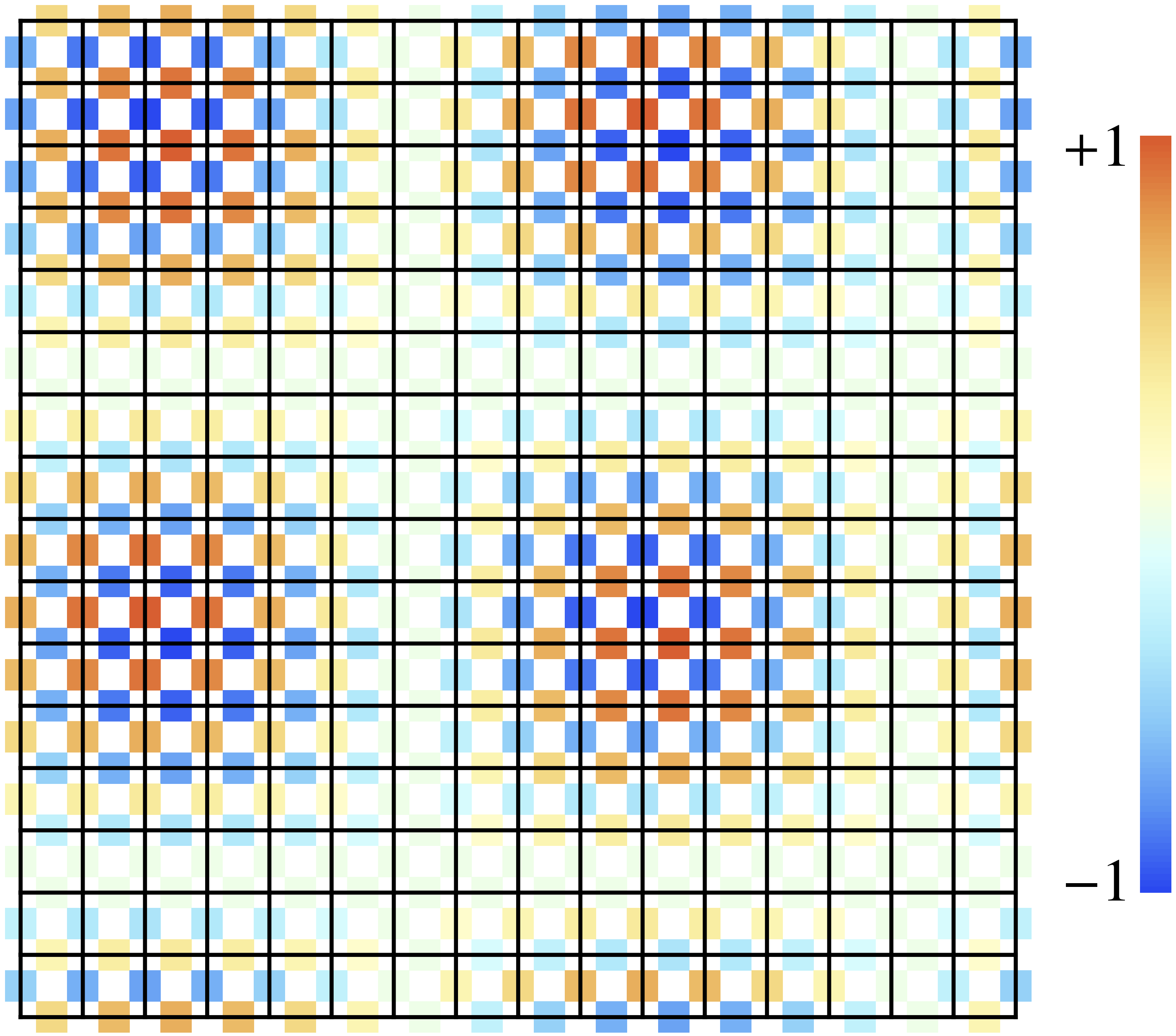
Bond-modulated charge order

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



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

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

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

