

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

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Max Metlitski



Erez Berg





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Erez Berg



Sean Hartnoll

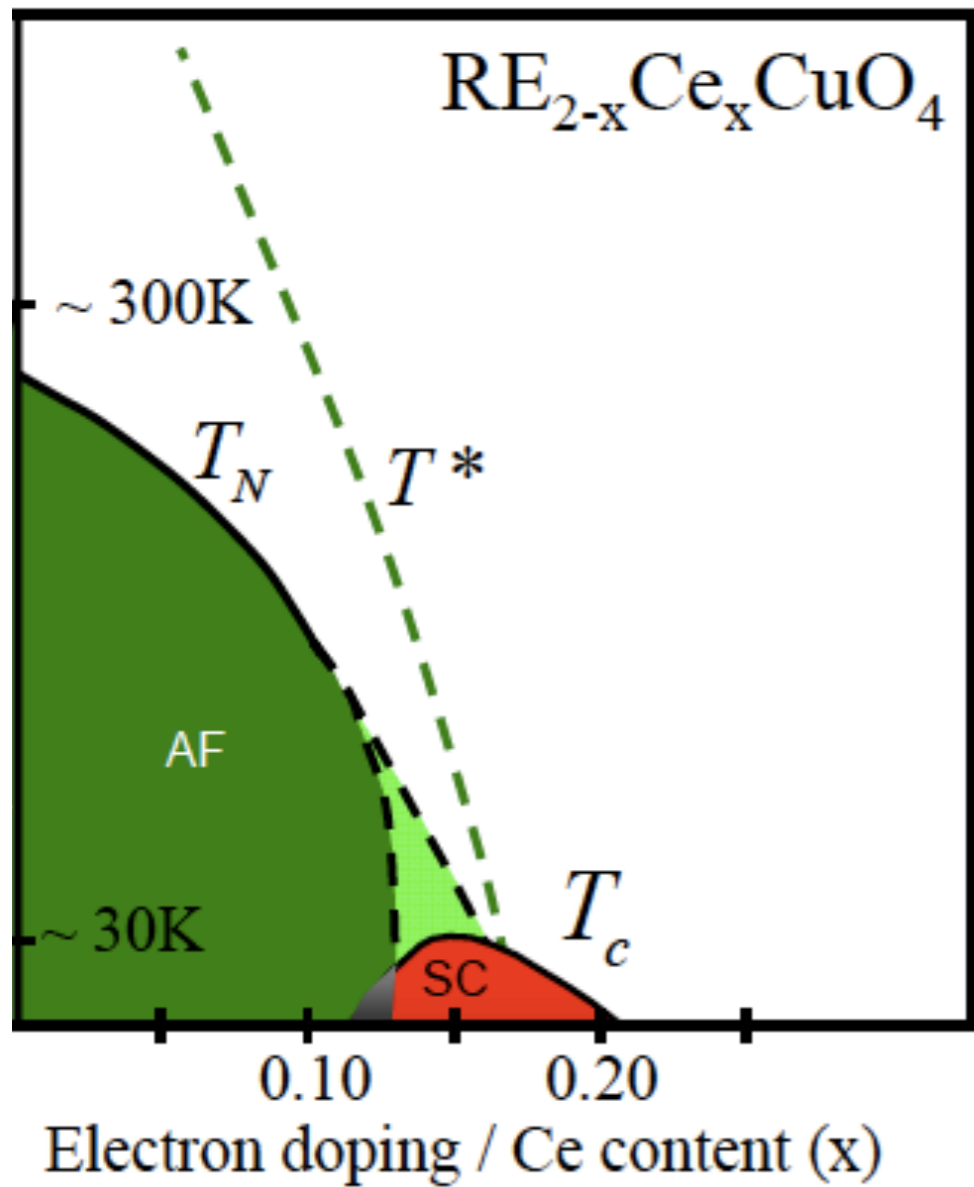


Diego Hofman



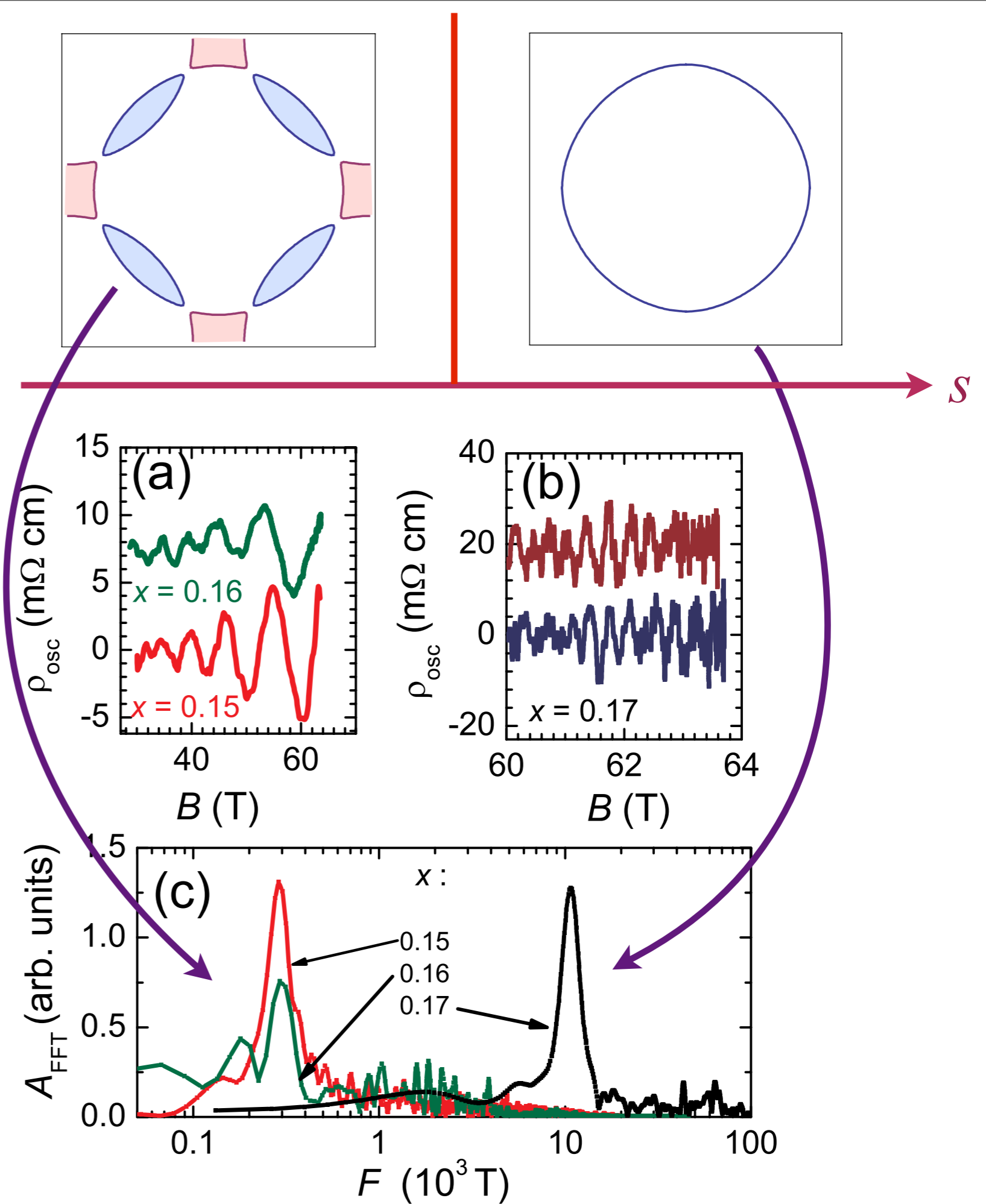
Matthias Punk



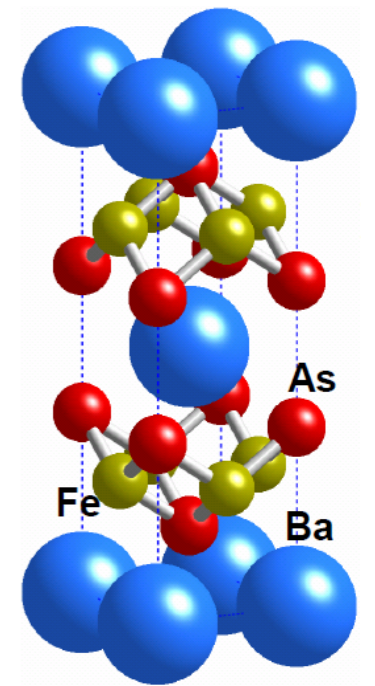
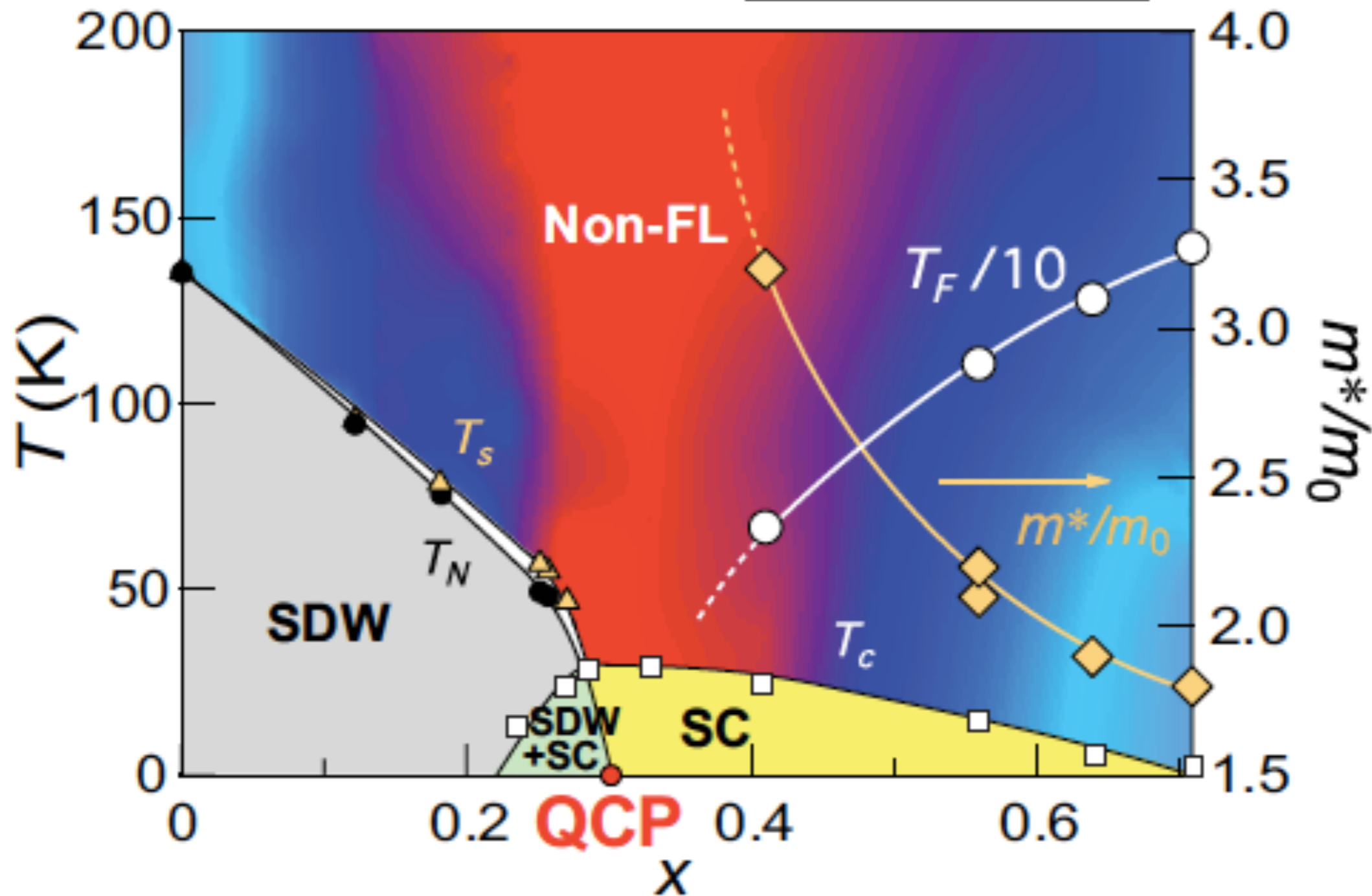


$\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$

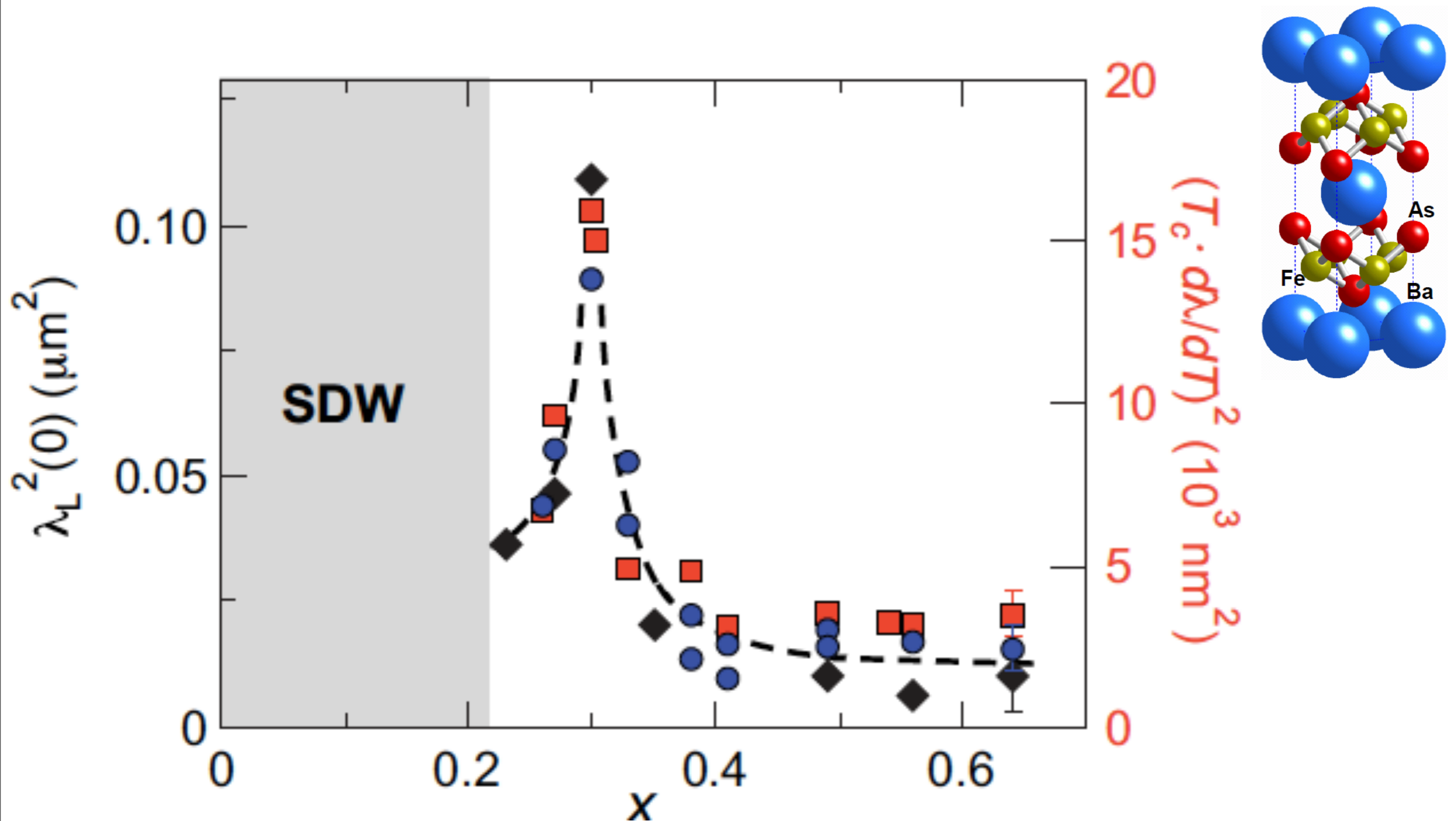
T. Helm, M.V. Kartsovnik,
M. Bartkowiak, N. Bittner,
M. Lambacher, A. Erb, J. Wosnitza,
and R. Gross,
Phys. Rev. Lett. **103**, 157002 (2009).



Resistivity
 $\sim \rho_0 + AT^n$

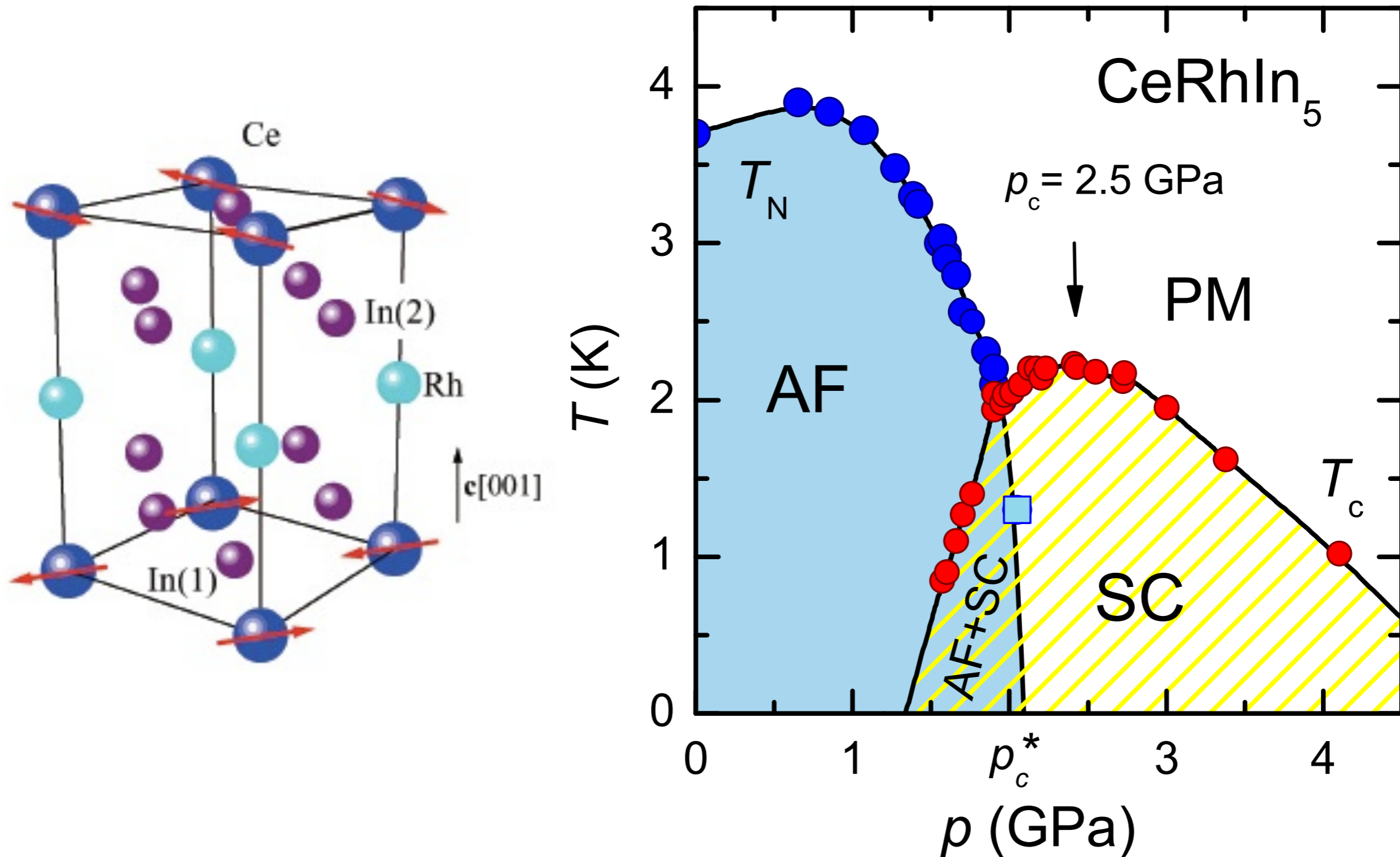


K. Hashimoto, K. Cho, T. Shibauchi, S. Kasahara, Y. Mizukami, R. Katsumata, Y. Tsuruhara, T. Terashima, H. Ikeda, M.A. Tanatar, H. Kitano, N. Salovich, R.W. Giannetta, P. Walmsley, A. Carrington, R. Prozorov, and Y. Matsuda, *Science* **336**, 1554 (2012).