Features of strong coupling

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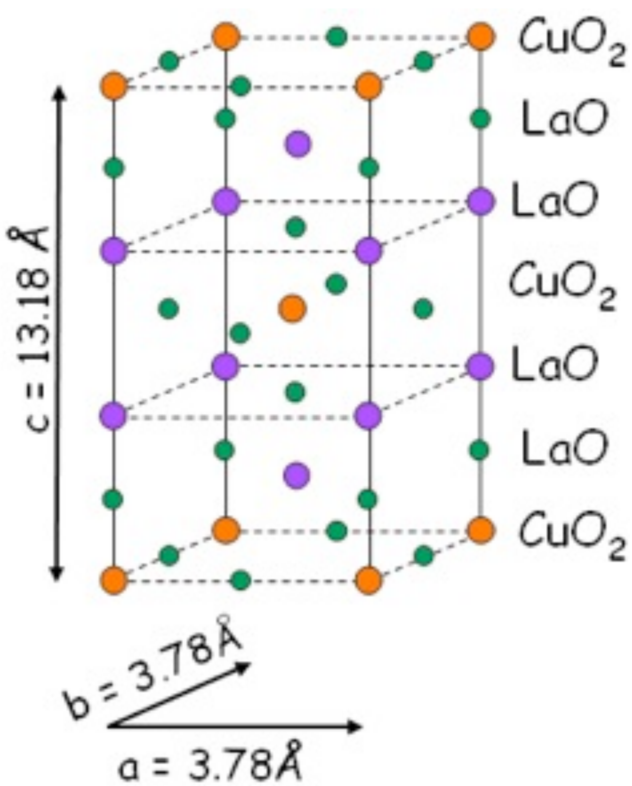
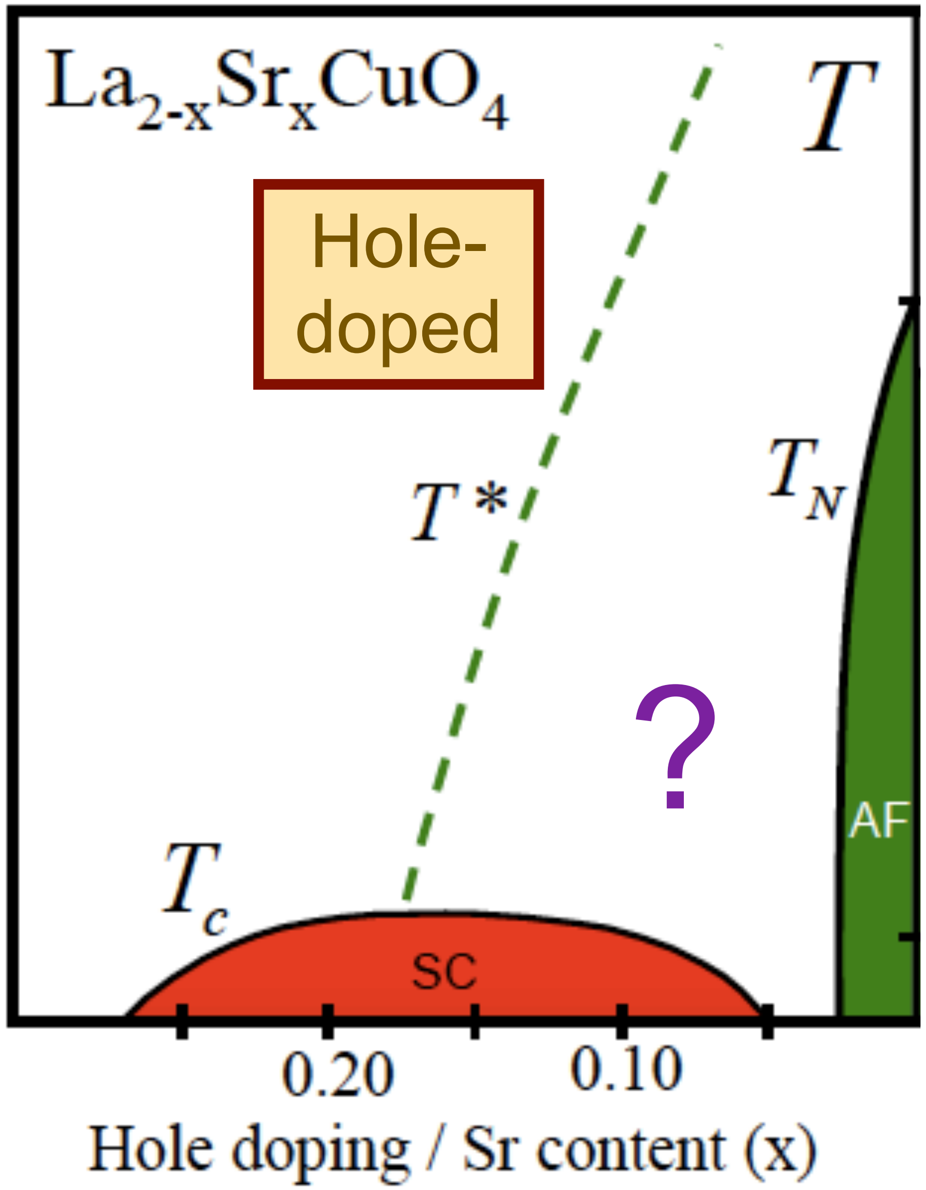
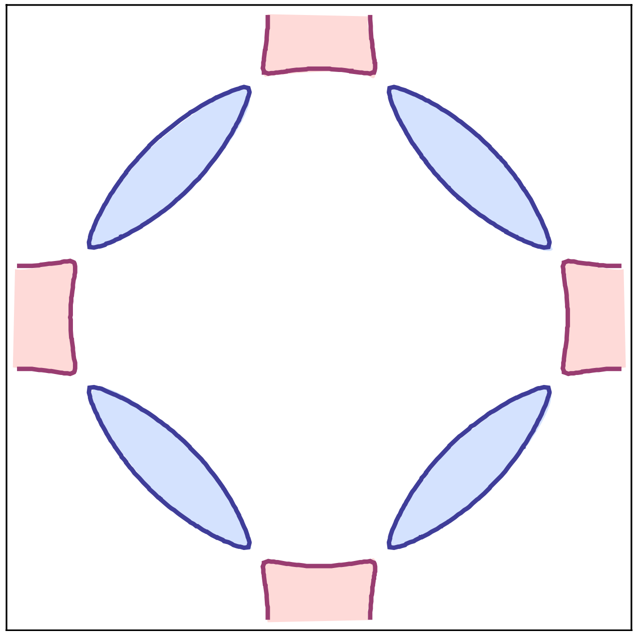


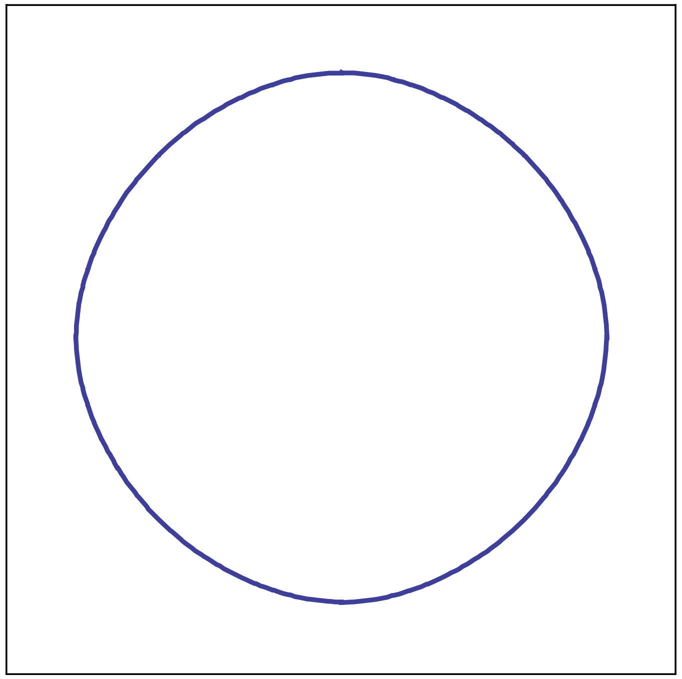
CuO2
LaO
LaO
CuO2
LaO
LaO
CuO2
c = 13.18 Å
b = 3.78Å
a = 3.78Å



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

Quantum phase transition with Fermi surface reconstruction





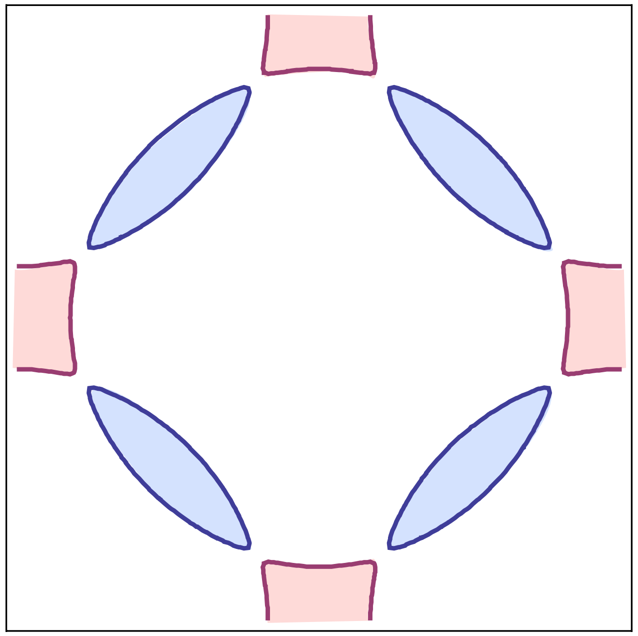
$\langle \vec{\varphi} \rangle \neq 0$

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

Metal with electron and hole pockets

Metal with "large" Fermi surface

Separating onset of SDW order and Fermi surface reconstruction



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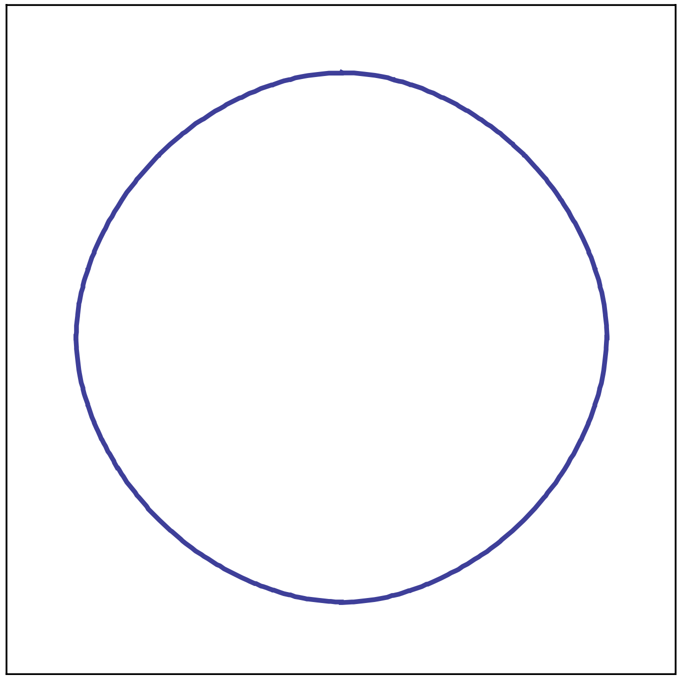
Metal with electron and hole pockets



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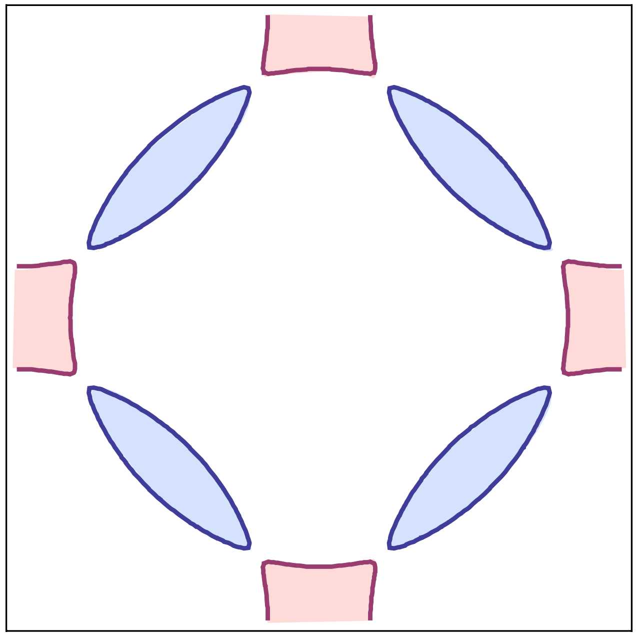
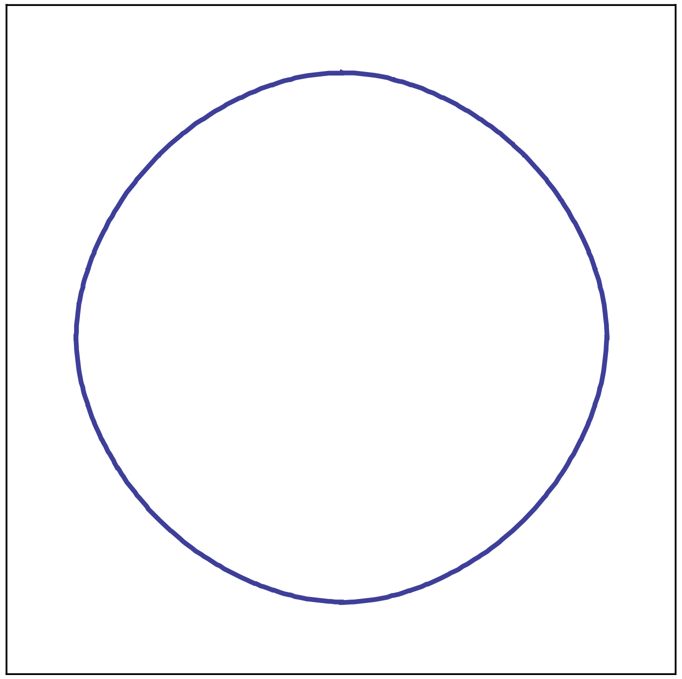


Electron and/or hole Fermi pockets form in "local" SDW order, but quantum fluctuations destroy long-range SDW order



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

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

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

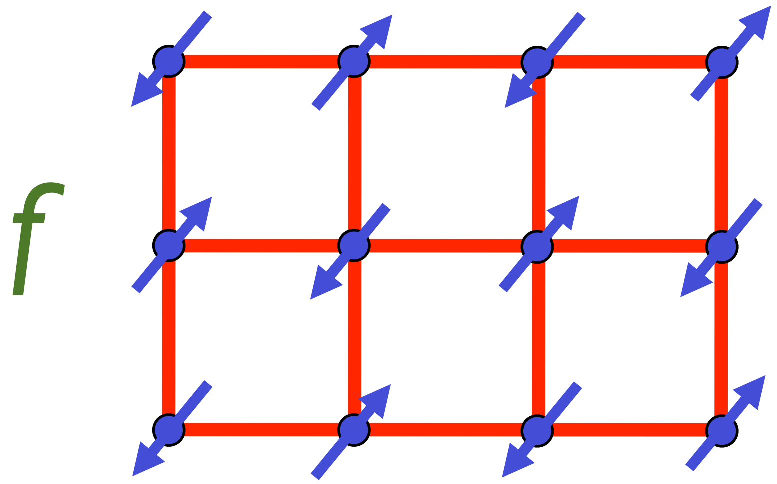
Metal with electron and hole pockets

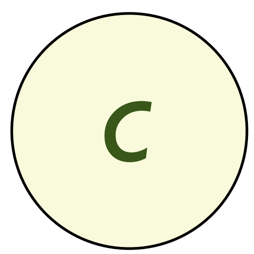
Fractionalized Fermi liquid (FL*) phase with no symmetry breaking and "small" Fermi surface