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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The Hubbard Model

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

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

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

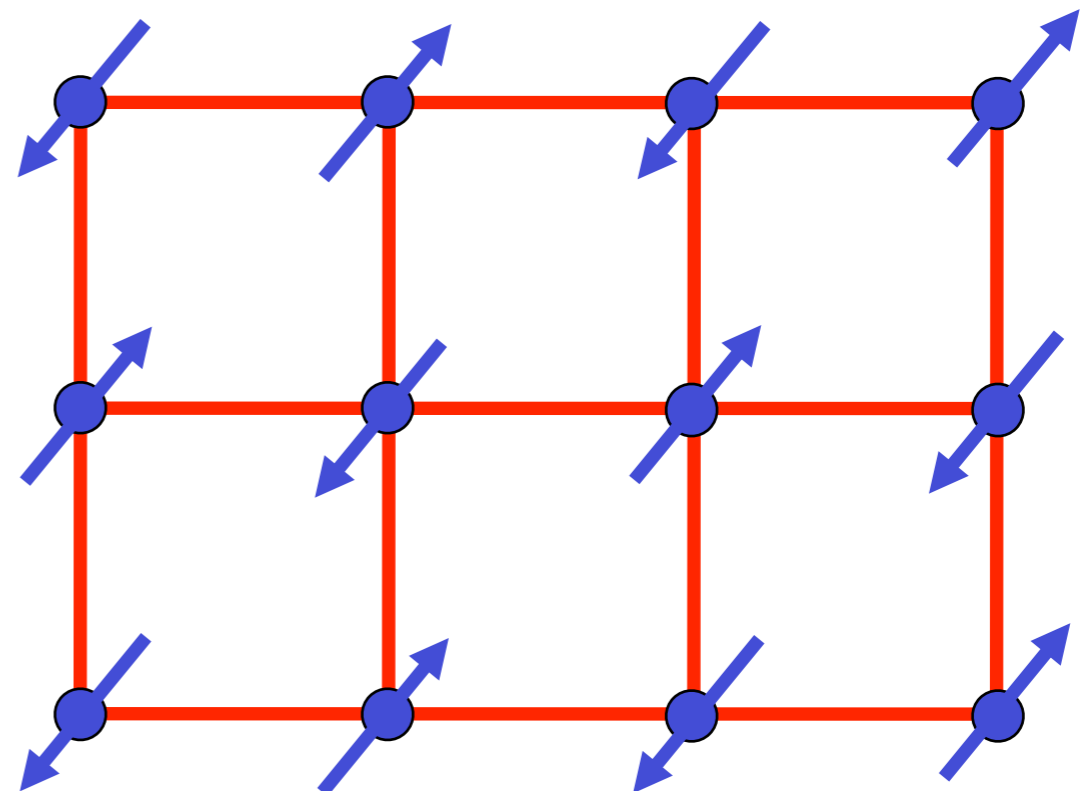
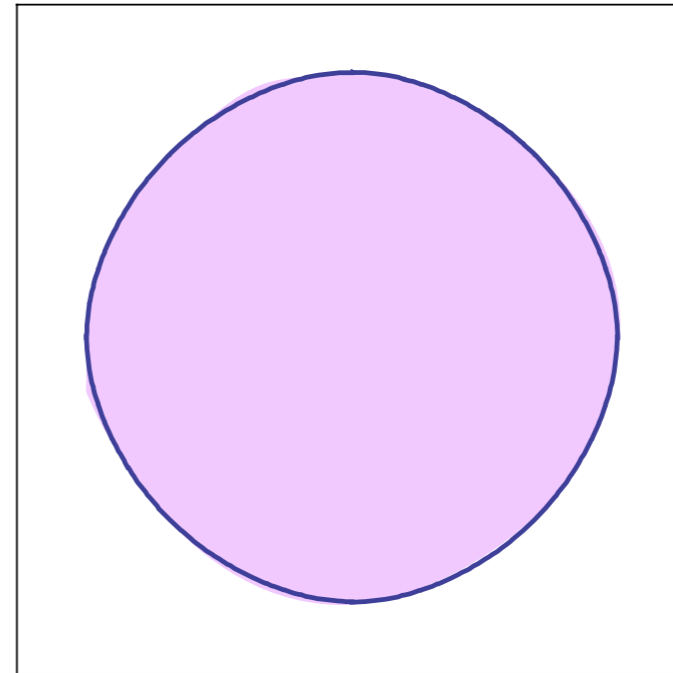
$$n_{i\alpha} = c_{i\alpha}^\dagger c_{i\alpha}$$

$$c_{i\alpha}^\dagger c_{j\beta} + c_{j\beta} c_{i\alpha}^\dagger = \delta_{ij} \delta_{\alpha\beta}$$

$$c_{i\alpha} c_{j\beta} + c_{j\beta} c_{i\alpha} = 0$$

Fermi surface+antiferromagnetism

Metal with “large”
Fermi surface



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.

The Hubbard Model

Decouple U term by a Hubbard-Stratanovich transformation

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

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

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

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

“Yukawa” coupling between fermions and antiferromagnetic order:

$$\lambda^2 \sim U, \text{ the Hubbard repulsion}$$

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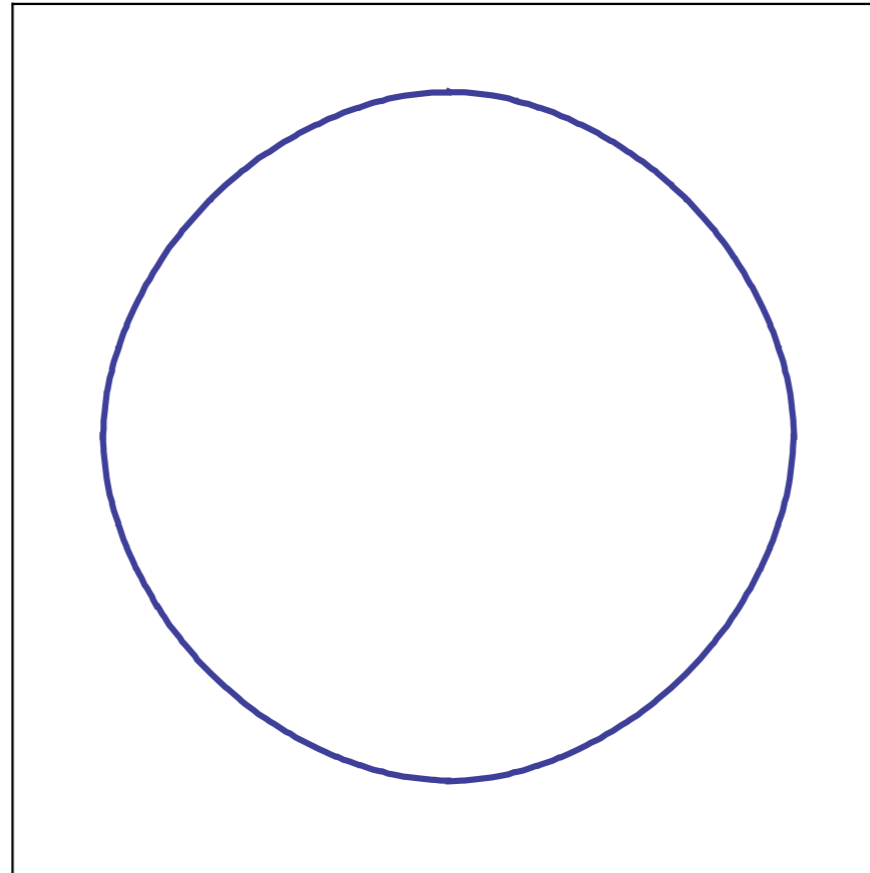
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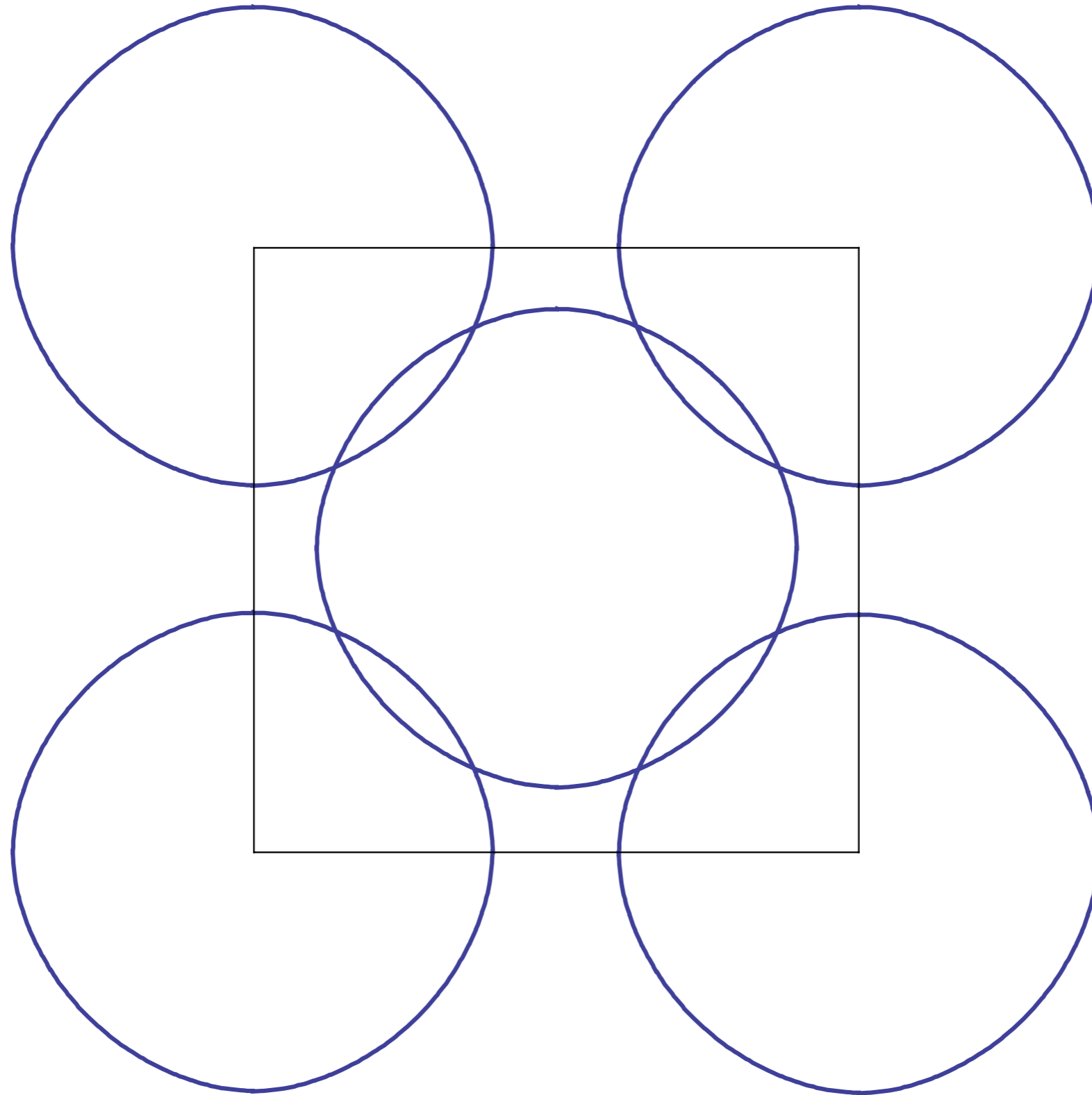
Hertz, Moriya, Millis: integrate out fermions, and focus on effective theory of damped excitations of the order parameter φ_α . Method fails in $d = 2$.

Fermi surface+antiferromagnetism



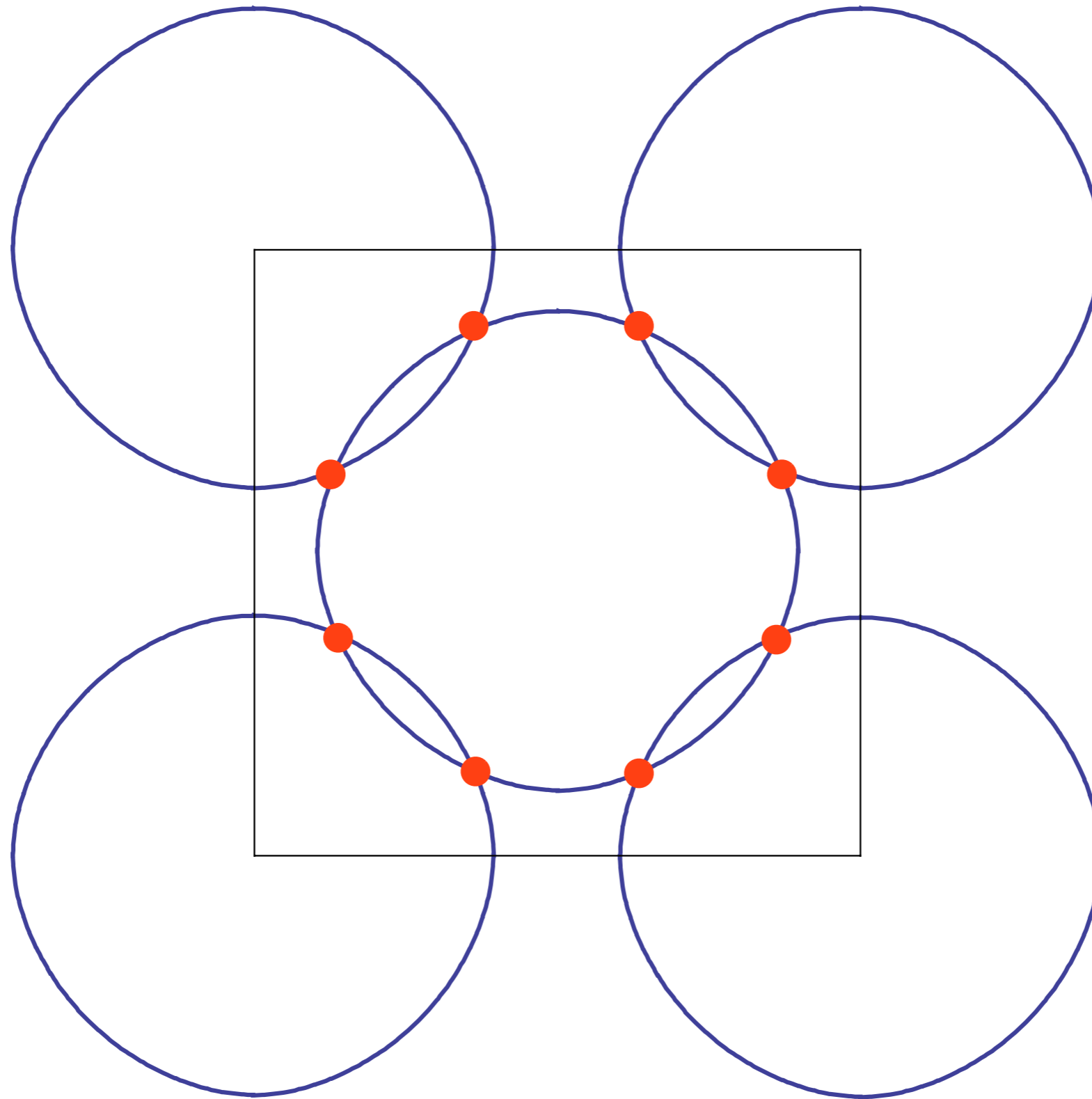
Metal with “large” Fermi surface

Fermi surface+antiferromagnetism



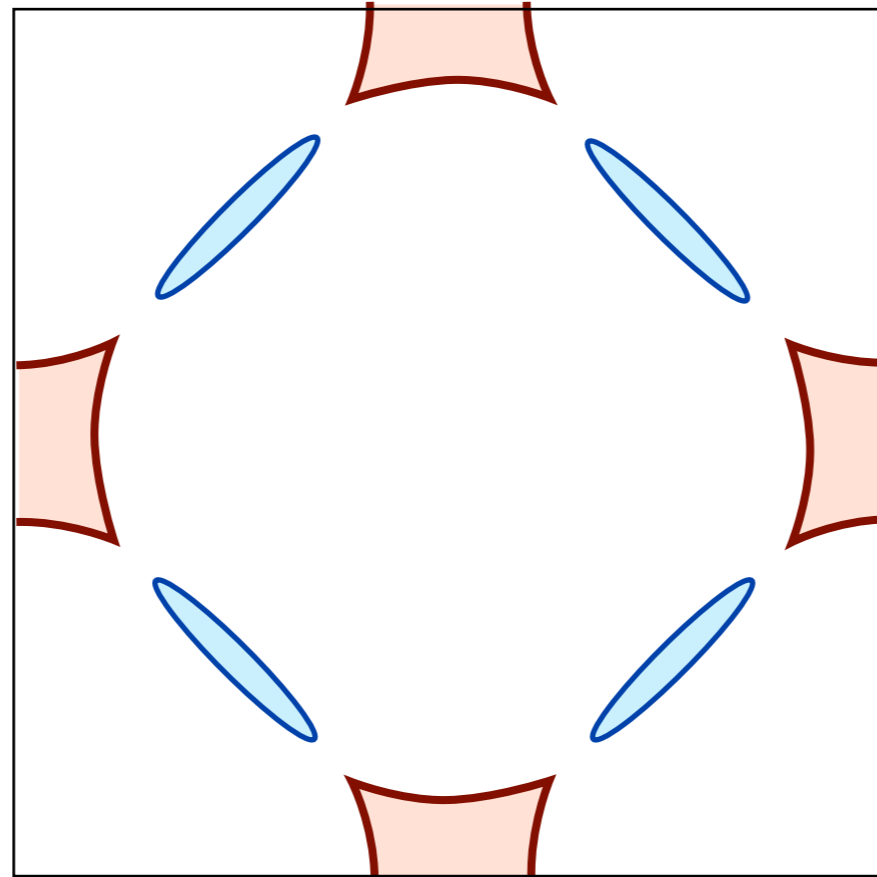
Fermi surfaces translated by $\mathbf{K} = (\pi, \pi)$.

Fermi surface+antiferromagnetism



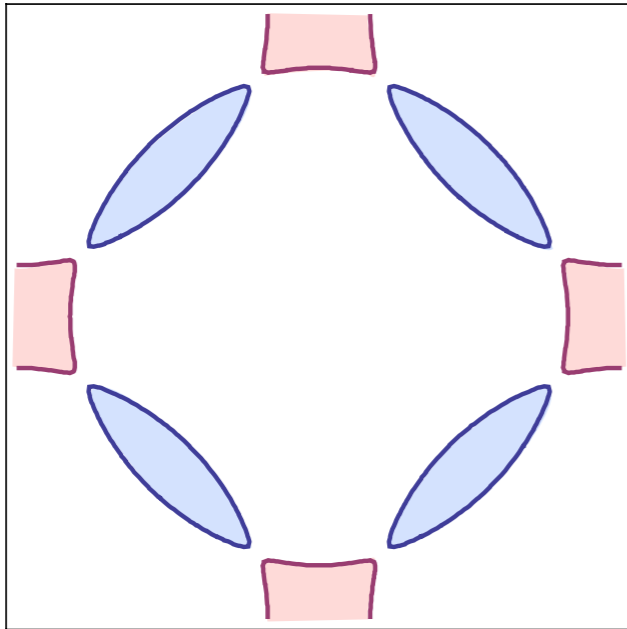
“Hot” spots

Fermi surface+antiferromagnetism



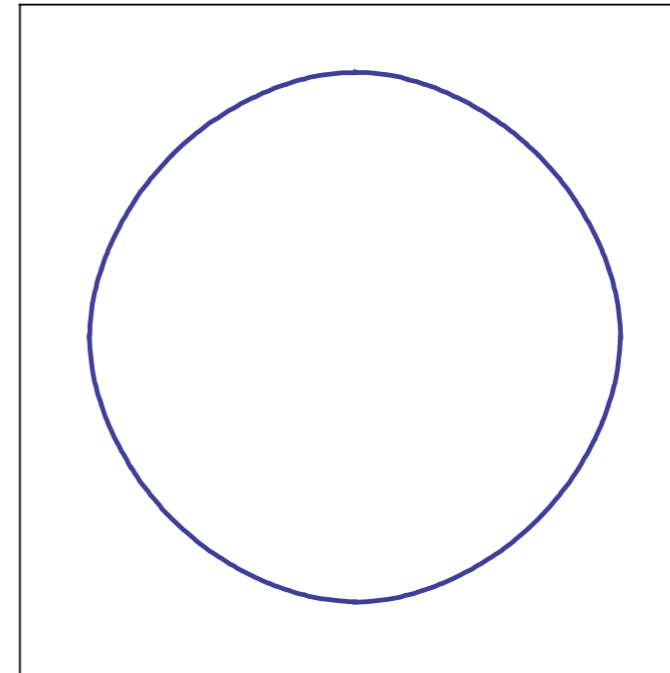
Electron and hole pockets in
antiferromagnetic phase with $\langle \vec{\varphi} \rangle \neq 0$