Metal with "large" Fermi surface

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

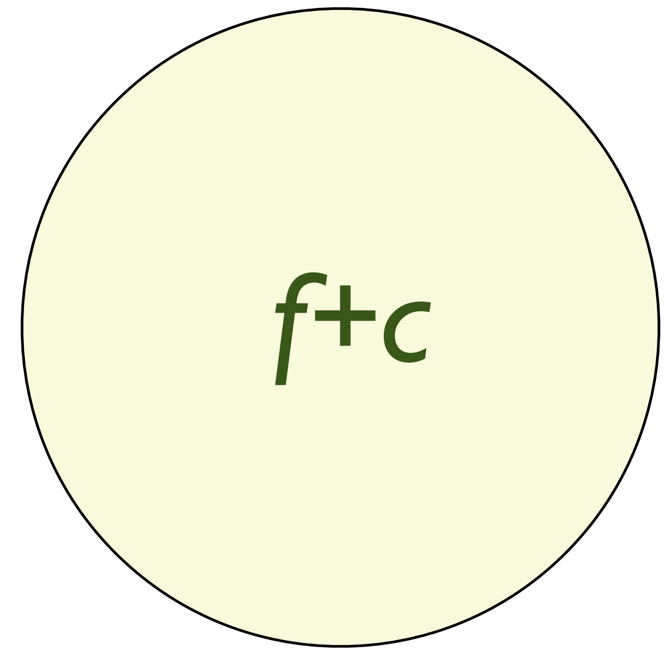
Magnetic order and the heavy Fermi liquid in the Kondo lattice





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

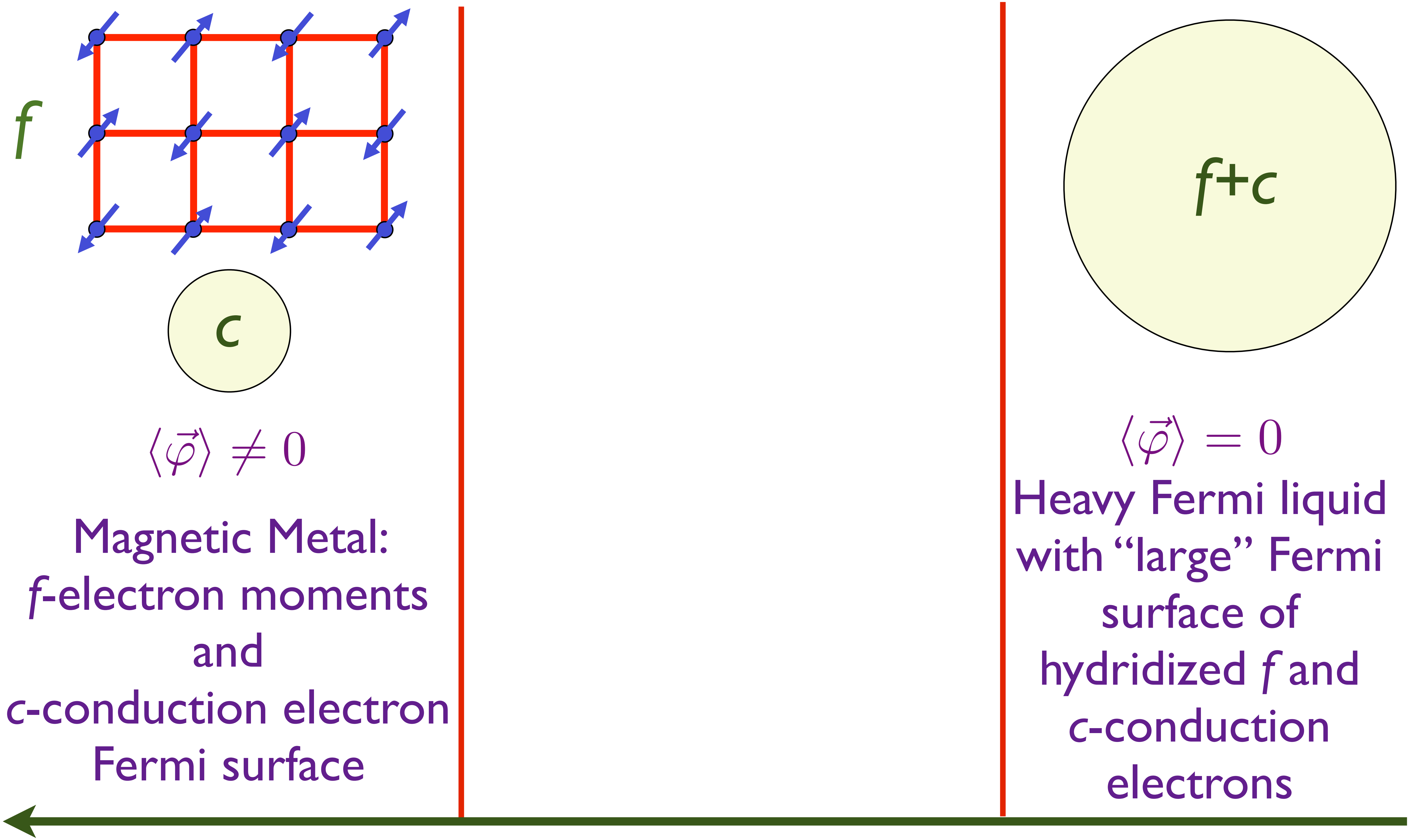
Magnetic Metal:
f-electron moments
and
c-conduction electron
Fermi surface