Fermi surface+antiferromagnetism



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

Metal with electron
and hole pockets



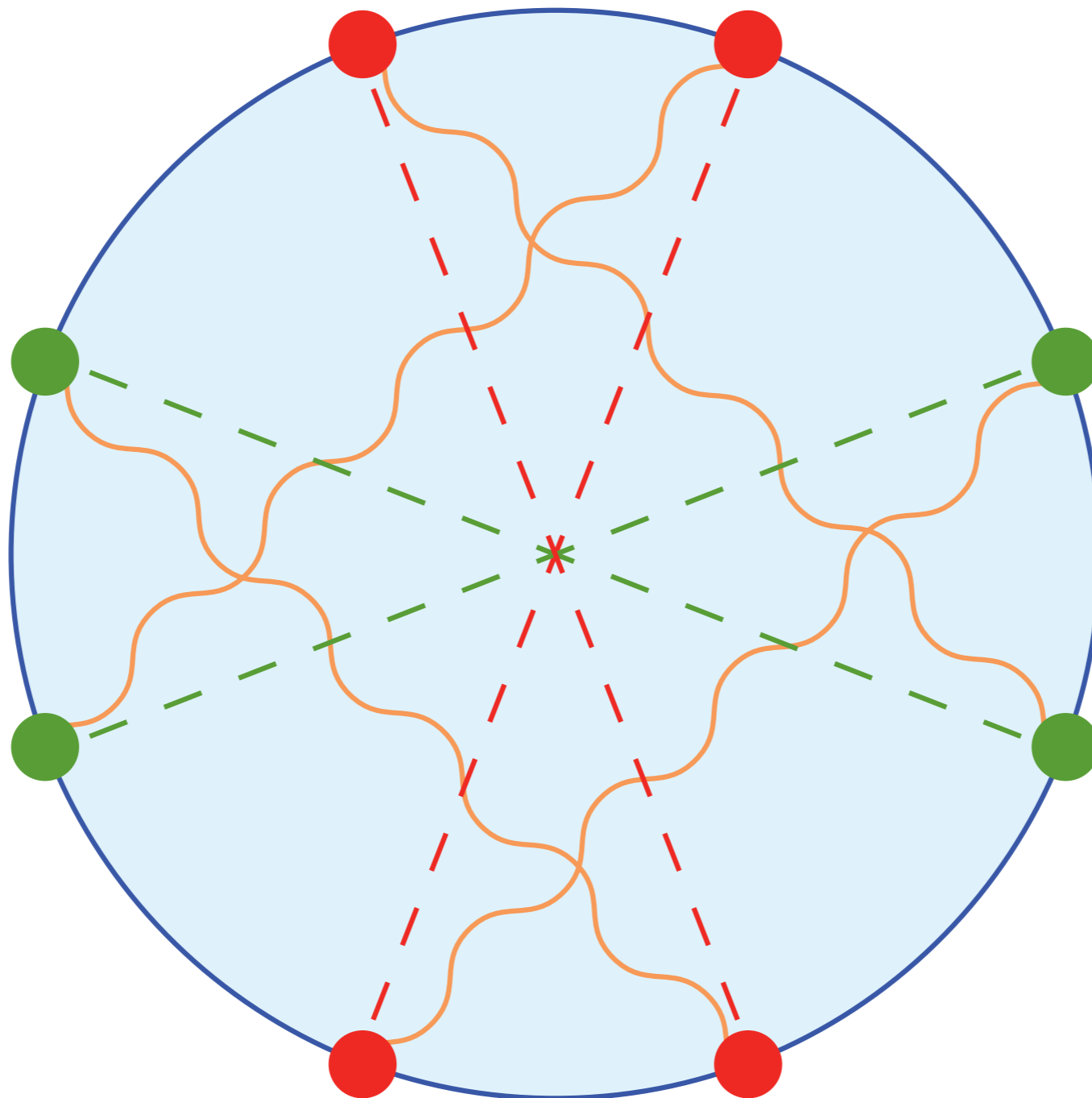
$$\langle \vec{\varphi} \rangle = 0$$

Metal with “large”
Fermi surface

← Increasing interaction

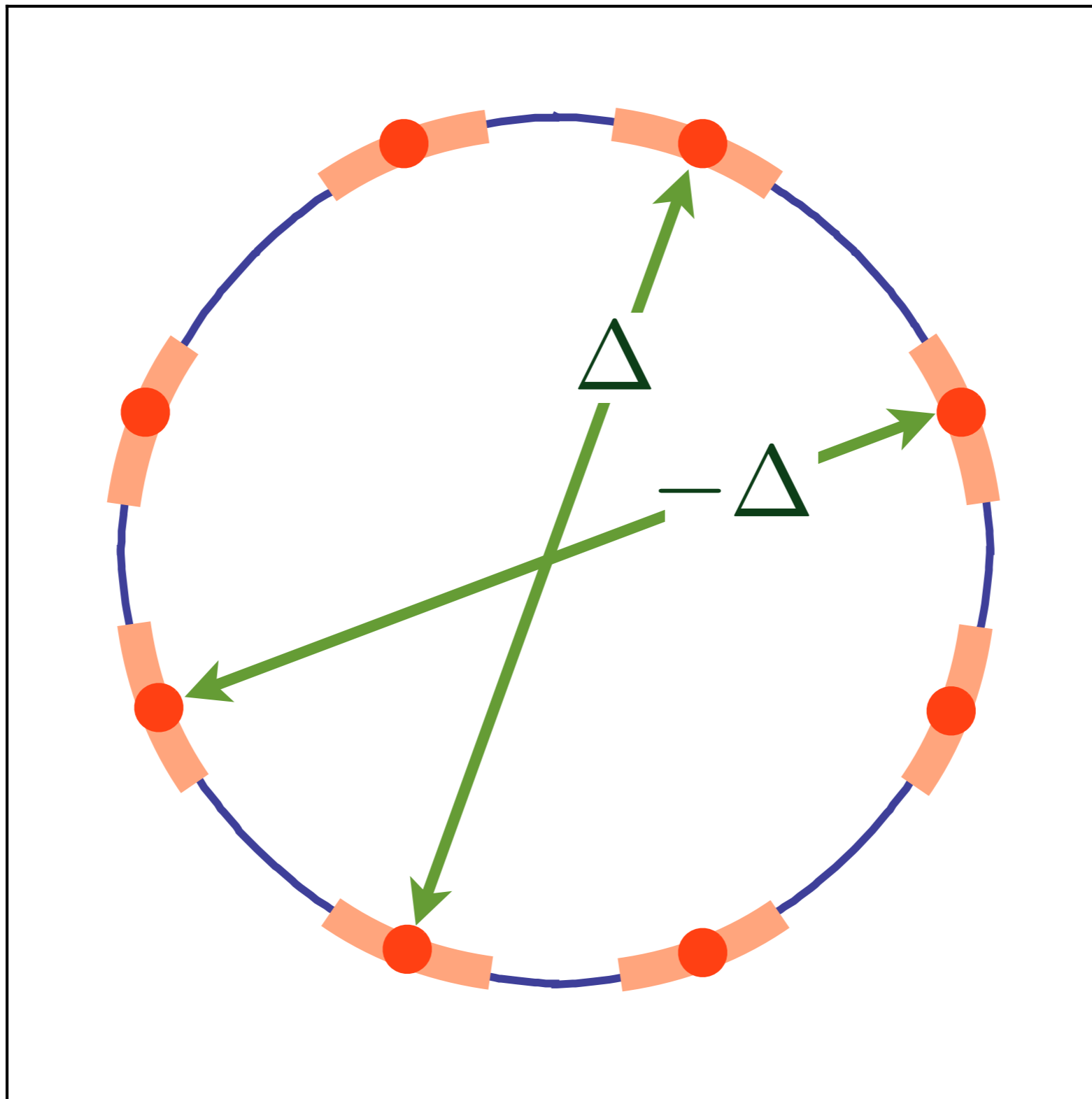
S. Sachdev, A. V. Chubukov, and A. Sokol, *Phys. Rev. B* **51**, 14874 (1995).
A. V. Chubukov and D. K. Morr, *Physics Reports* **288**, 355 (1997).

Pairing “glue” from antiferromagnetic fluctuations



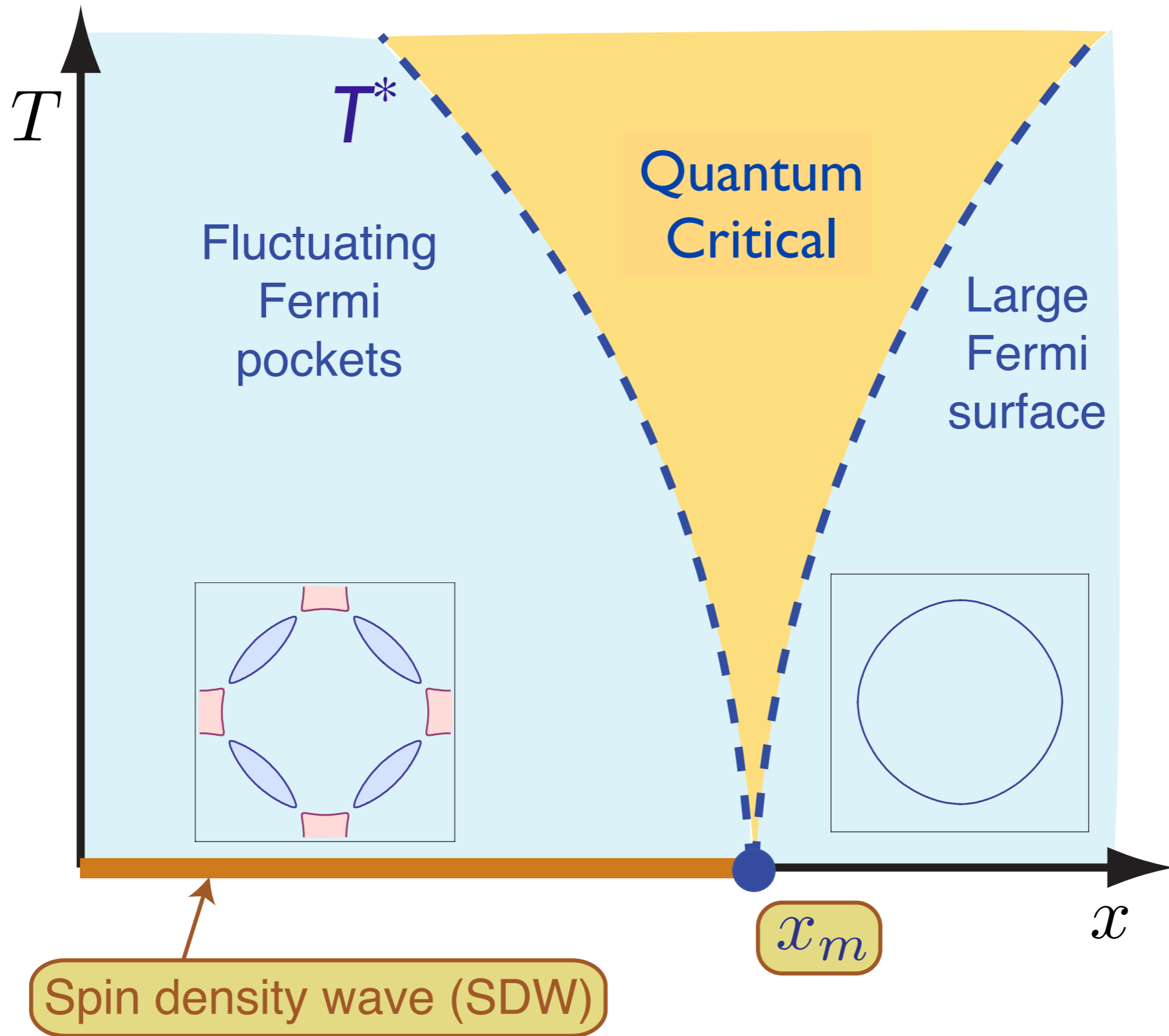
V. J. Emery, *J. Phys. (Paris) Colloq.* **44**, C3-977 (1983)
D. J. Scalapino, E. Loh, and J. E. Hirsch, *Phys. Rev. B* **34**, 8190 (1986)
K. Miyake, S. Schmitt-Rink, and C. M. Varma, *Phys. Rev. B* **34**, 6554 (1986)
S. Raghu, S. A. Kivelson, and D. J. Scalapino, *Phys. Rev. B* **81**, 224505 (2010)

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



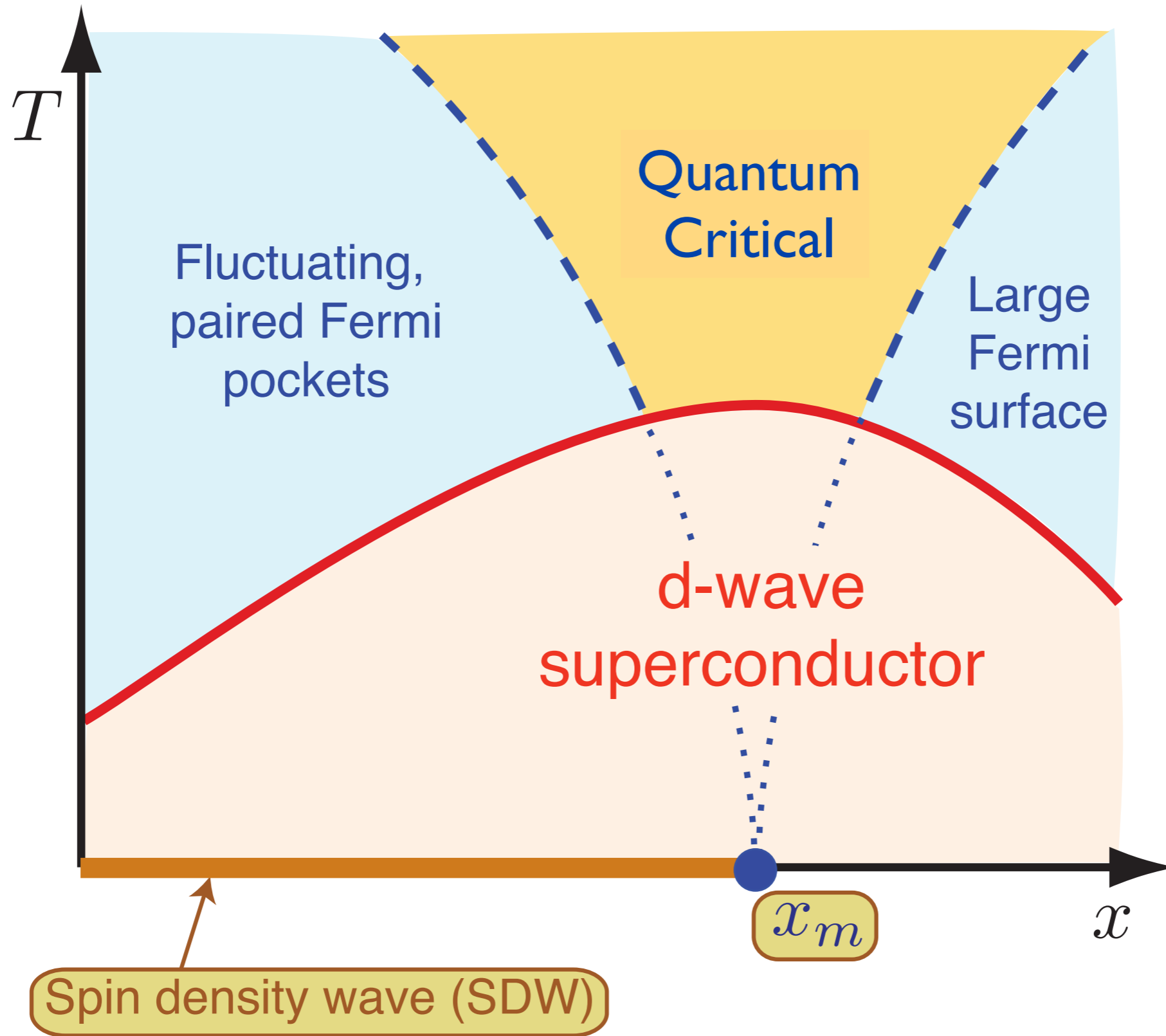
Unconventional pairing at and near hot spots

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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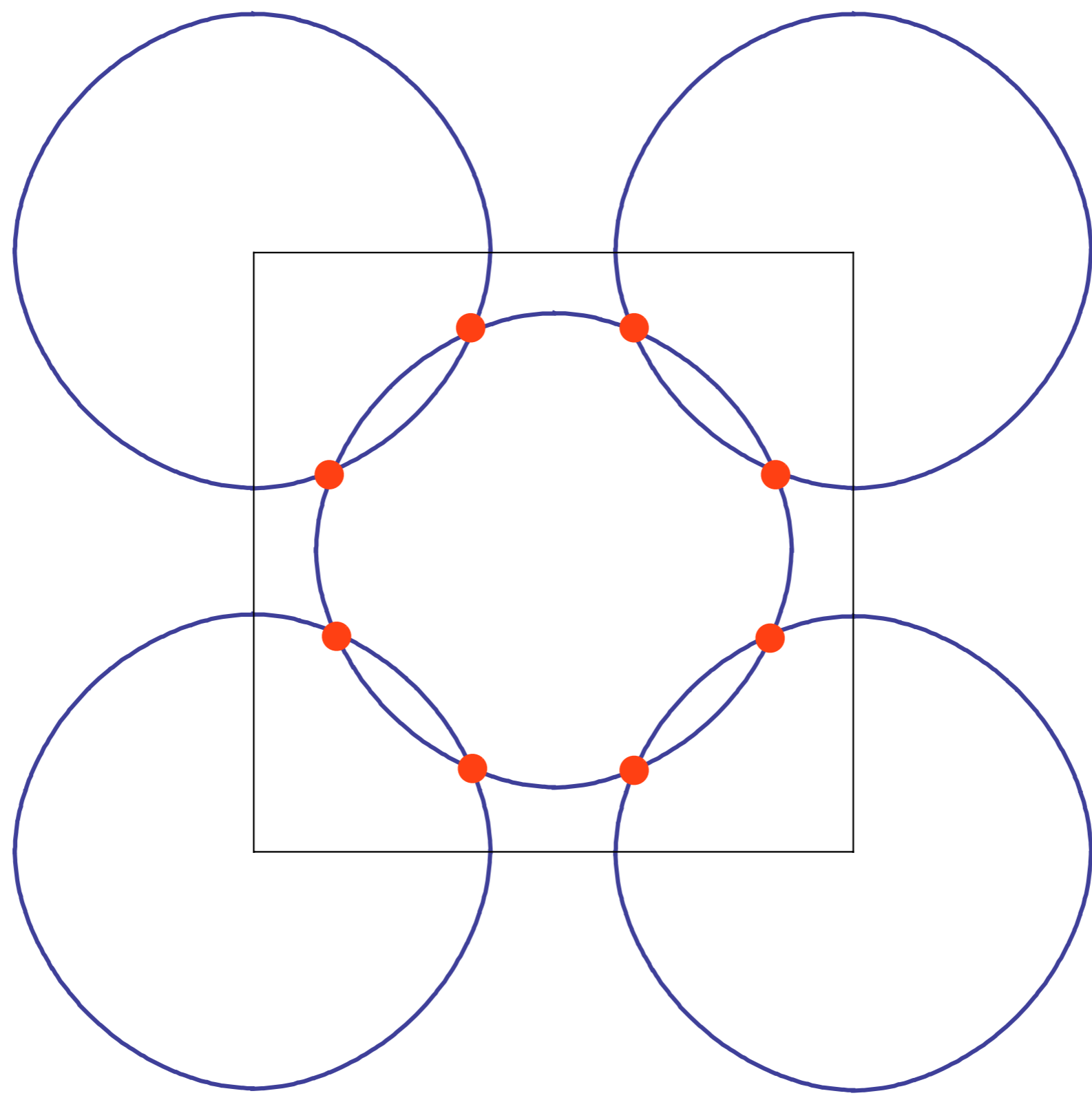
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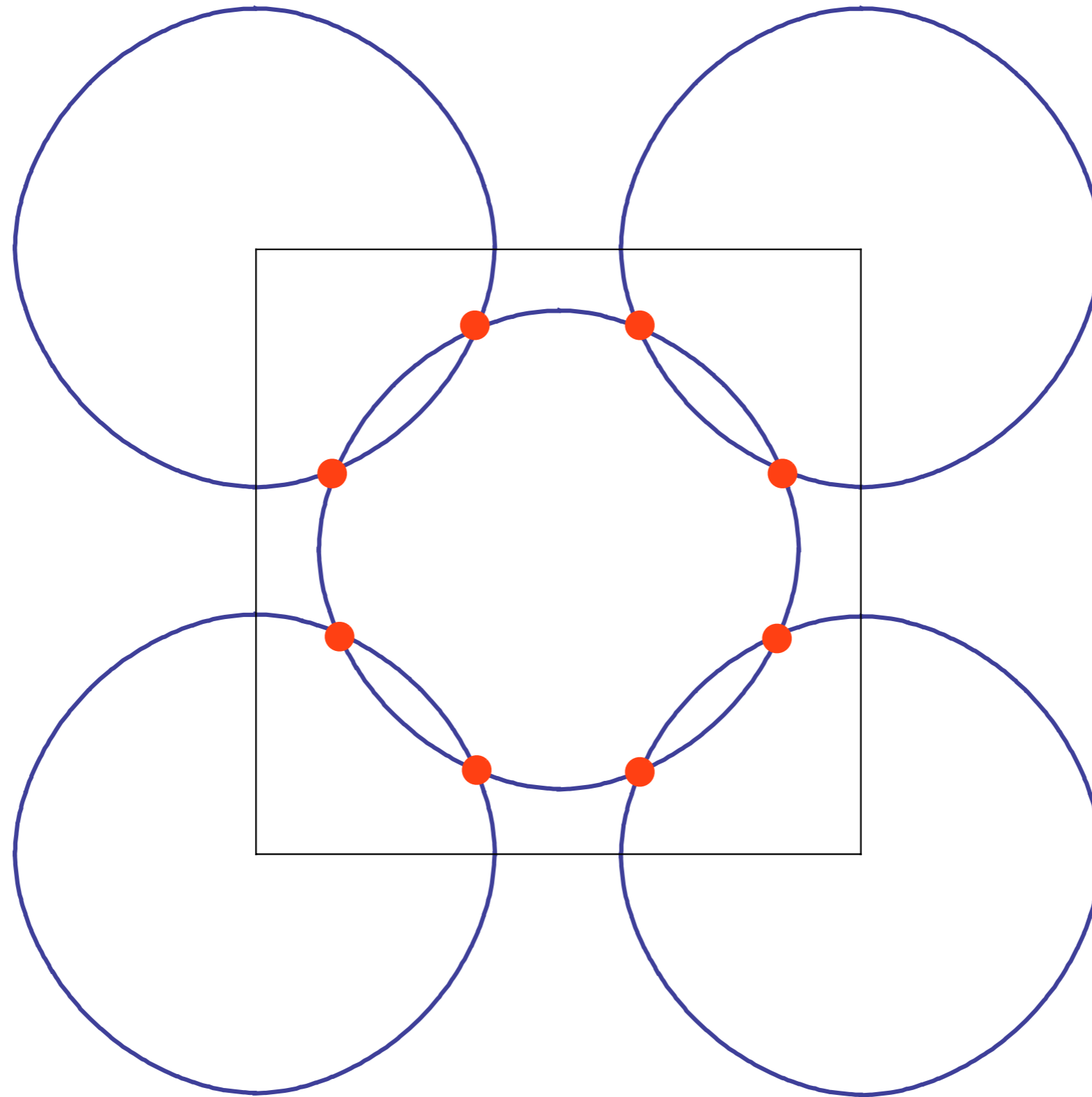
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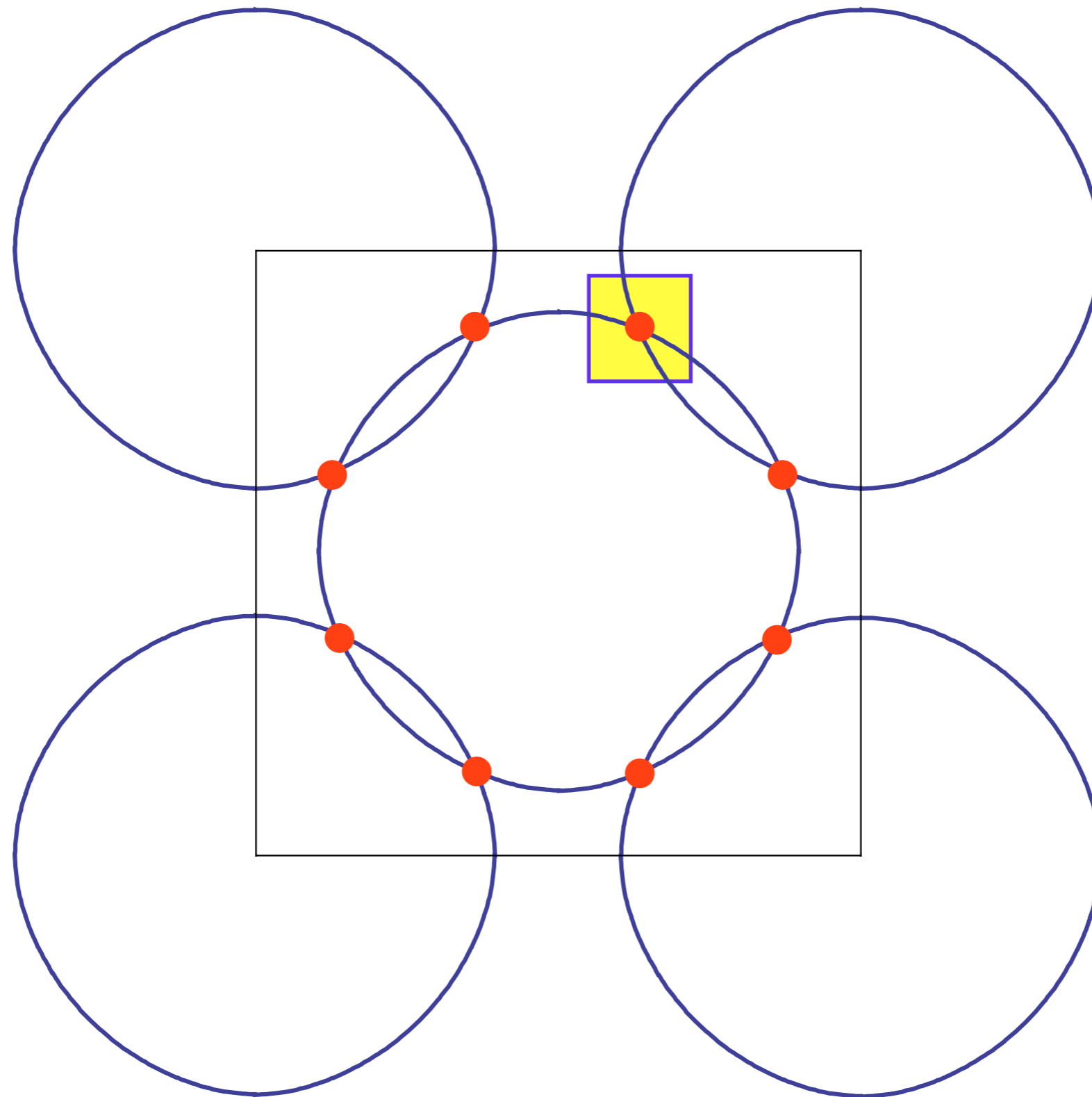
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“Hot” spots

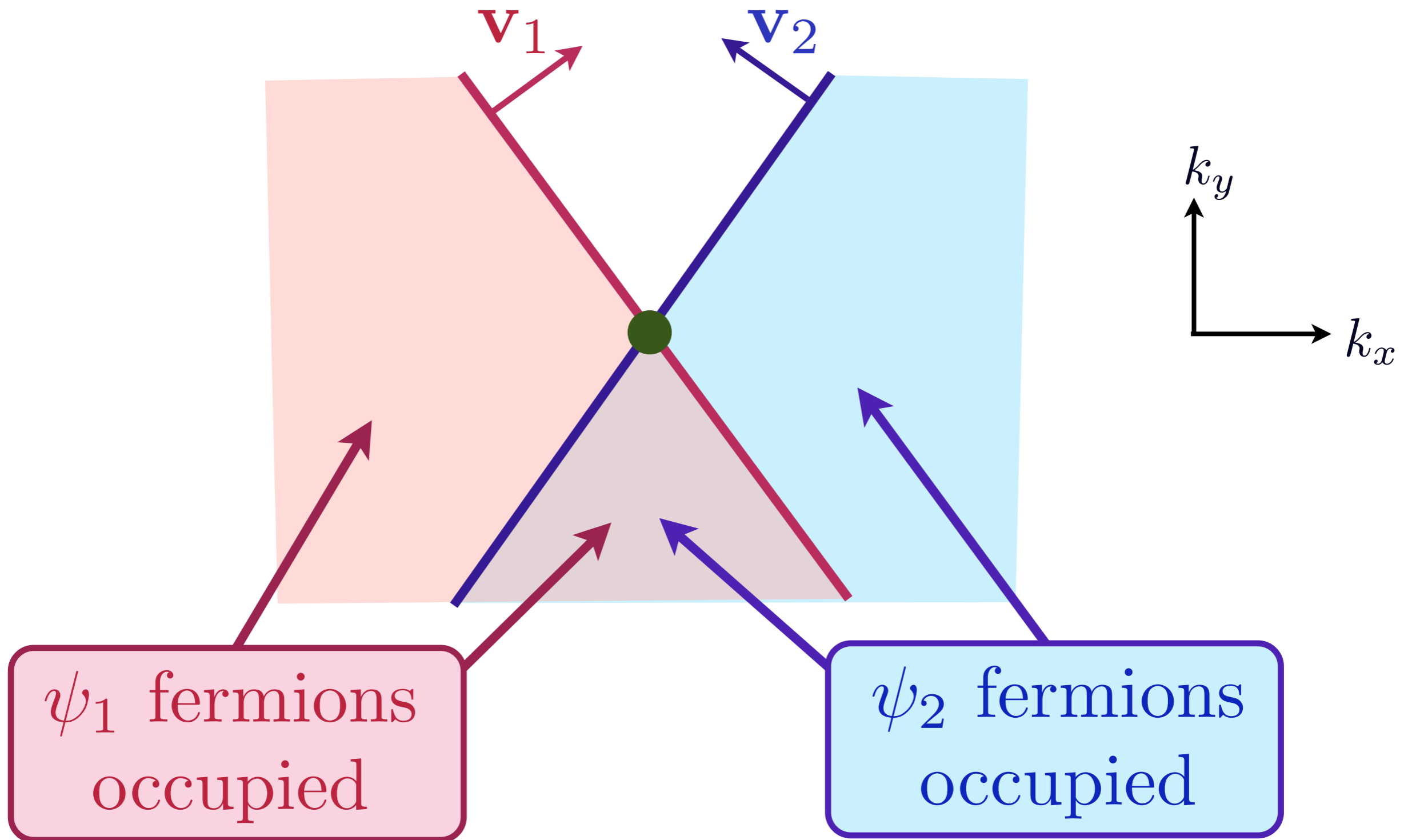


Low energy theory for critical point near hot spots



Low energy theory for critical point near hot spots

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



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

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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)

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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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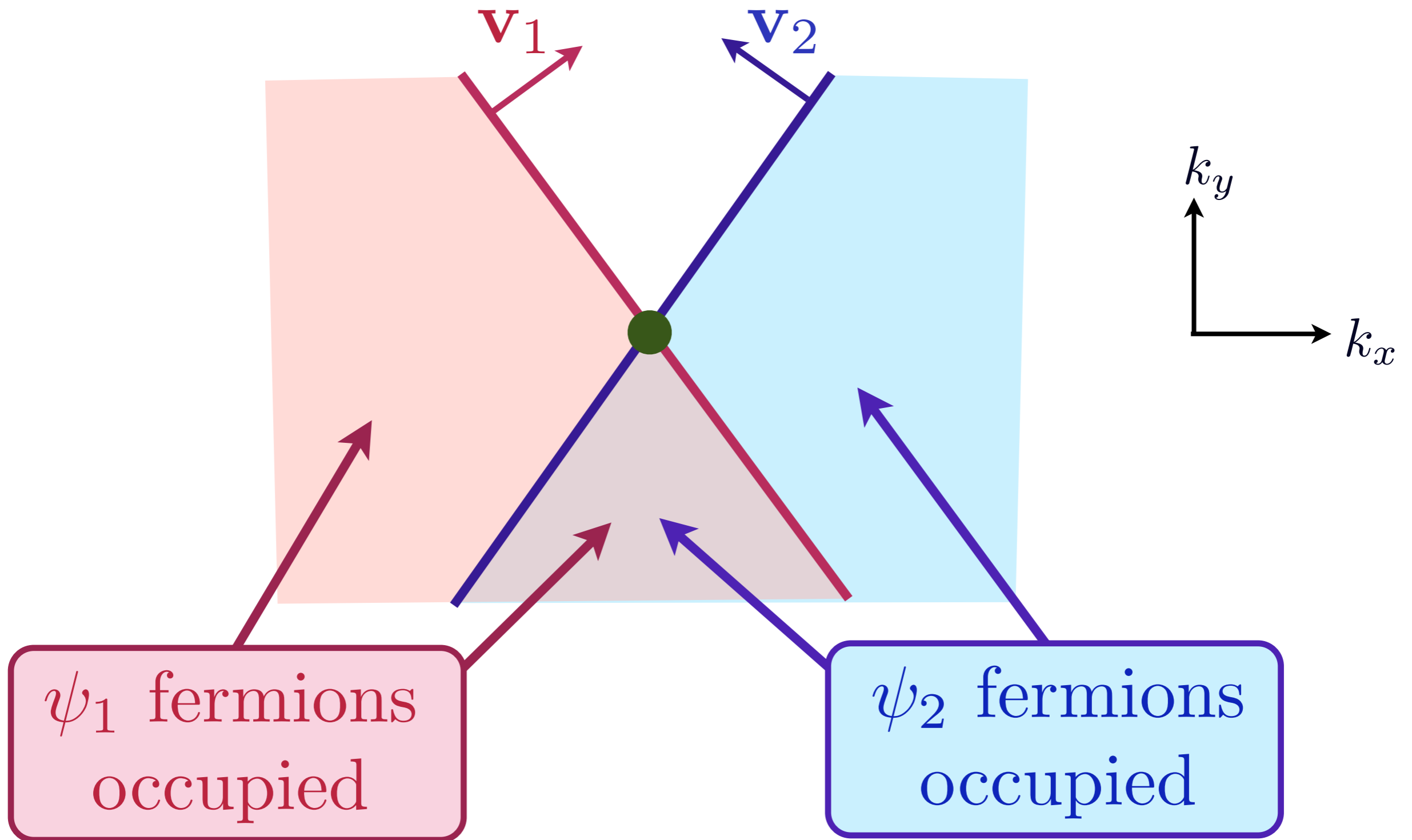
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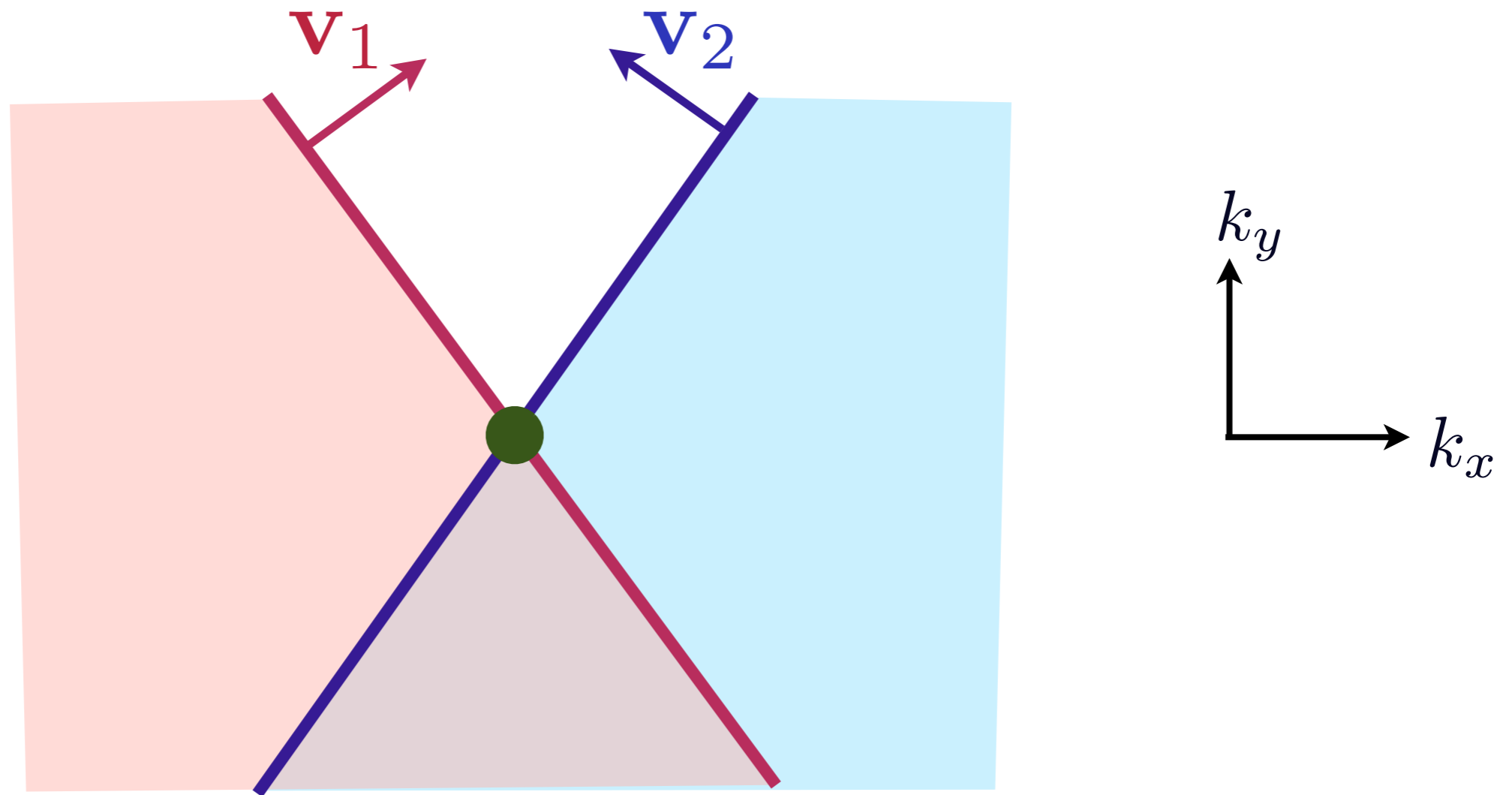
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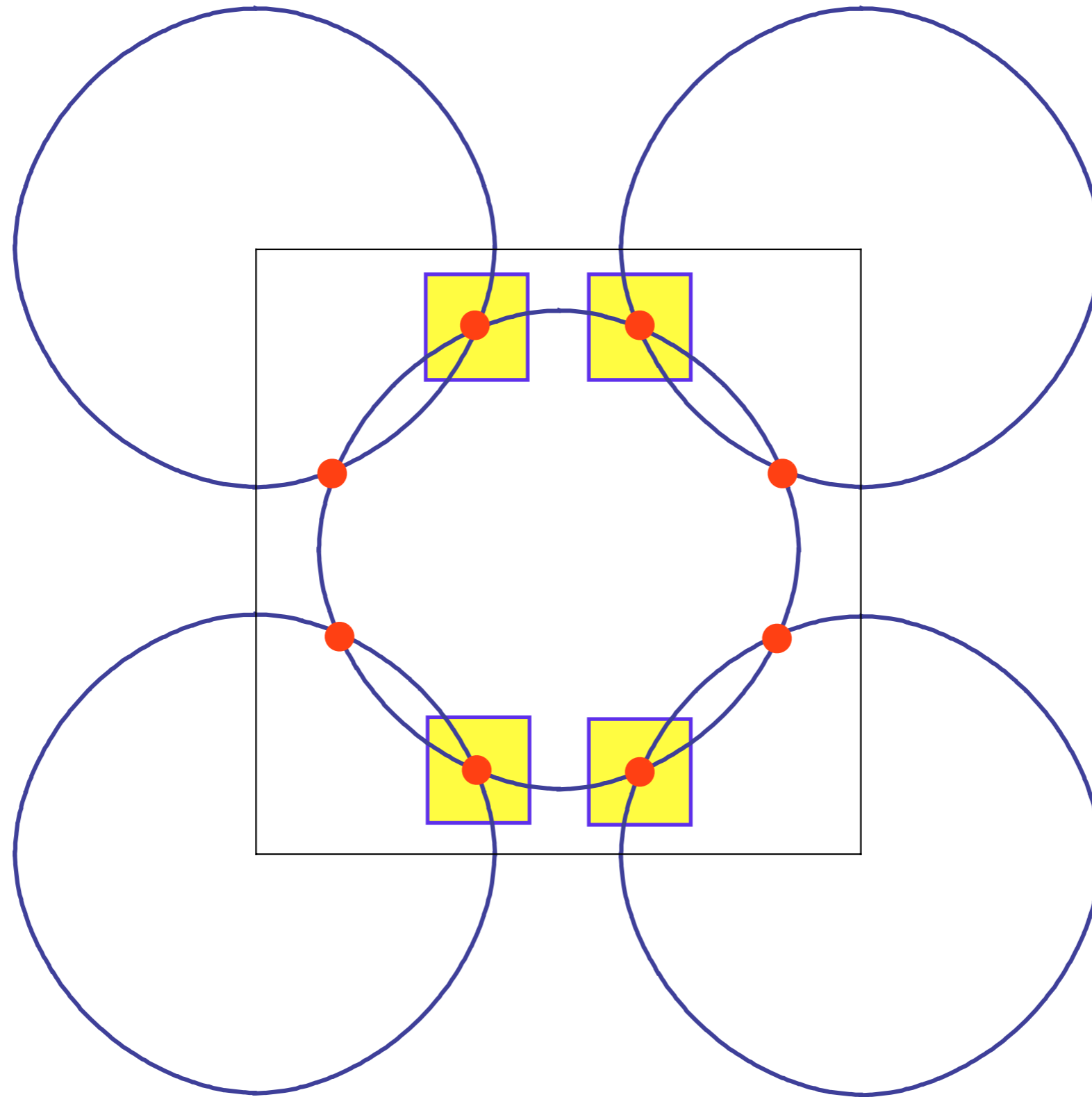
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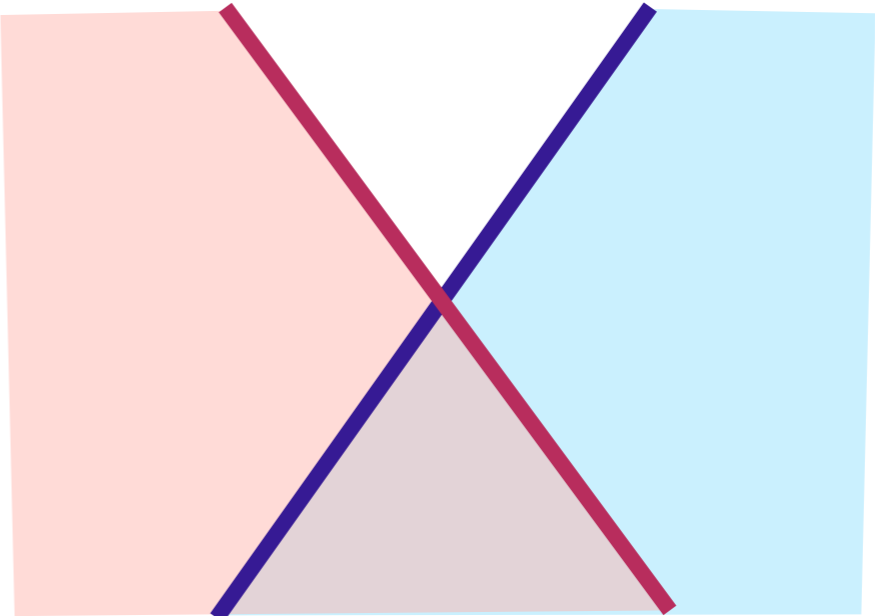
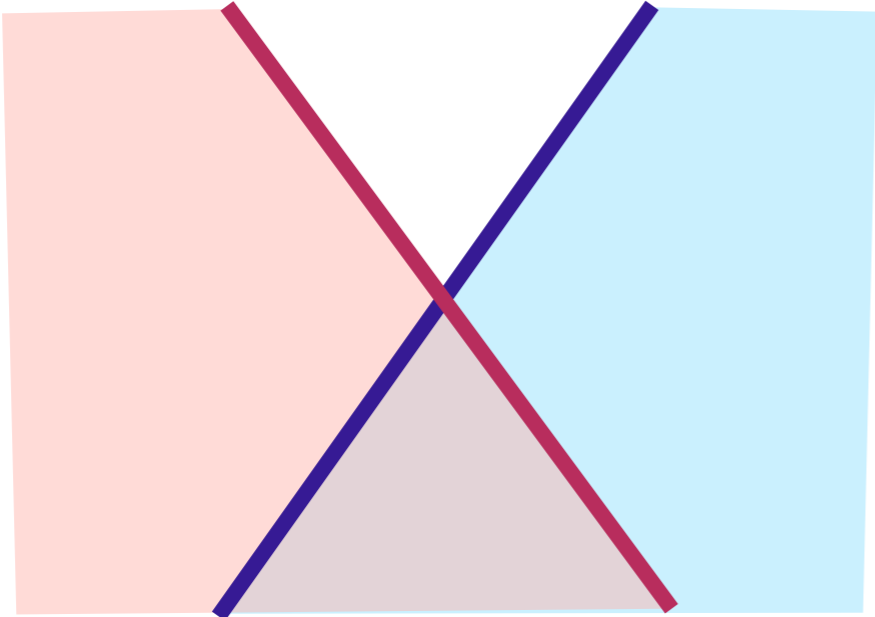
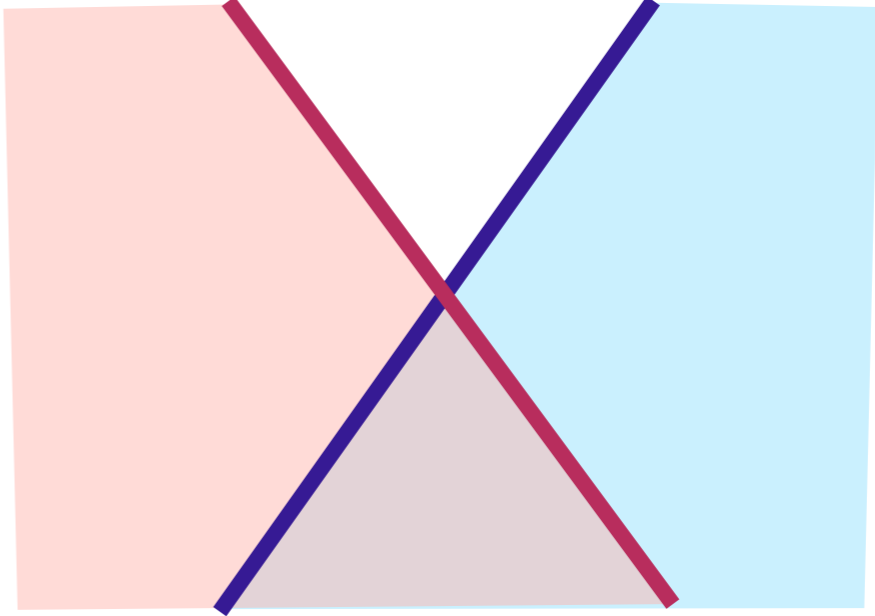
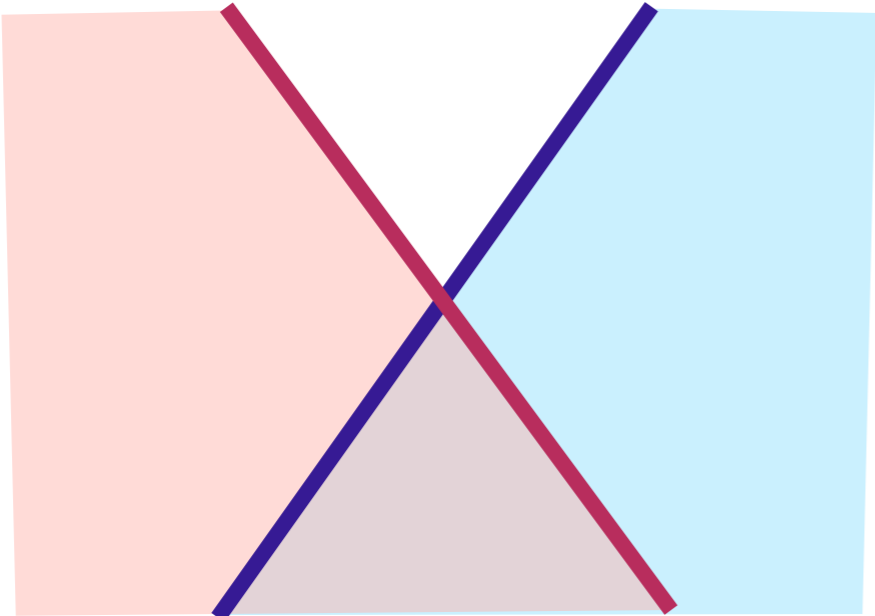


To faithfully realize low energy theory in quantum Monte Carlo,
we need a UV completion in which Fermi lines don't end
and all weights are positive.