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

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

Separating onset of SDW order and the heavy Fermi liquid in the Kondo lattice



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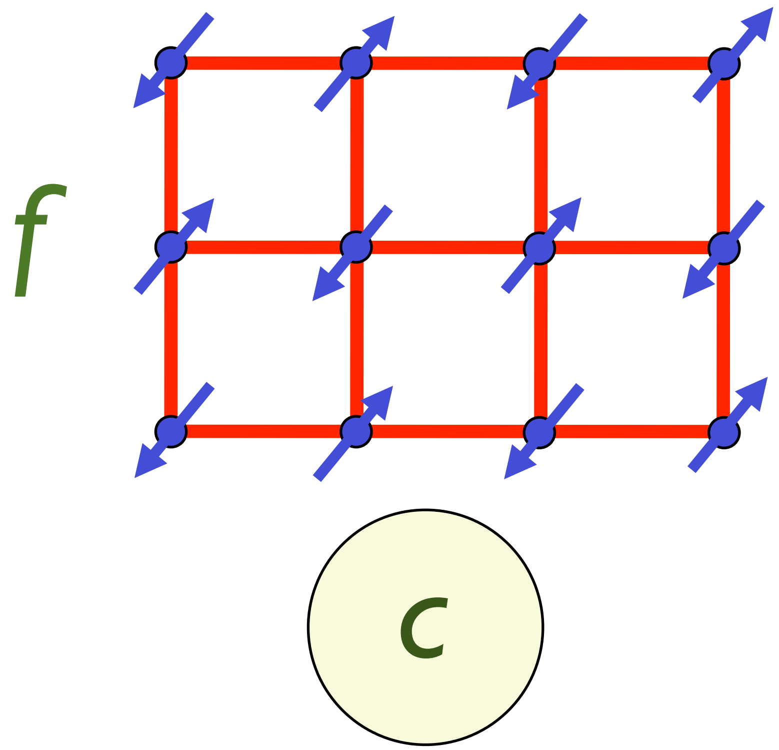
Fermi surface

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

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

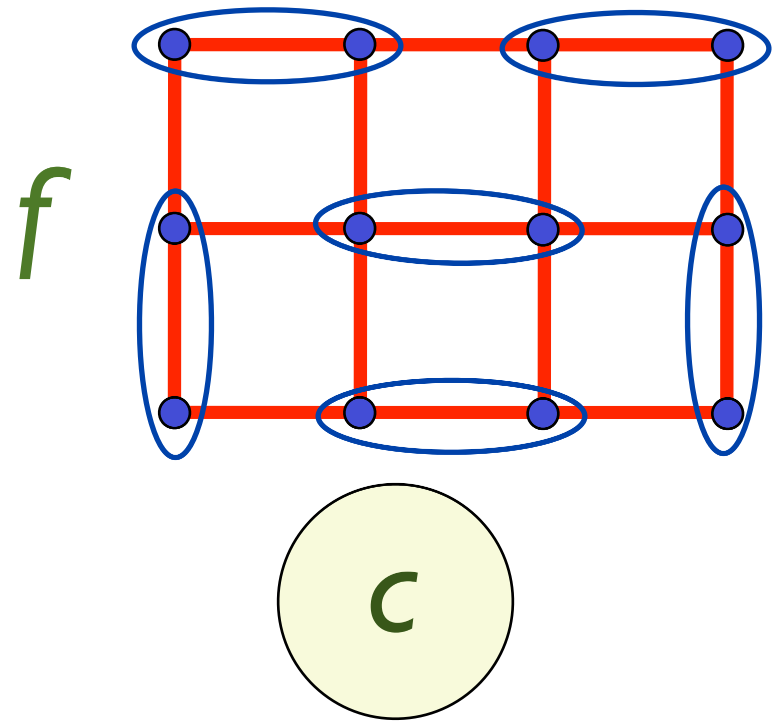
T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

Separating onset of SDW order and the heavy Fermi liquid in the Kondo lattice



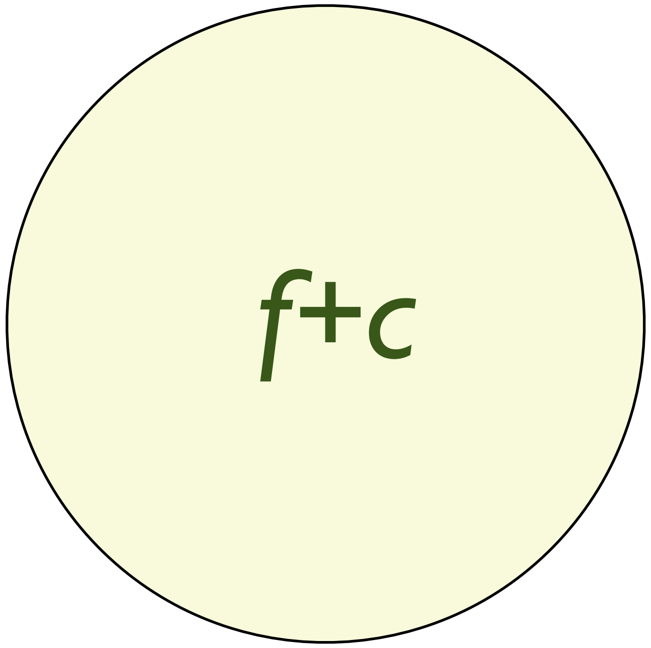
$$\langle \vec{\varphi} \rangle \neq 0$$

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



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

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



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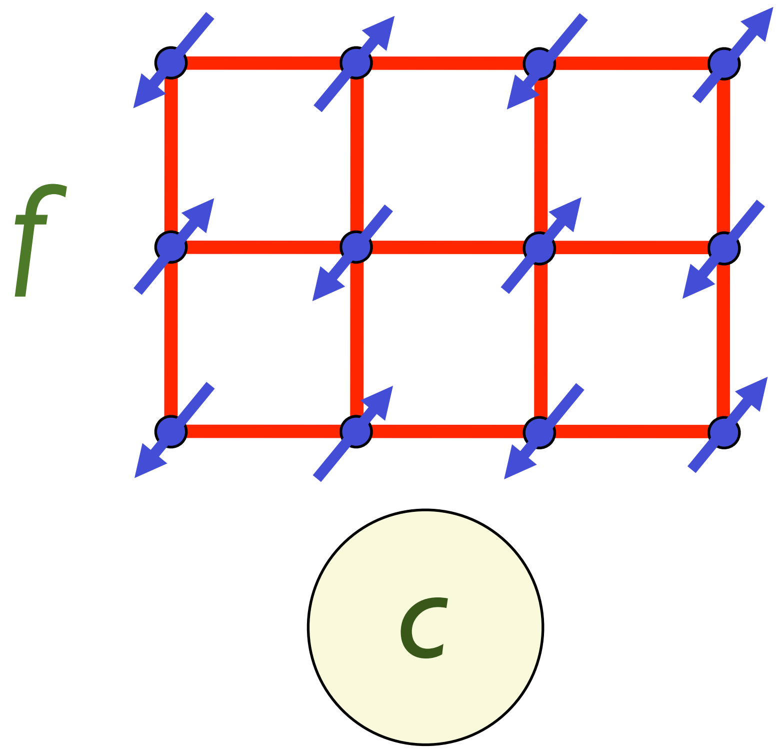