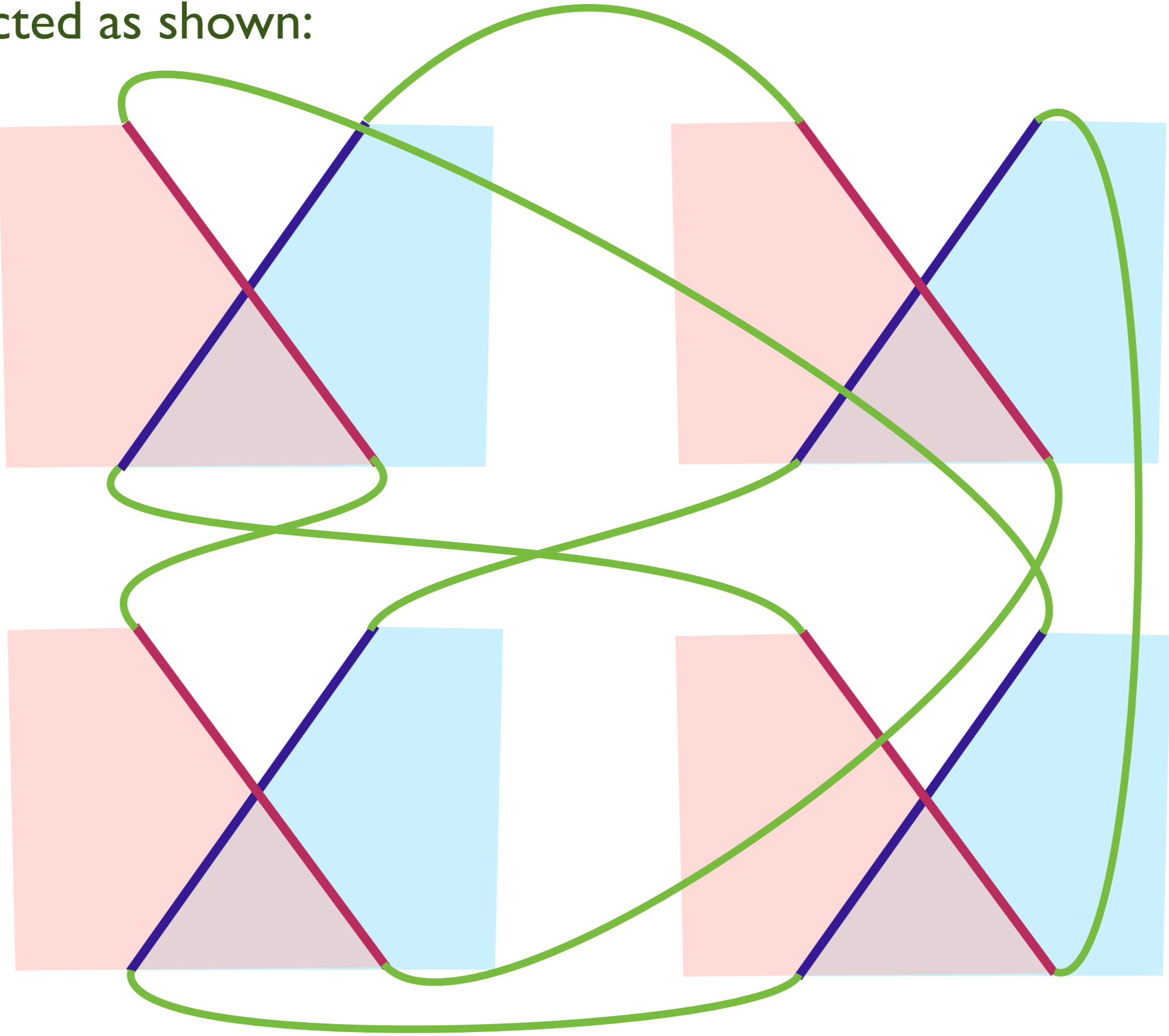


Low energy theory for critical point near hot spots

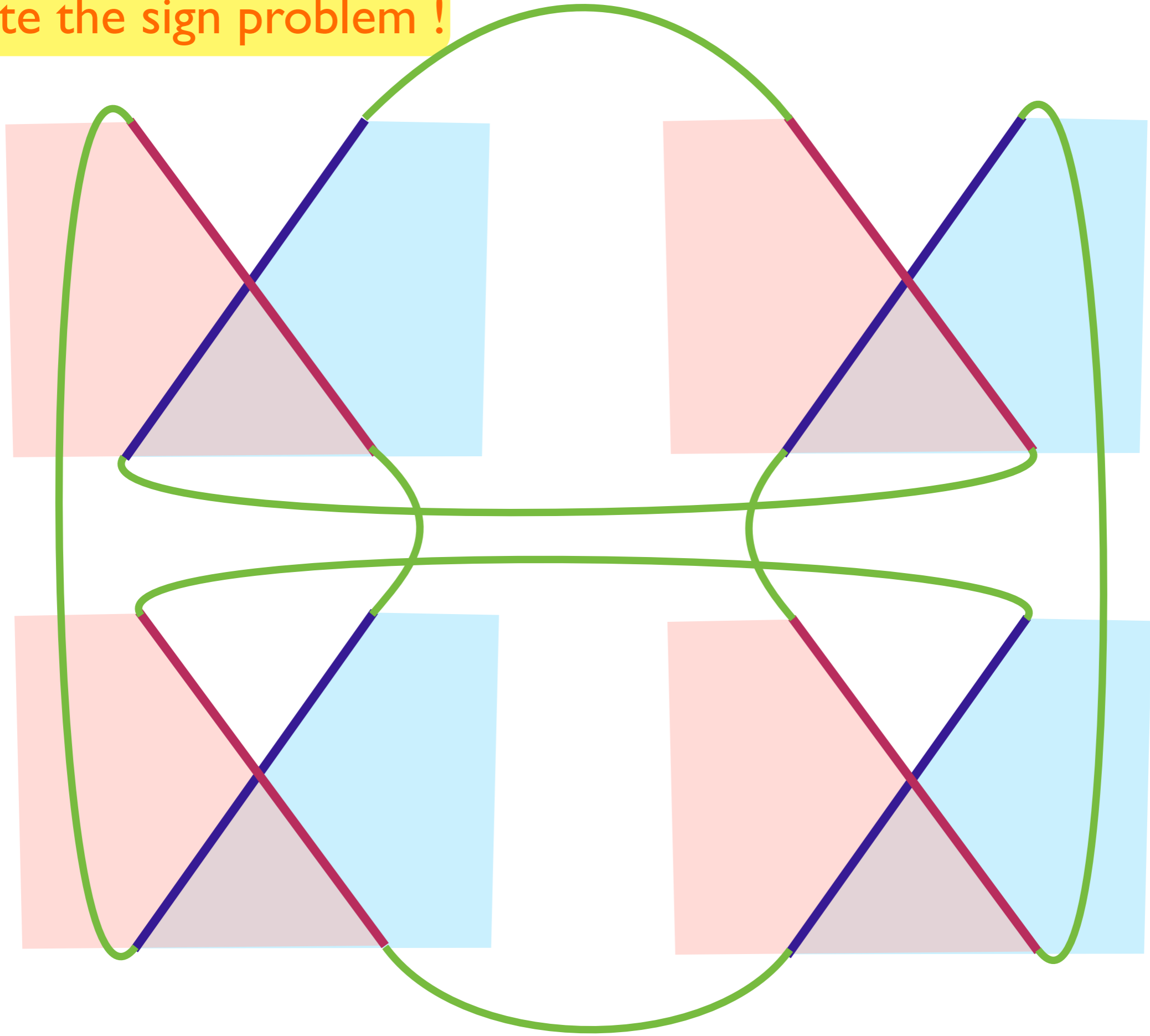
We have 4 copies
of the hot spot theory.....



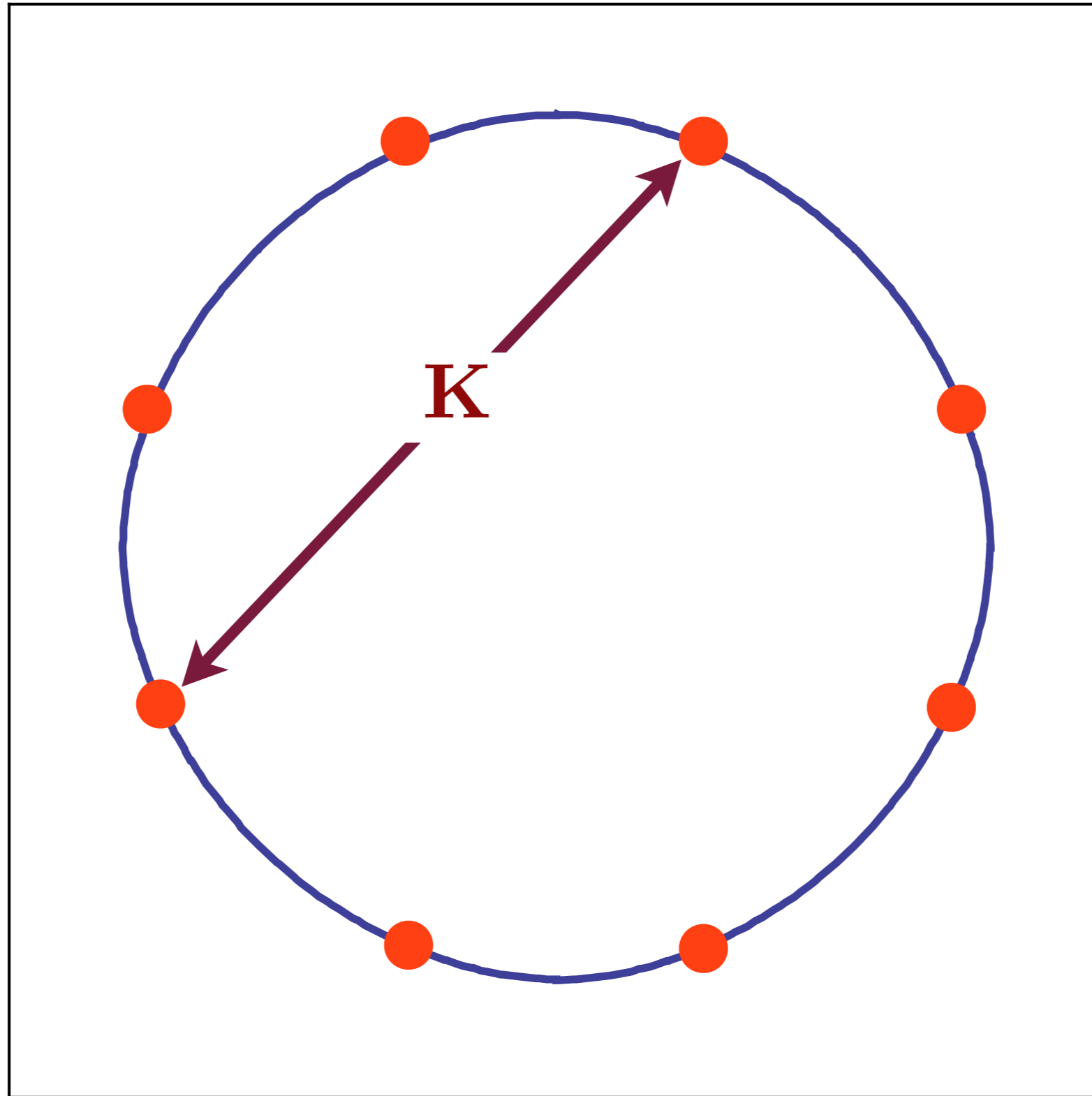
and their Fermi lines are connected as shown:



Reconnect Fermi lines and eliminate the sign problem !

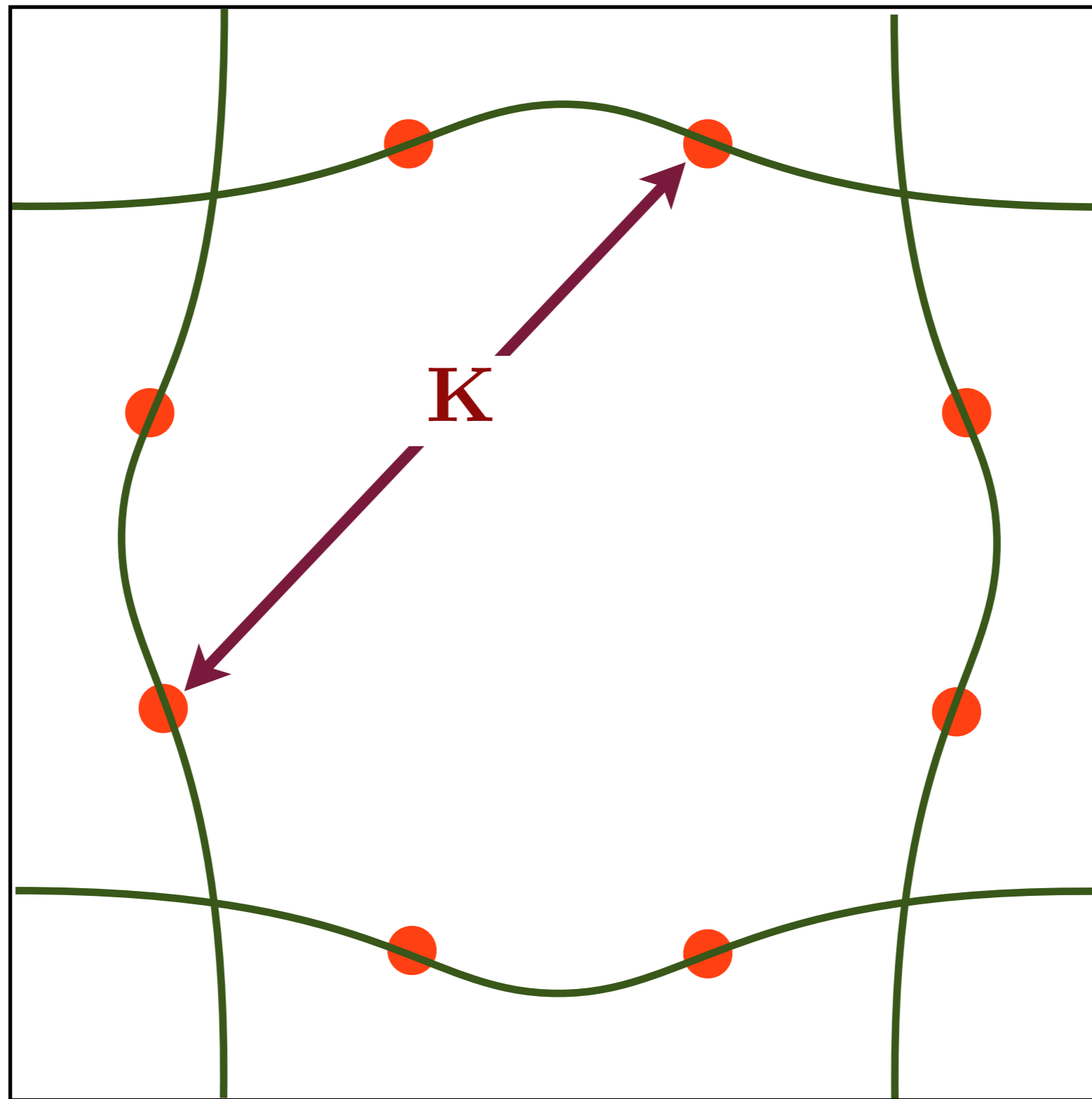


QMC for the onset of antiferromagnetism



Hot spots in a single band model

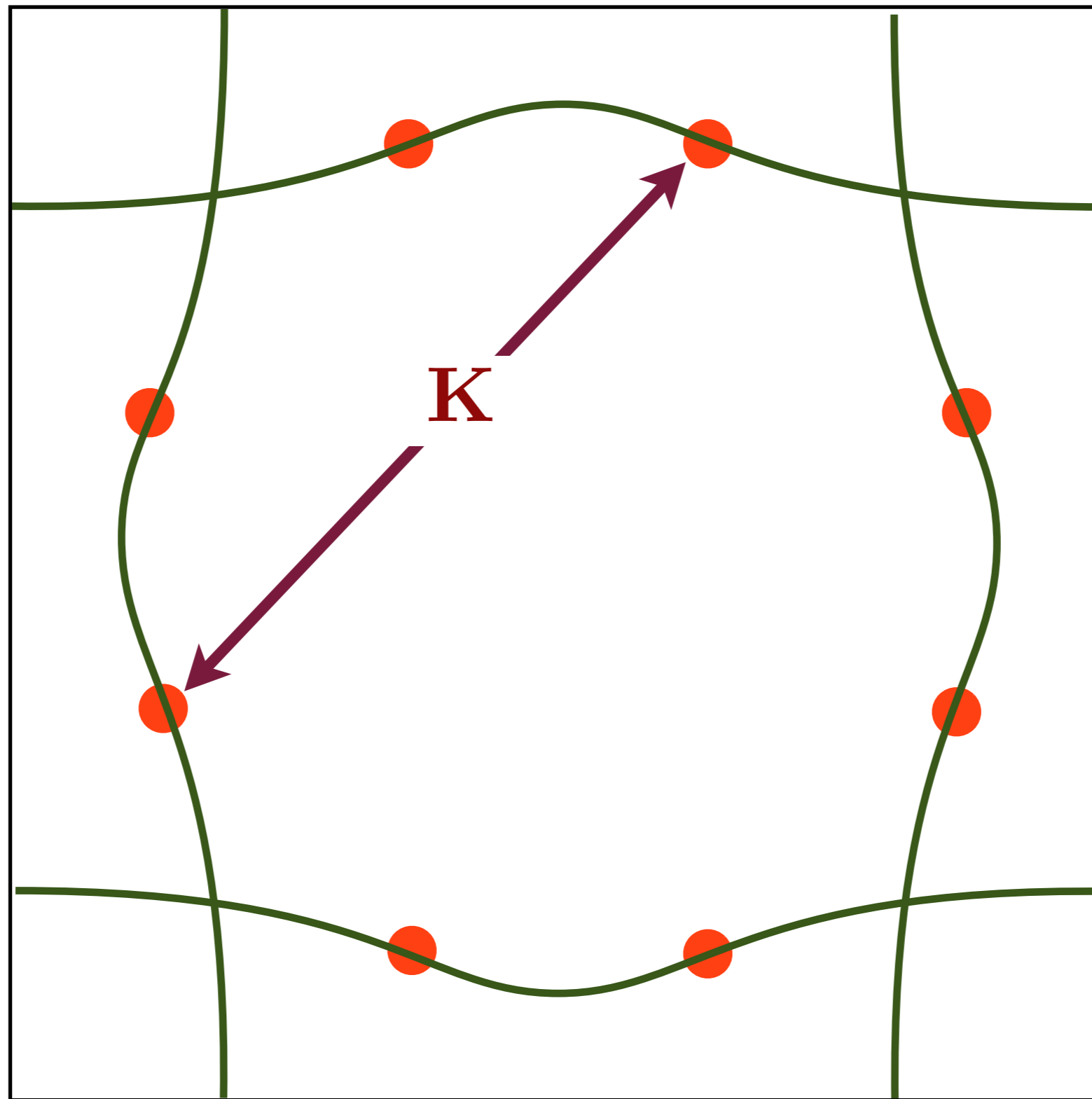
QMC for the onset of antiferromagnetism



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

Hot spots in a two band model

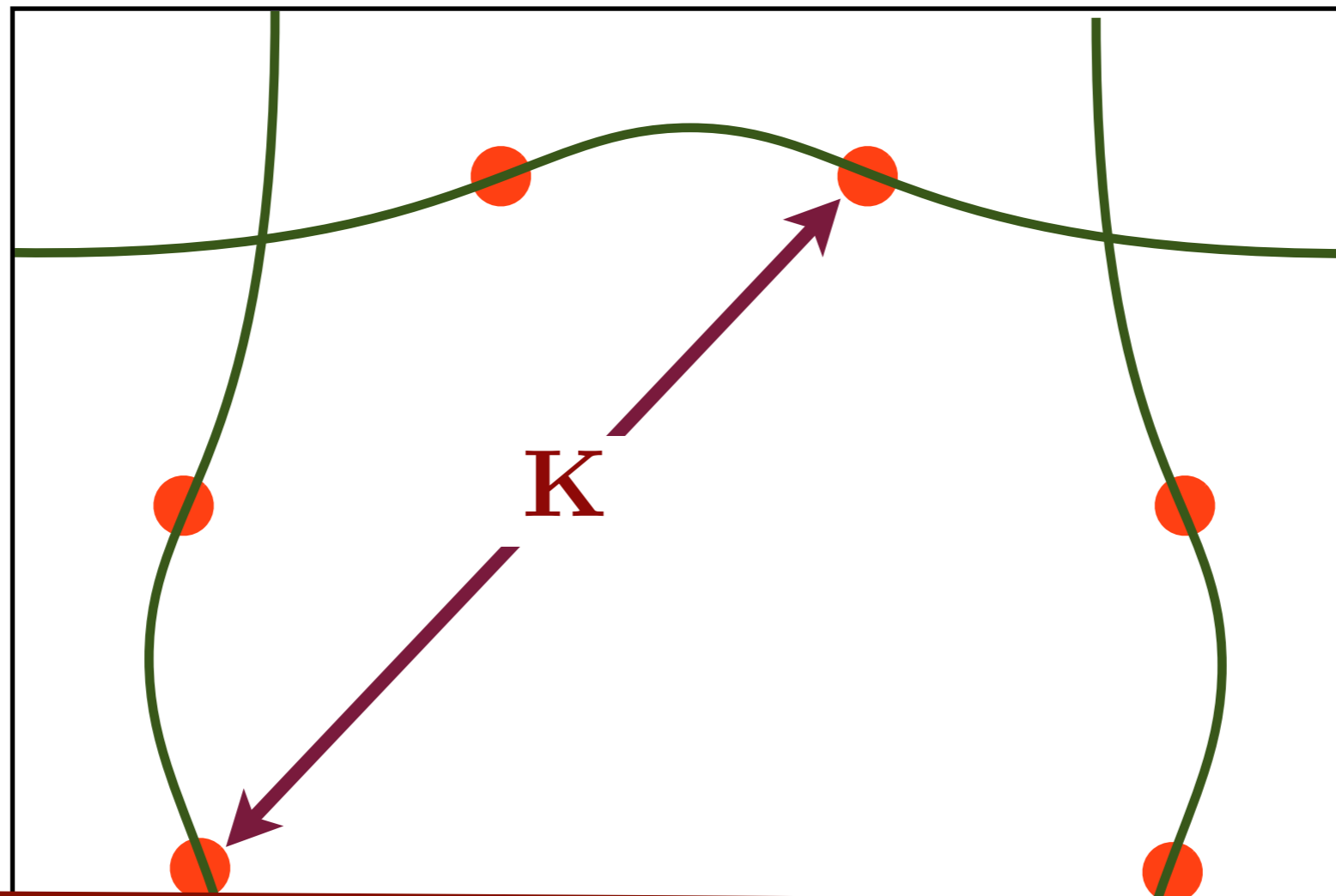
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No sign problem in
fermion determinant Monte Carlo !
Determinant is positive because of Kramer's
degeneracy, and no additional symmetries are needed; holds for
arbitrary band structure and band filling, provided **K** only
connects hot spots in distinct bands

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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QMC for the onset of antiferromagnetism

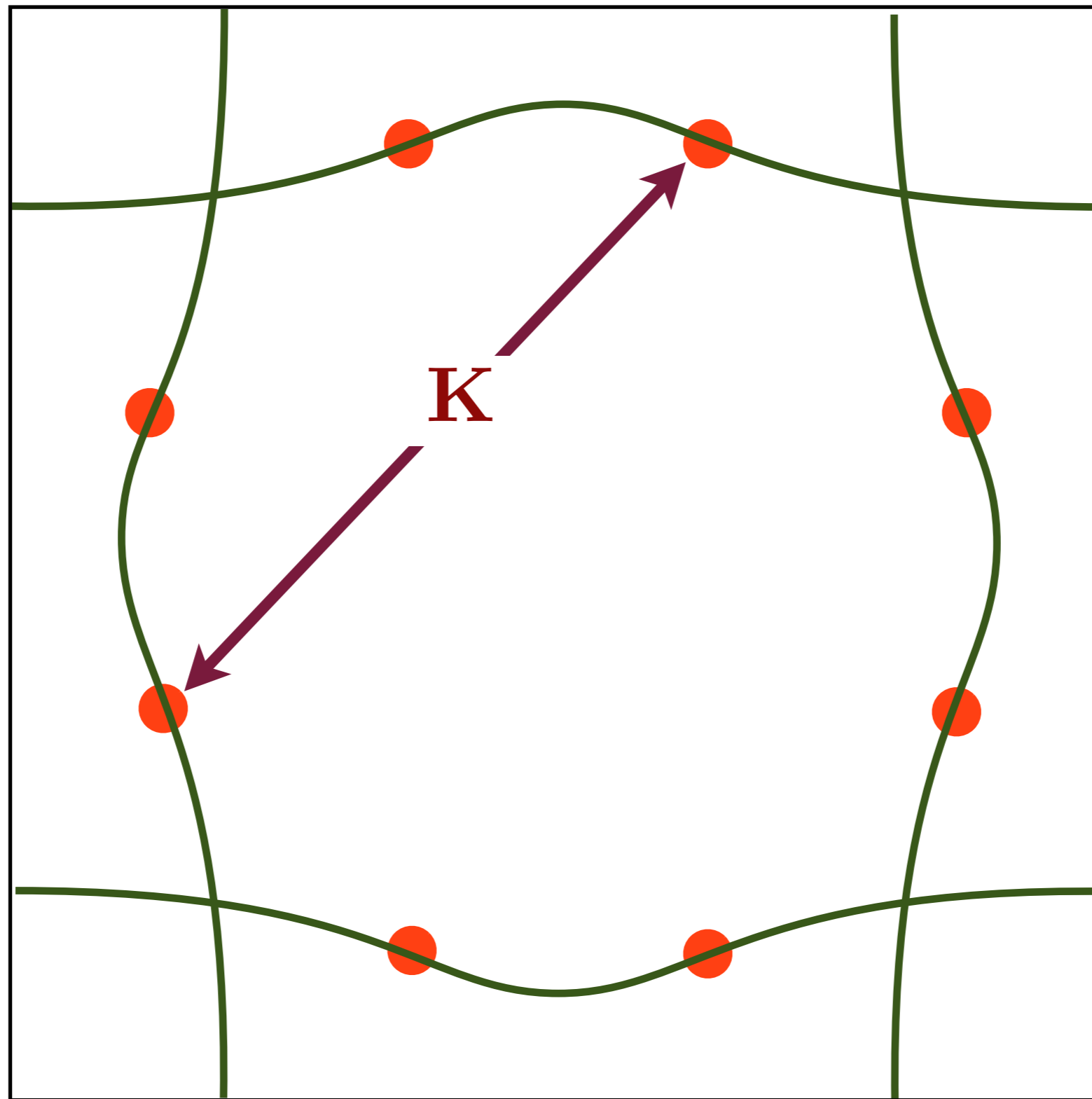
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No sign problem !

QMC for the onset of antiferromagnetism

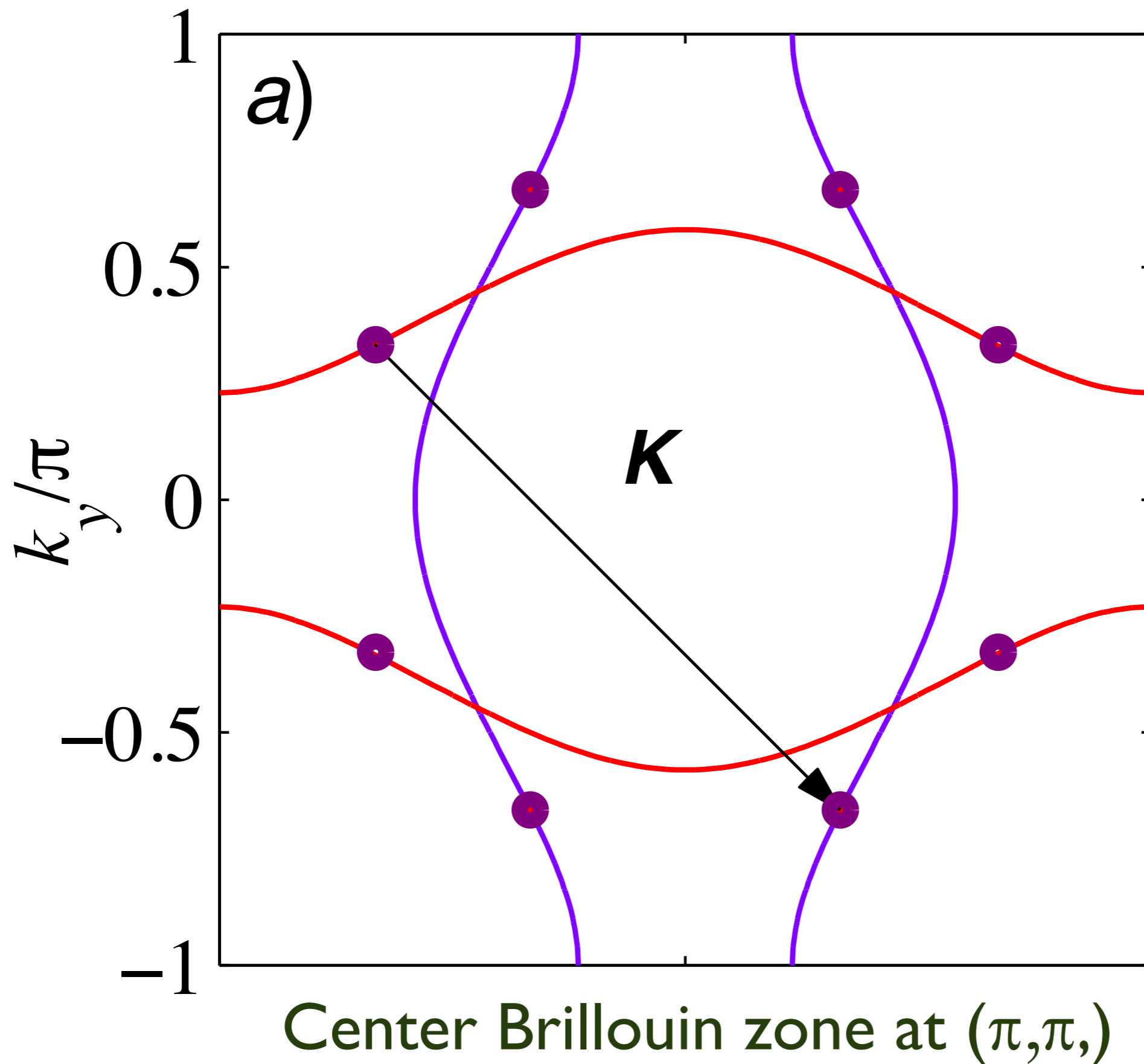


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Hot spots in a two band model

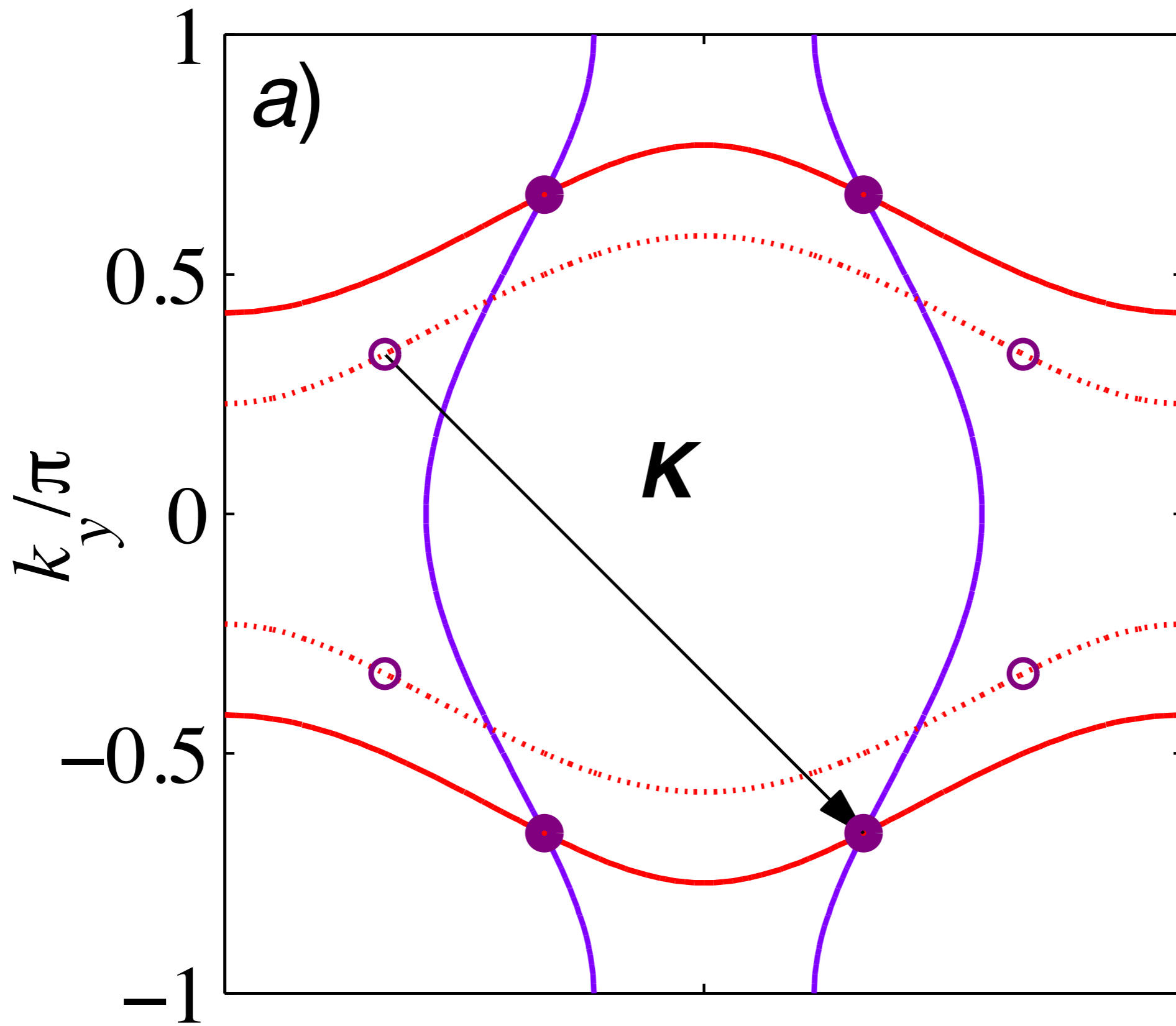
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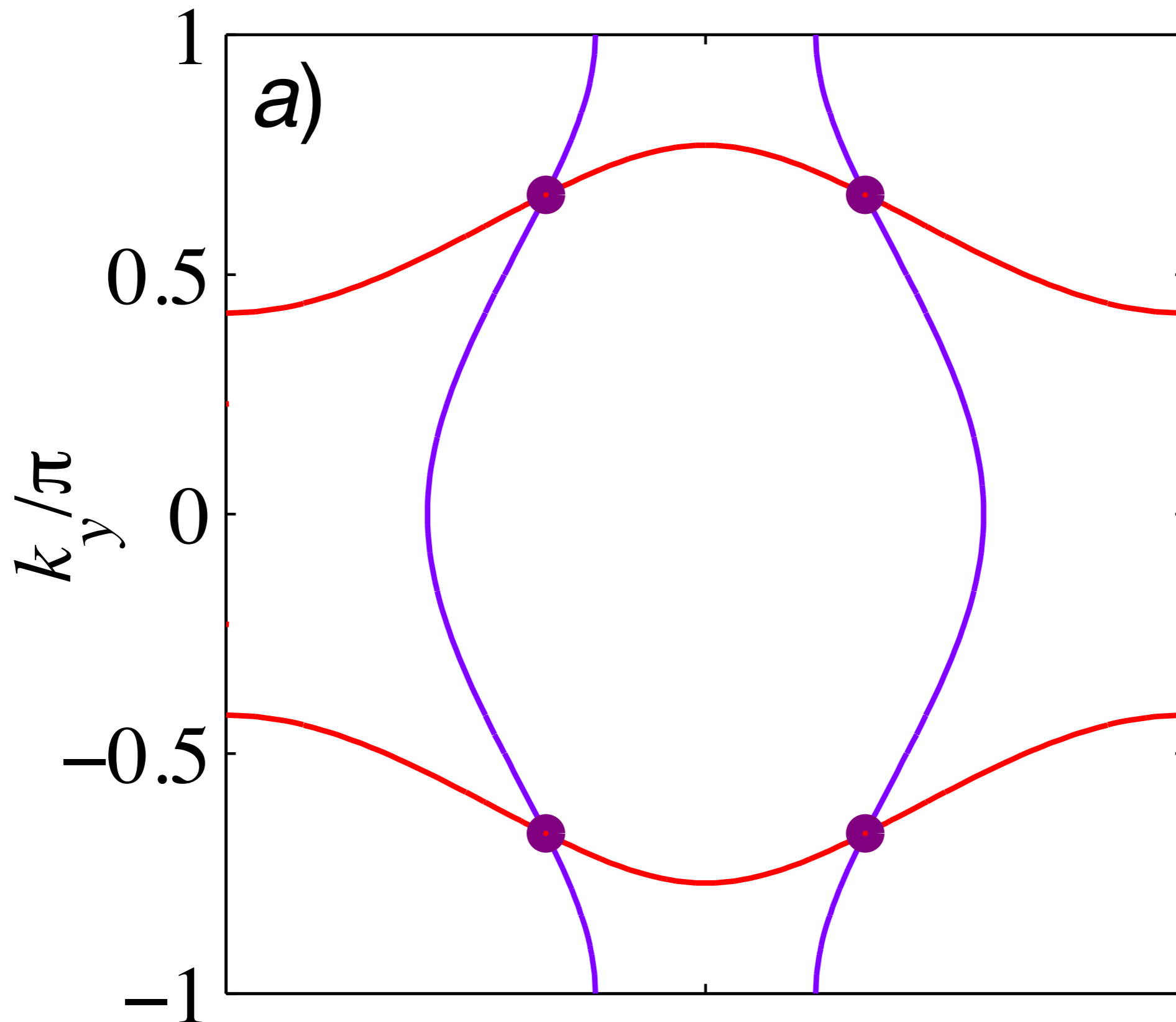
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Move one of the Fermi surface by (π, π)

QMC for the onset of antiferromagnetism

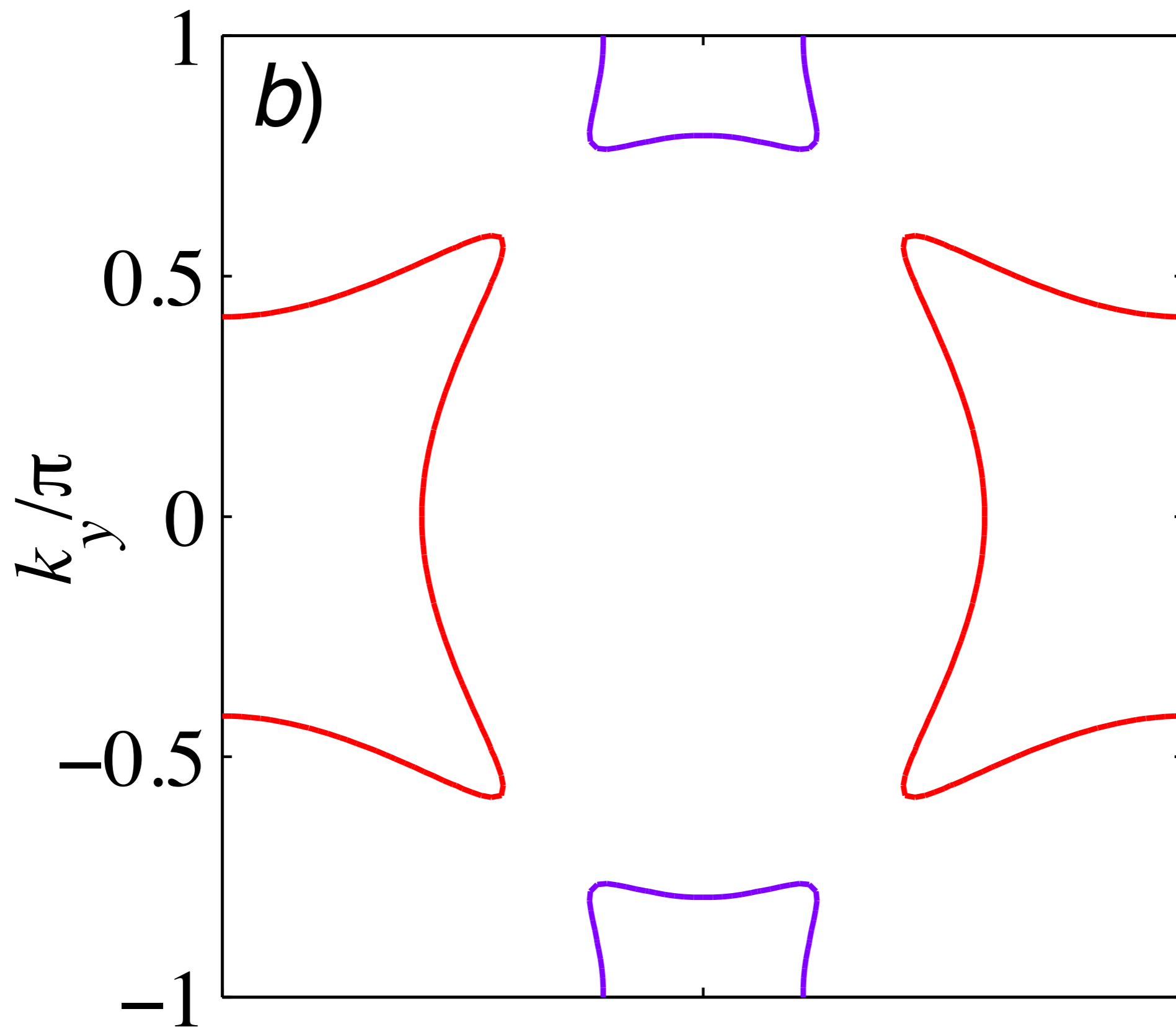
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arXiv:1206.0742