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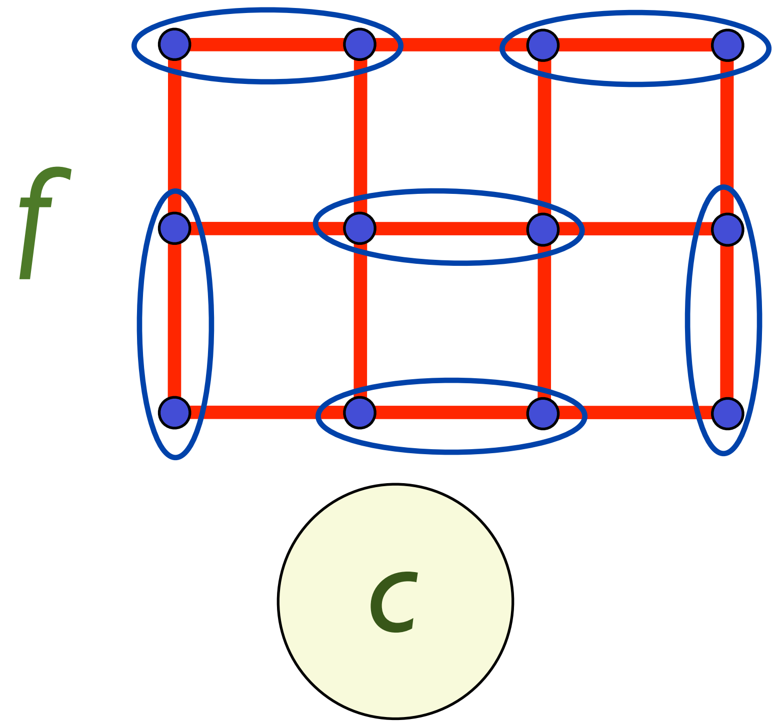
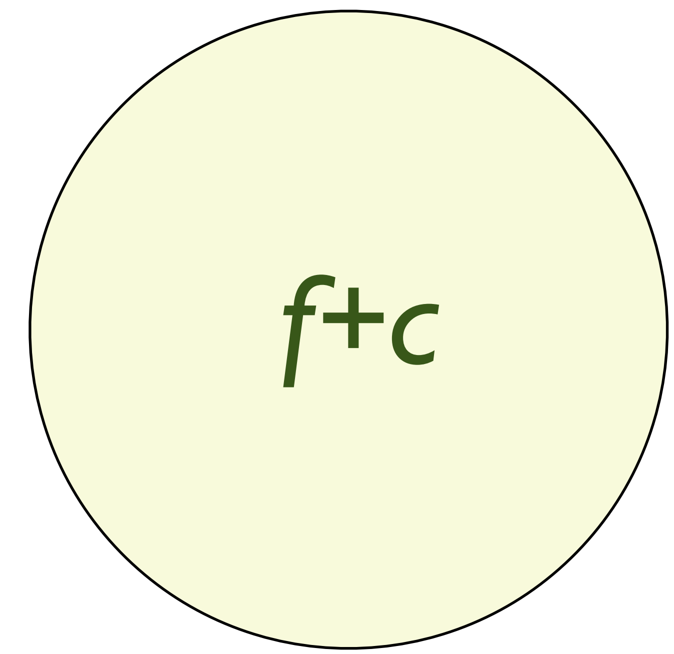


$\langle \vec{\varphi} \rangle = 0$

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



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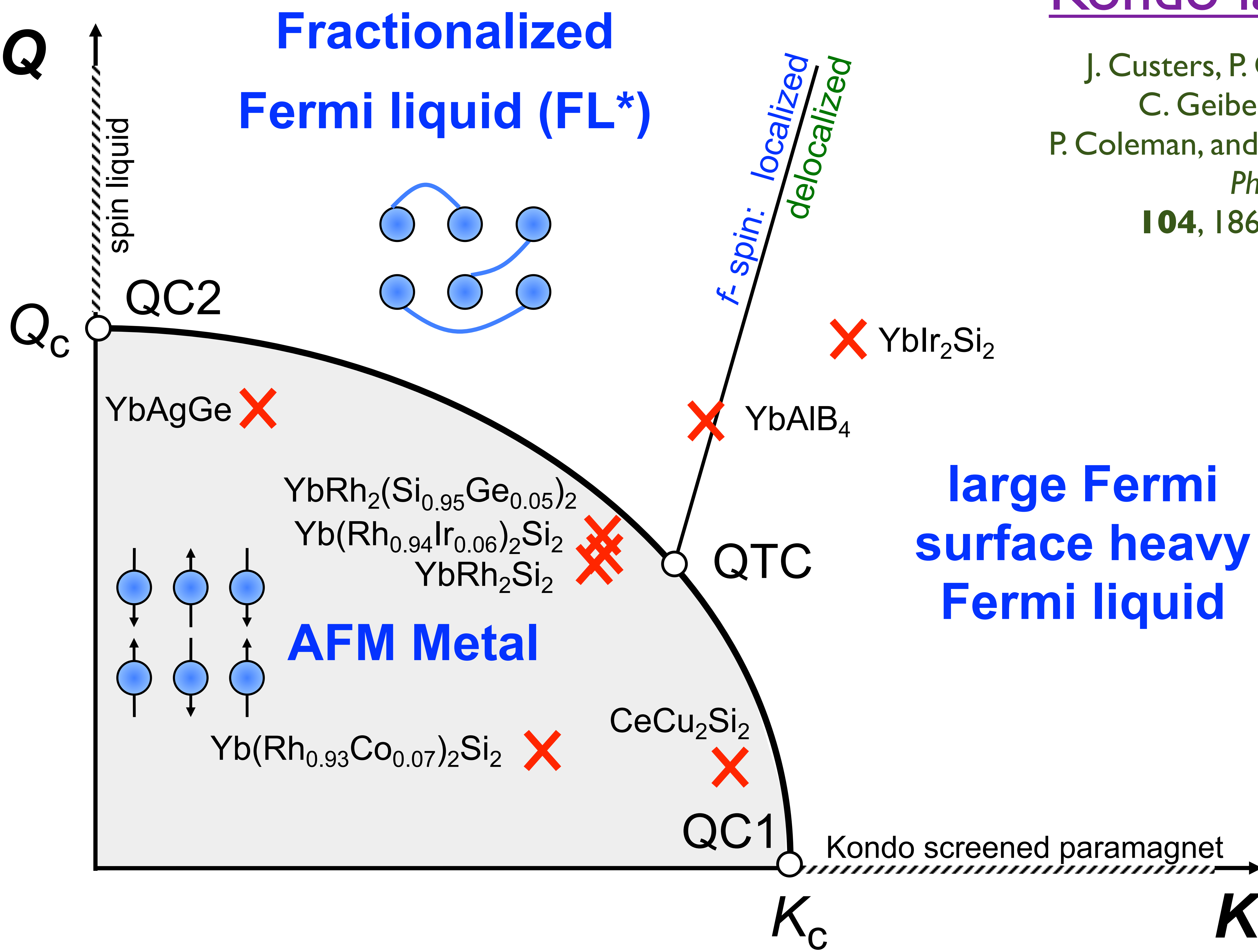
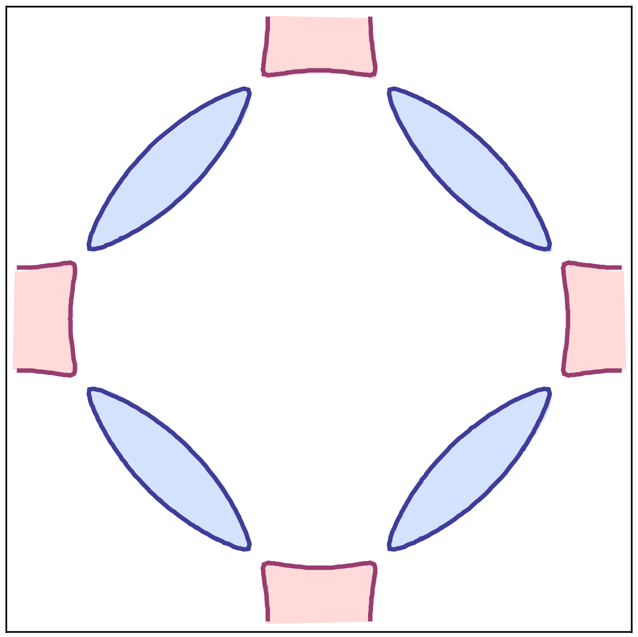
T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