Now hot spots are at Fermi surface intersections

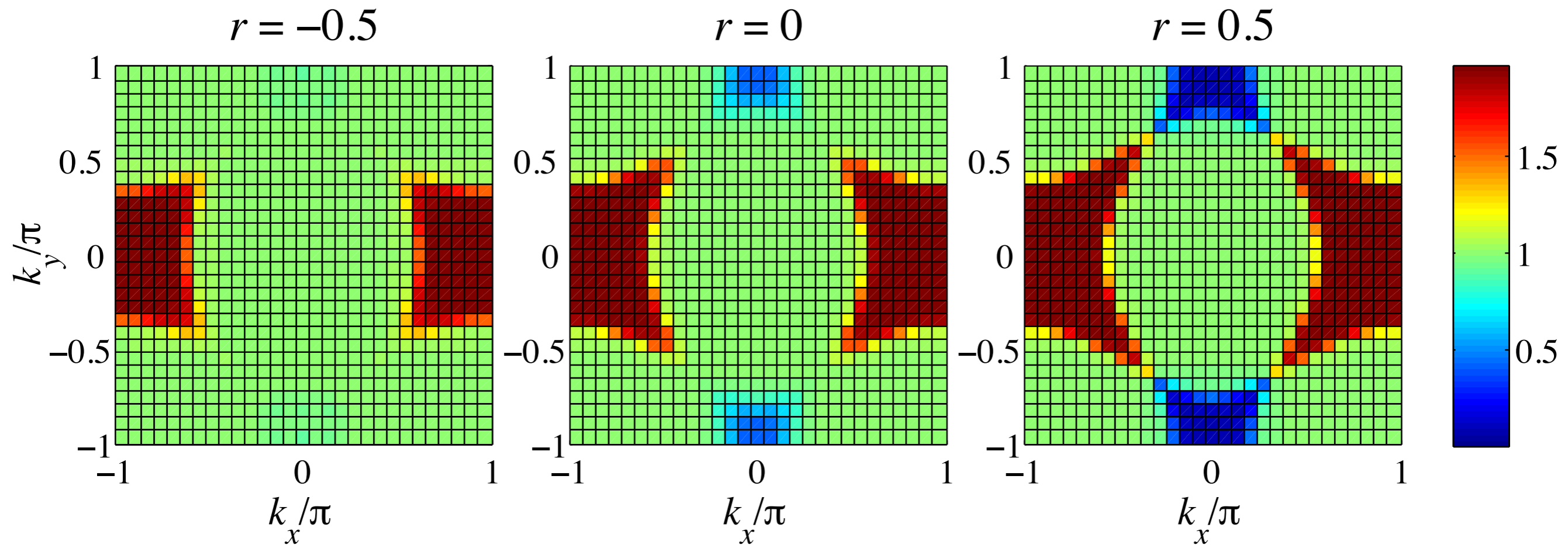
QMC for the onset of antiferromagnetism

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



Expected Fermi surfaces in the AFM ordered phase

QMC for the onset of antiferromagnetism

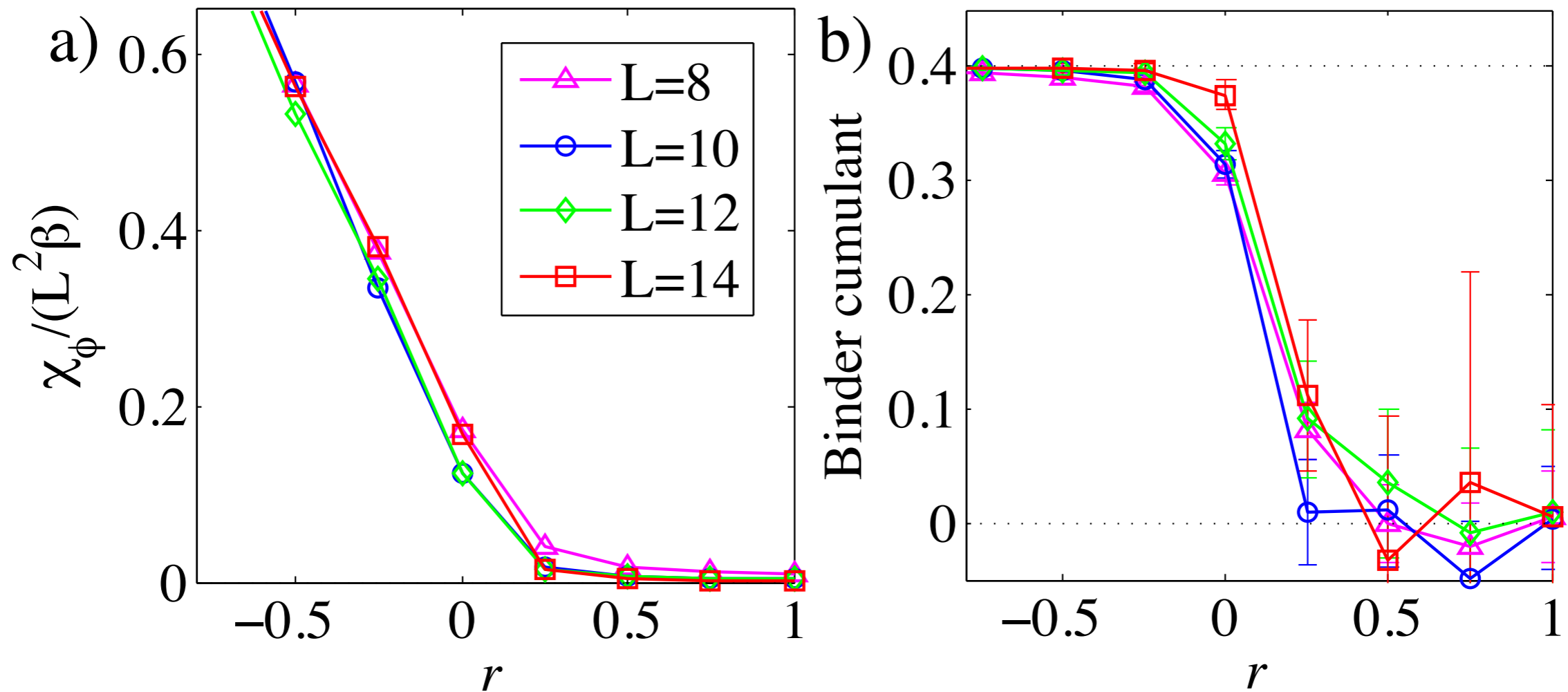


Electron occupation number $n_{\mathbf{k}}$
as a function of the tuning parameter r



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

QMC for the onset of antiferromagnetism

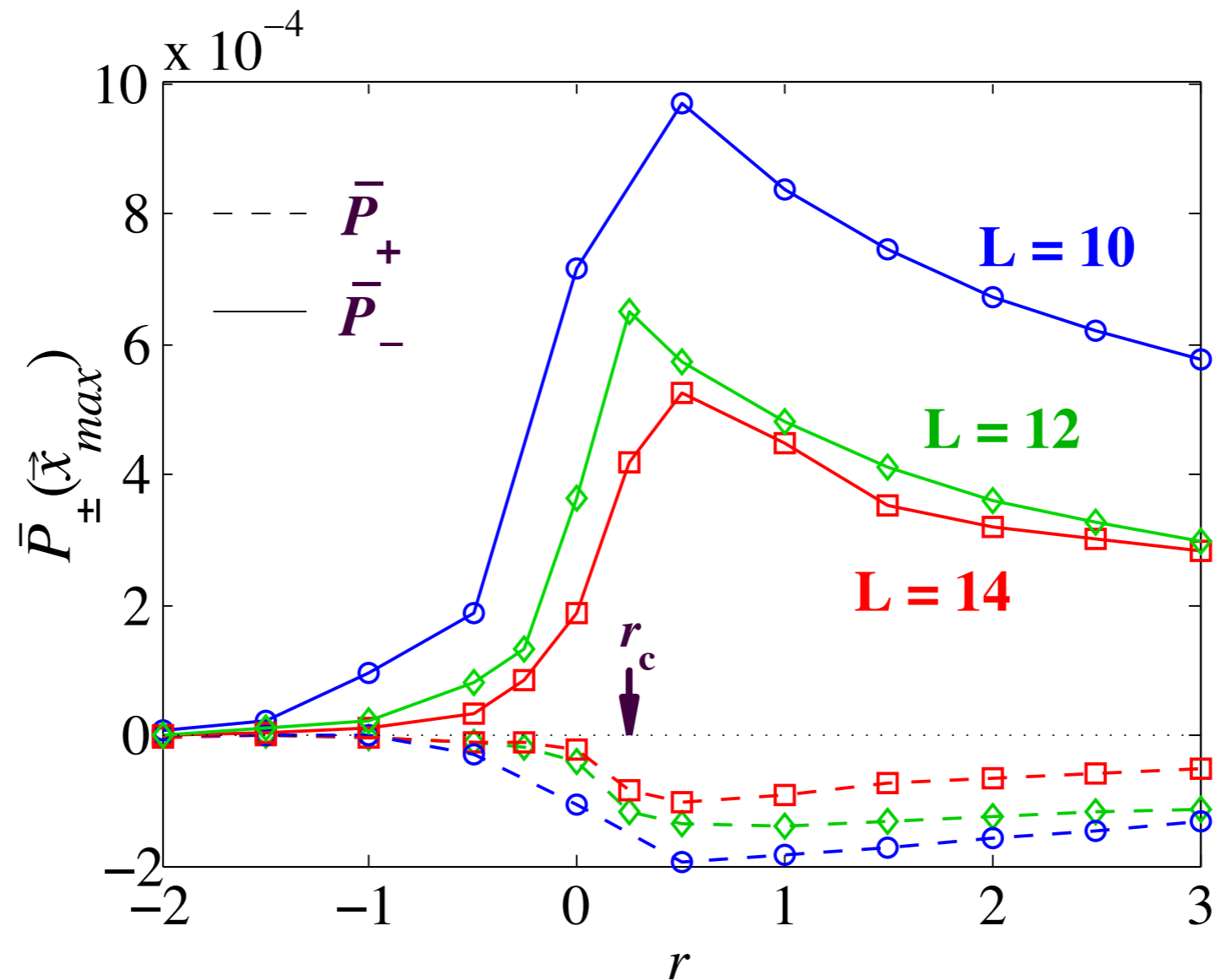


AF susceptibility, χ_ϕ , and Binder cumulant
as a function of the tuning parameter r



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

Outline

1. Weak coupling theory

2. Universal critical theory

3. Quantum Monte Carlo
without the sign problem

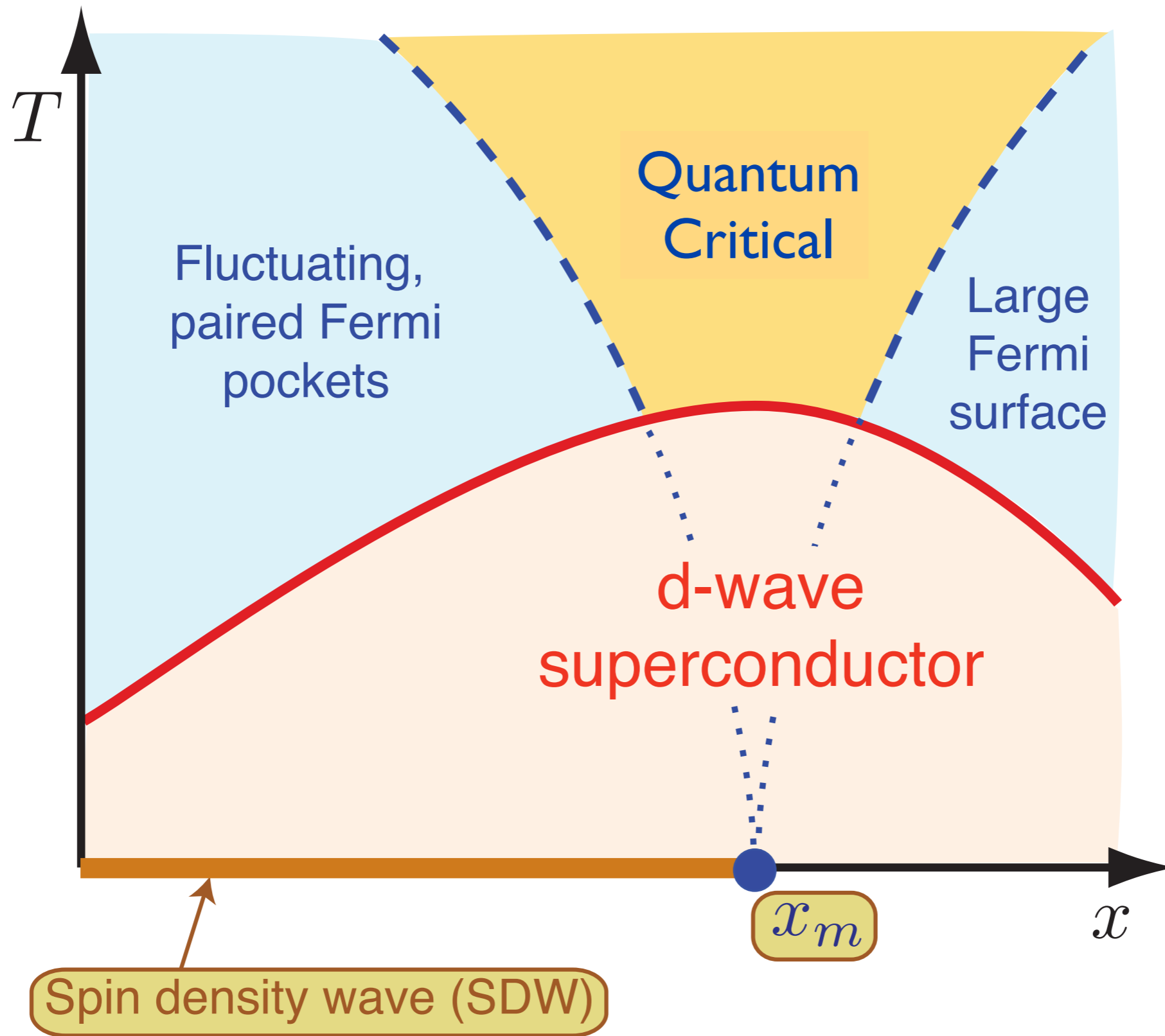
4. Features of strong coupling

Features of strong coupling

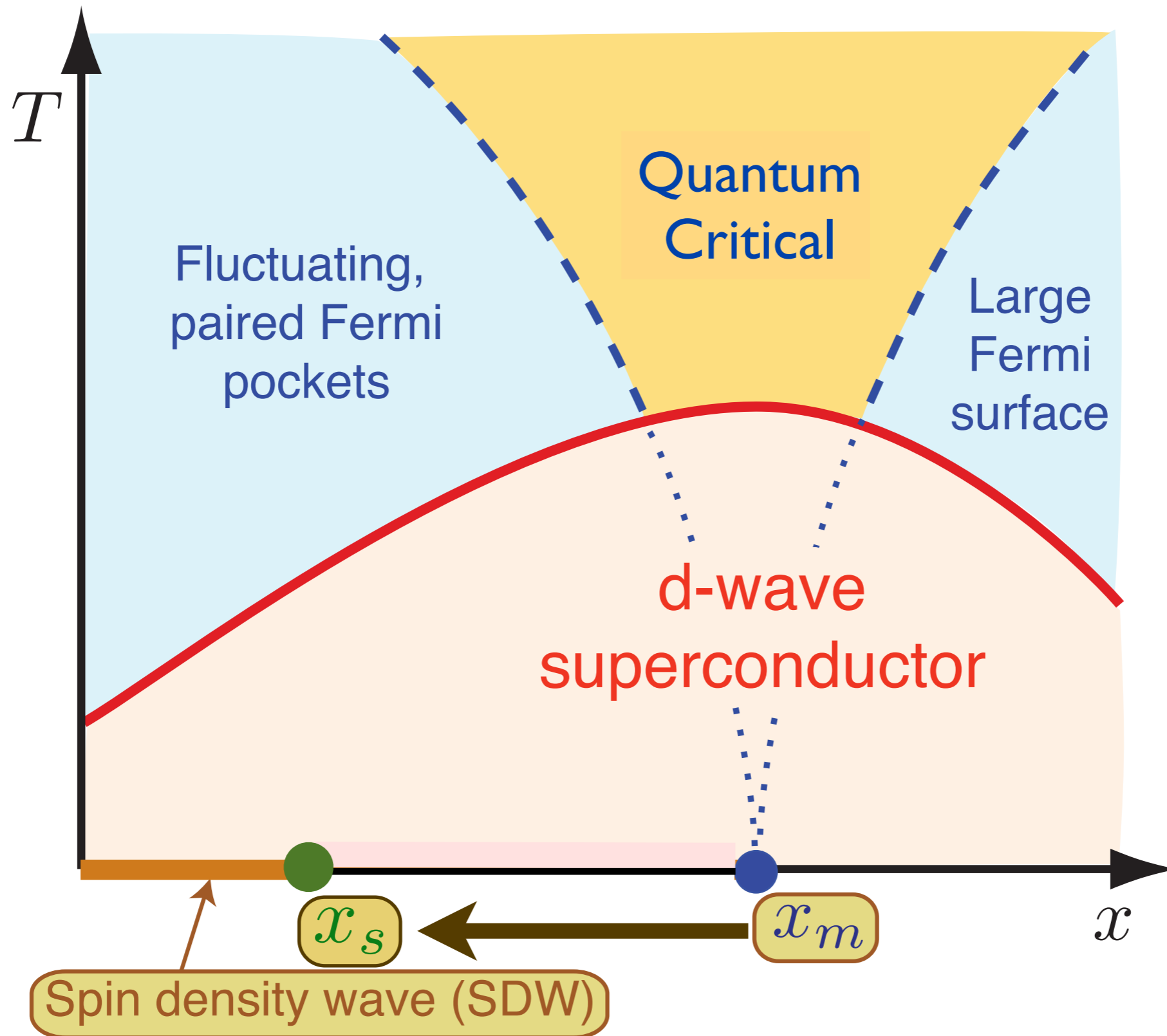
- Shift in QCP due to superconductivity: “backbending” of SDW order.
- Pairing instability is $(\log)^2$ with universal co-efficient.
- Leading subdominant instability is bond-modulated charge order.
- Intermediate “fractionalized Fermi liquid (FL*)” state with hole pockets and no broken symmetry.

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

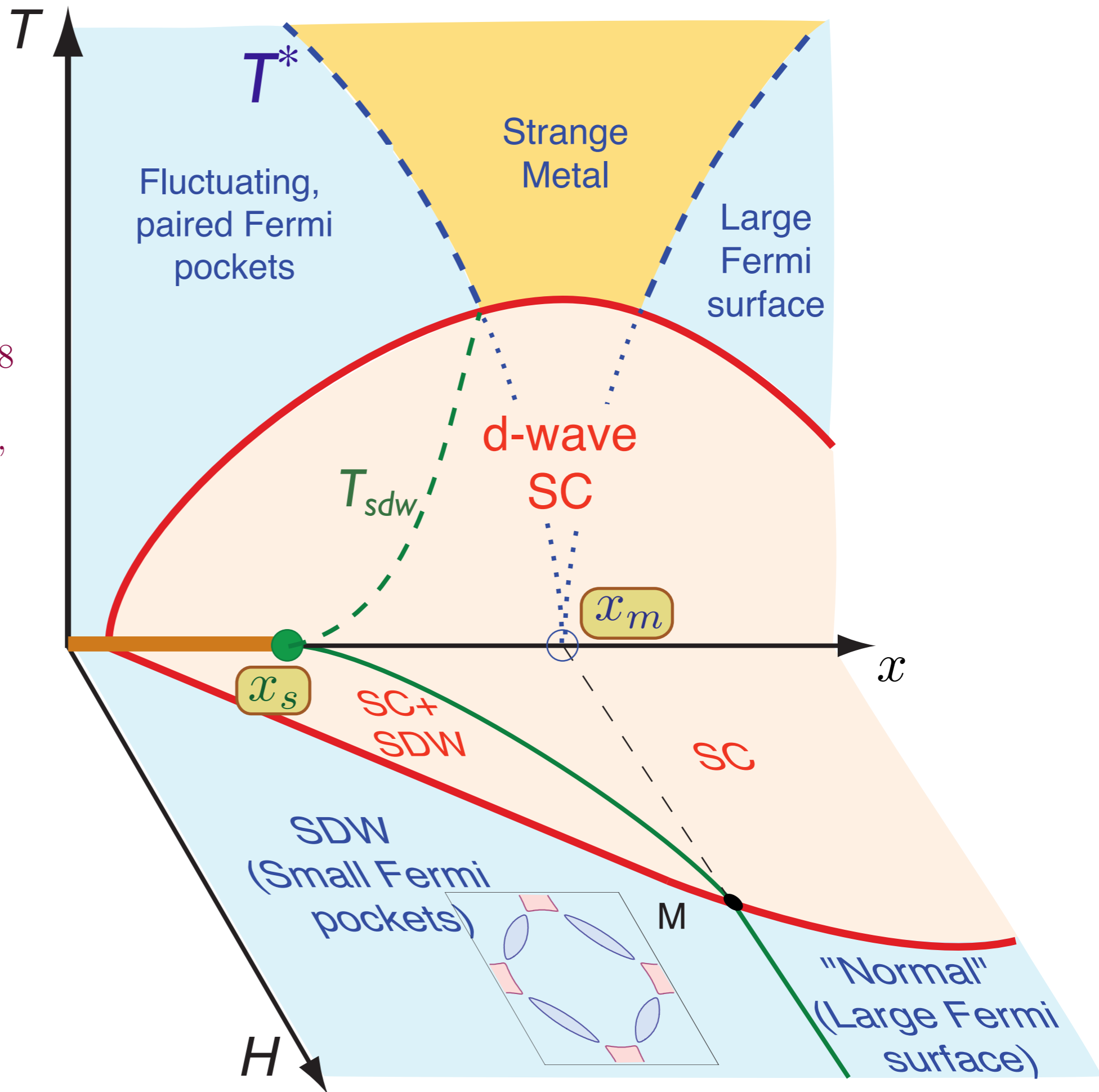


Competition between SDW order and superconductivity moves the actual quantum critical point to $x = x_s < x_m$.