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)



Separating onset of SDW order and Fermi surface reconstruction



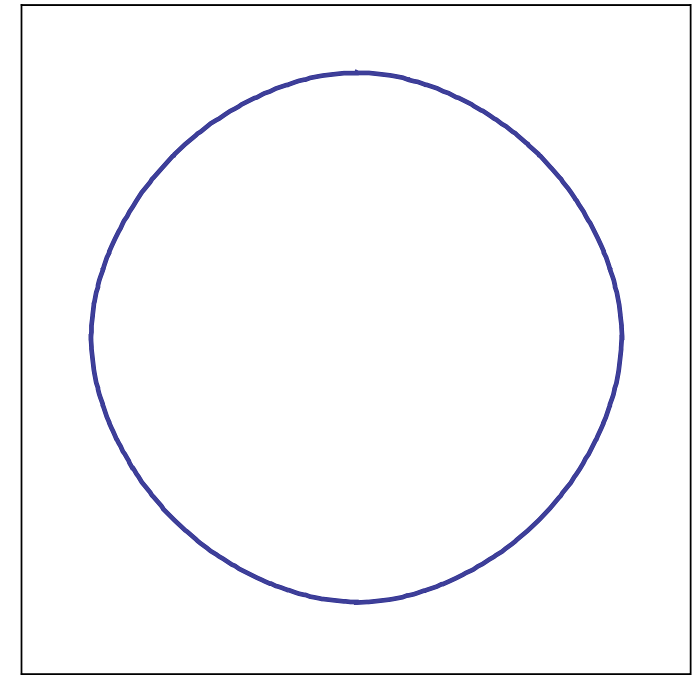
$$\langle \vec{\varphi} \rangle \neq 0$$

Metal with electron and hole pockets

Electron and/or hole Fermi pockets form in "local" SDW order, but quantum fluctuations destroy long-range SDW order

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

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



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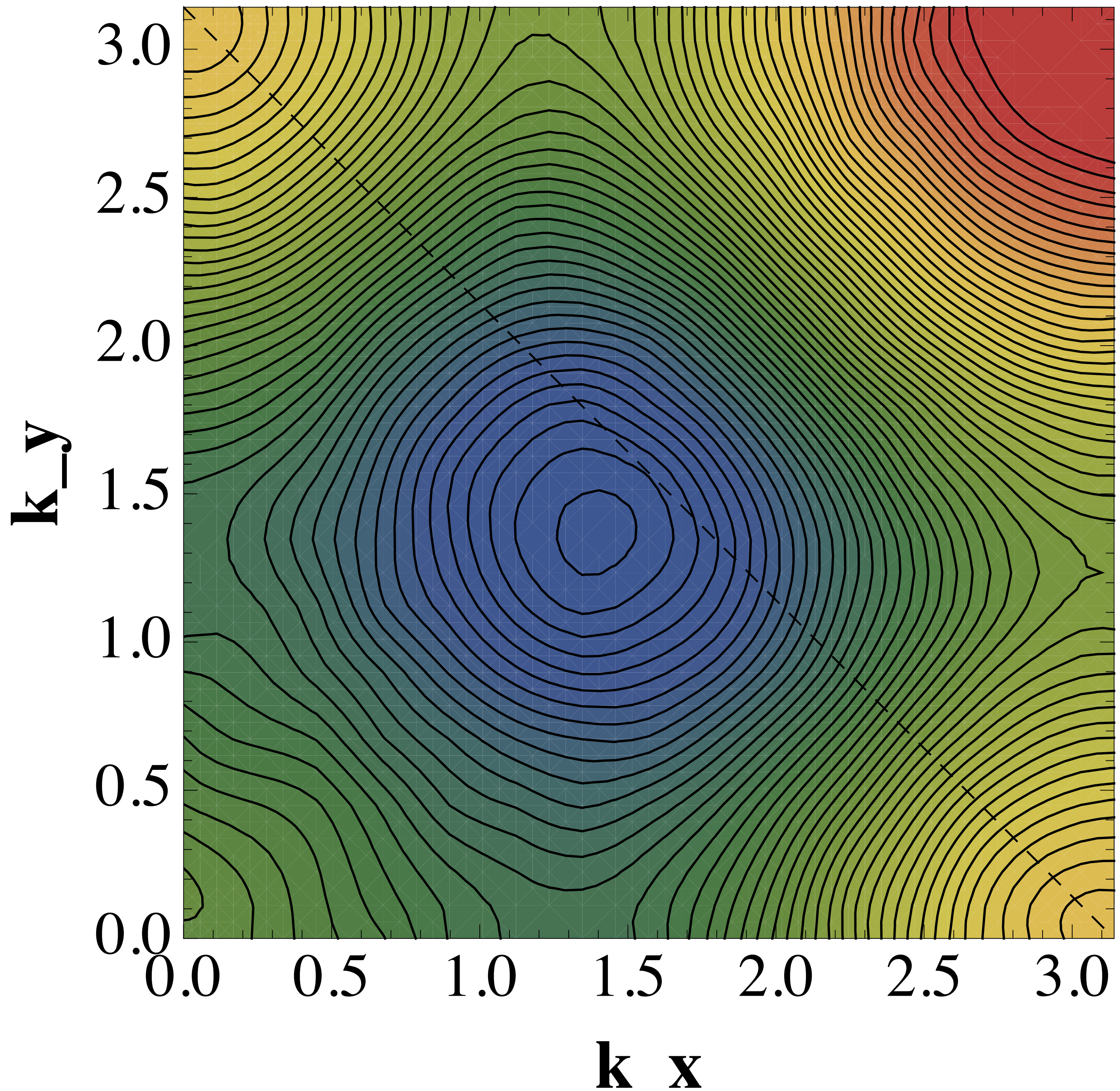
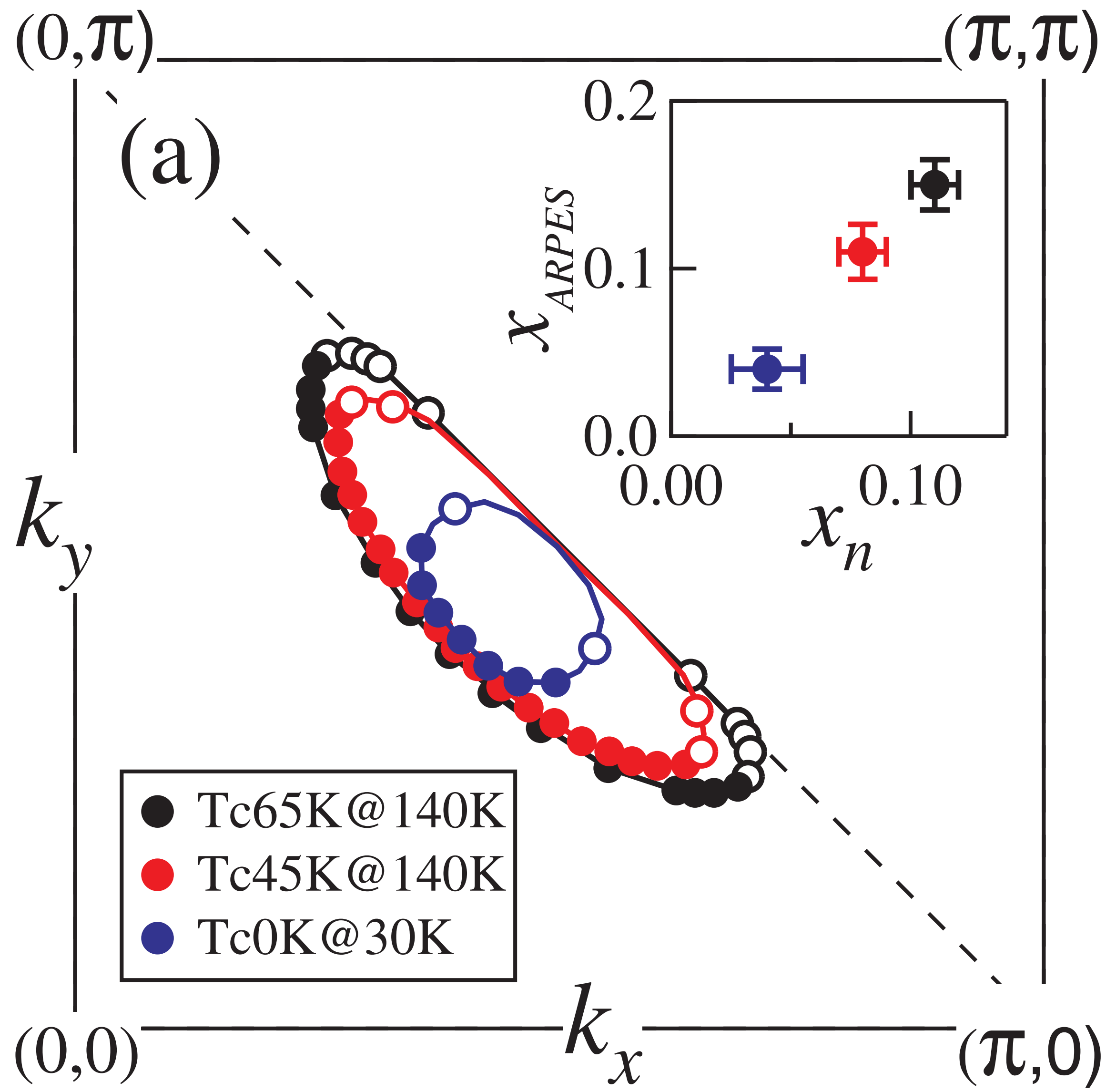
Metal with "large" Fermi surface

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



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)



PRL **107,** 047003 (2011) PHYSICAL REVIEW LETTERS week ending 22 JULY 2011

Reconstructed Fermi Surface of Underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ Cuprate Superconductors

H.-B. Yang,[1] J. D. Rameau,[1] Z.-H. Pan,[1] G. D. Gu,[1] P. D. Johnson,[1] H. Claus,[2] D. G. Hinks,[2] and T. E. Kidd[3]

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)

Characteristics of FL* phase

- Fermi surface volume does not count all electrons.

- Such a phase *must* have neutral $S = 1/2$ excitations (”spinons”), and collective spinless gauge excitations (“topological” order).

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.

- Such a phase *must* have neutral $S = 1/2$ excitations (”spinons”), and collective spinless gauge excitations (“topological” order).

- 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" order.