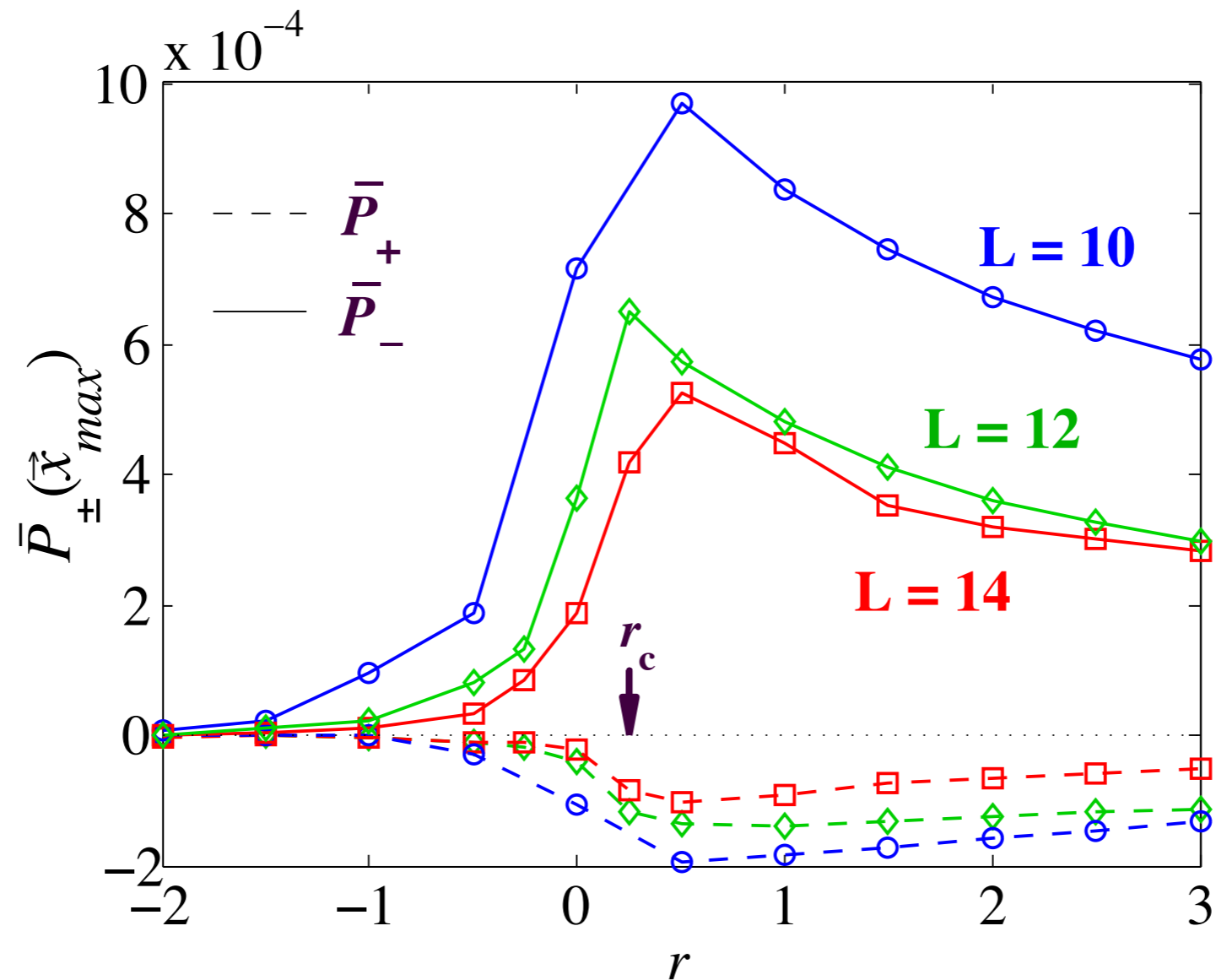
E. Demler, S. Sachdev
and Y. Zhang, *Phys.
Rev. Lett.* **87**,
067202 (2001).

S. Sachdev, arXiv:0907.0008

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



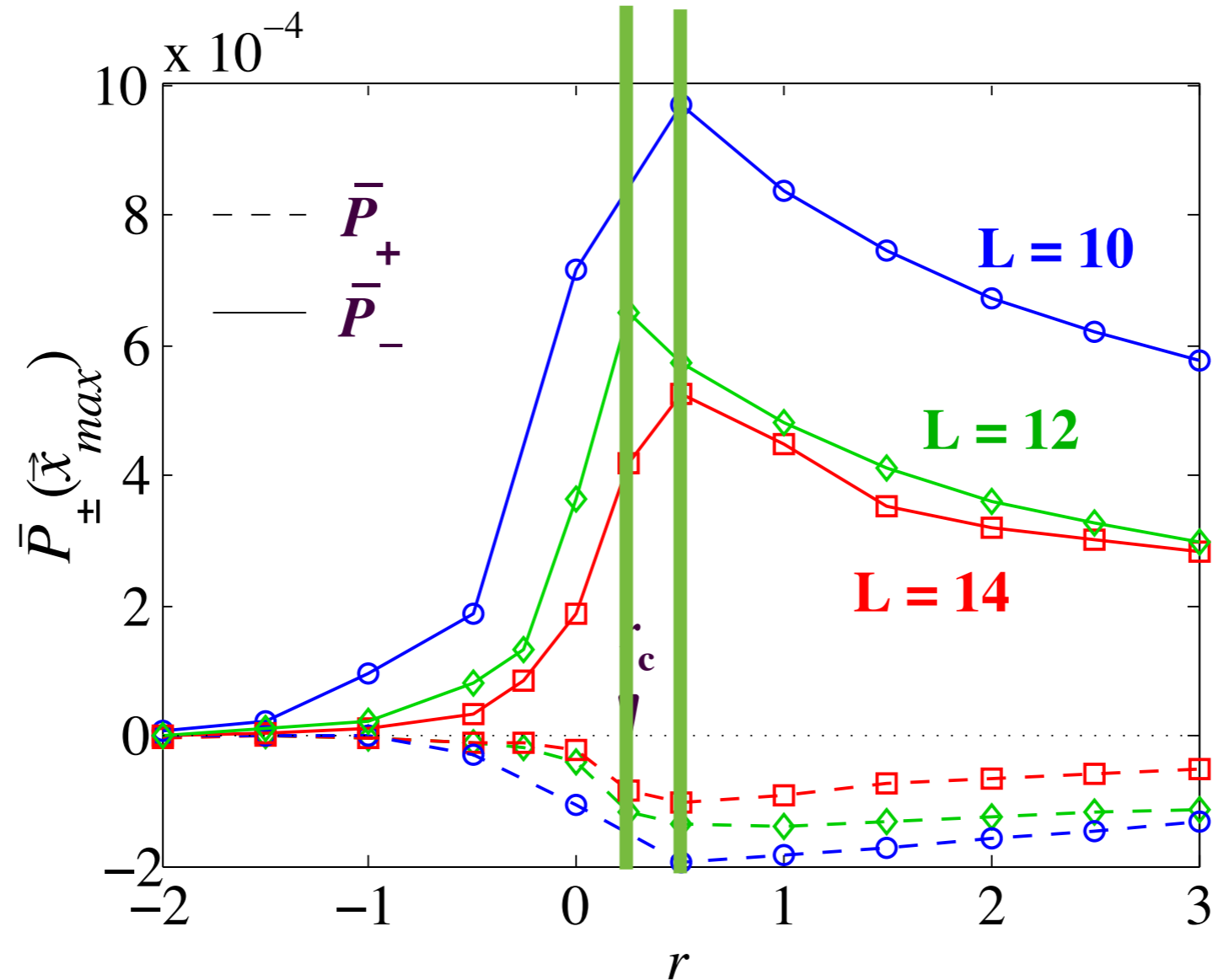
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s/d pairing amplitudes P_+/P_-
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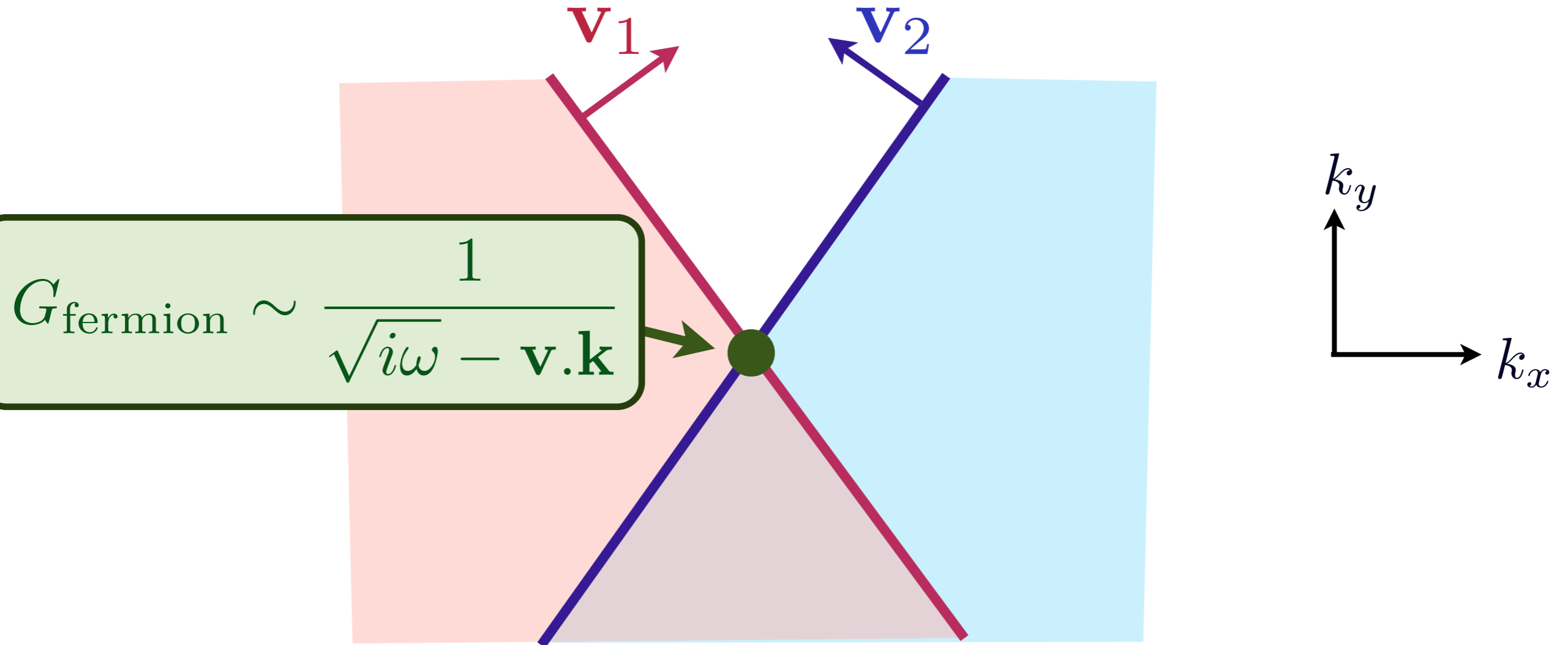
Notice shift between the position of the QCP in the superconductor, and the position of maximum pairing. This is found in numerous experiments.

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

Features of strong coupling

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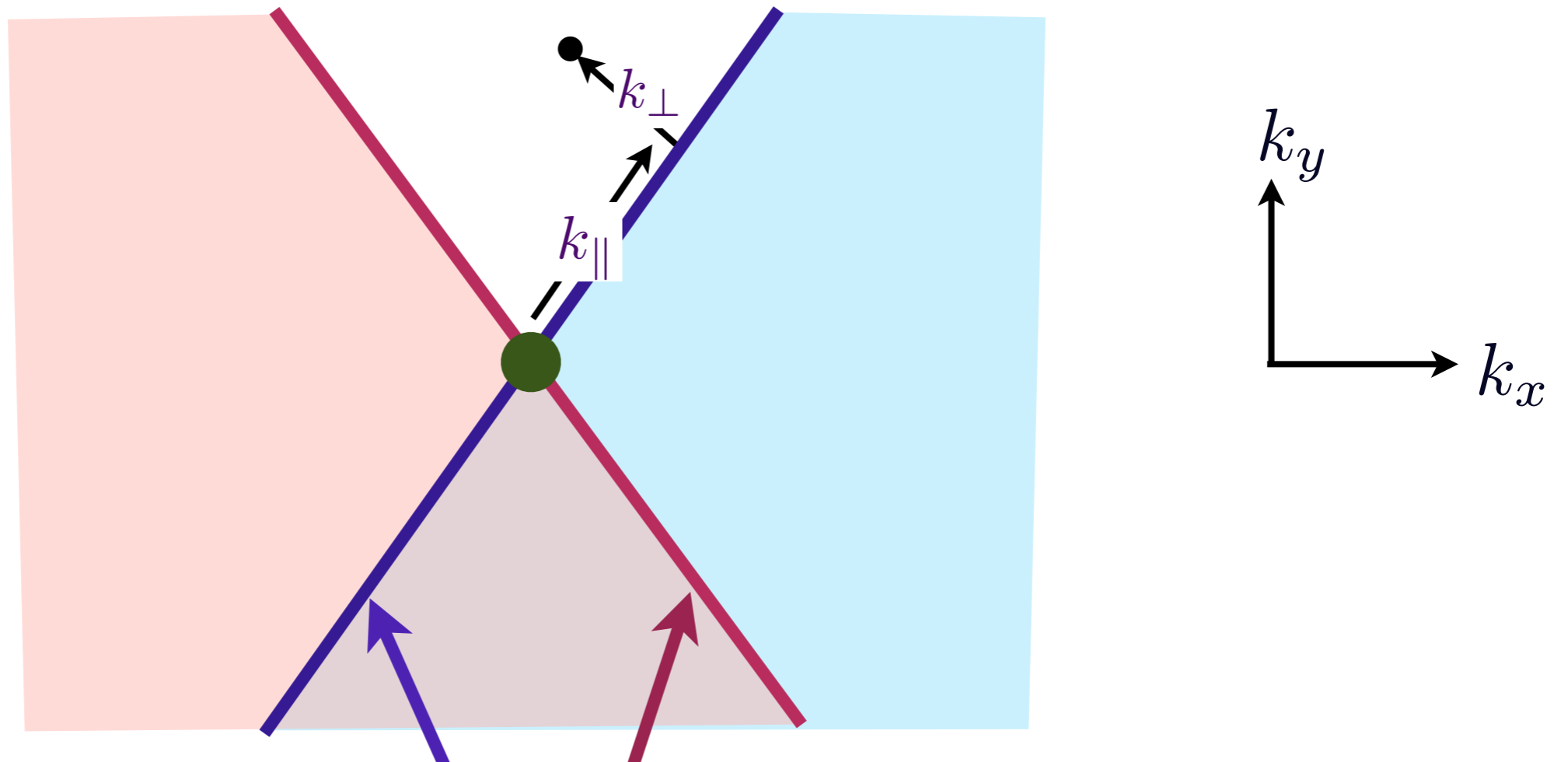
Two loop results: Non-Fermi liquid spectrum at hot spots



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)

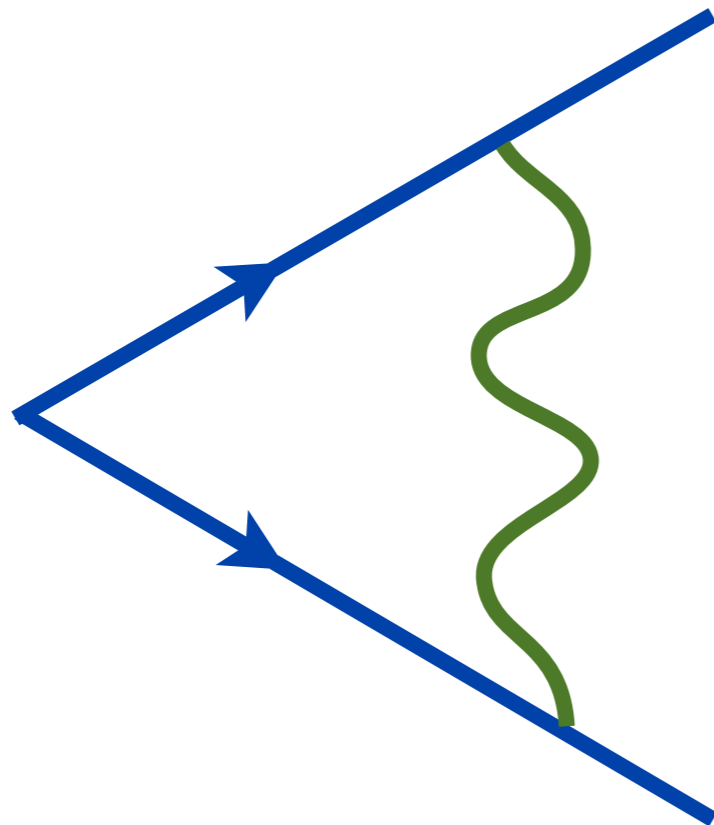
Pairing by SDW fluctuation exchange

Weak-coupling theory

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

Fermi energy

Density of states at Fermi energy



Pairing by SDW fluctuation exchange

Antiferromagnetic critical point

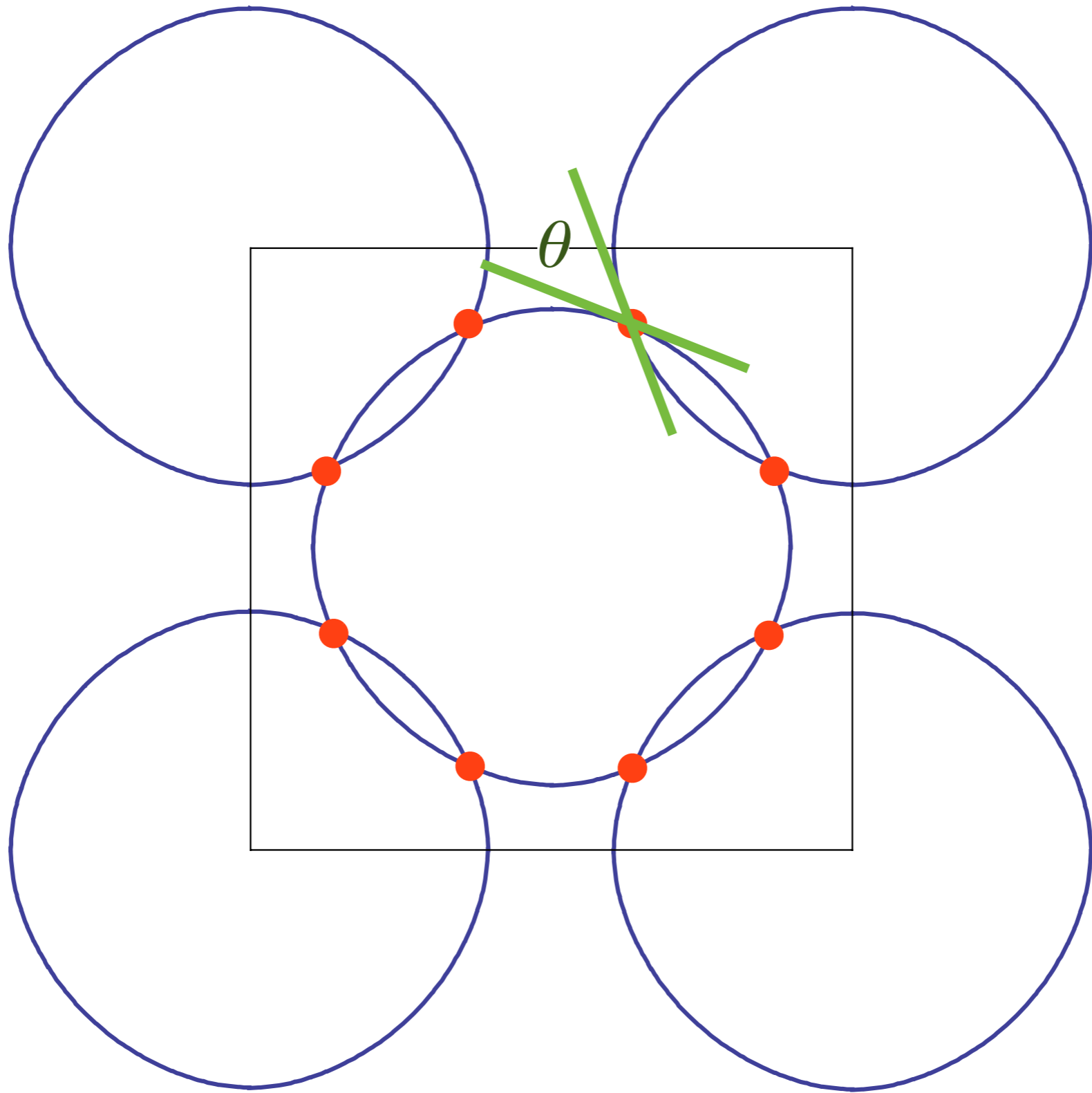
Fermi
energy

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



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)



Pairing by SDW fluctuation exchange

Antiferromagnetic critical point

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



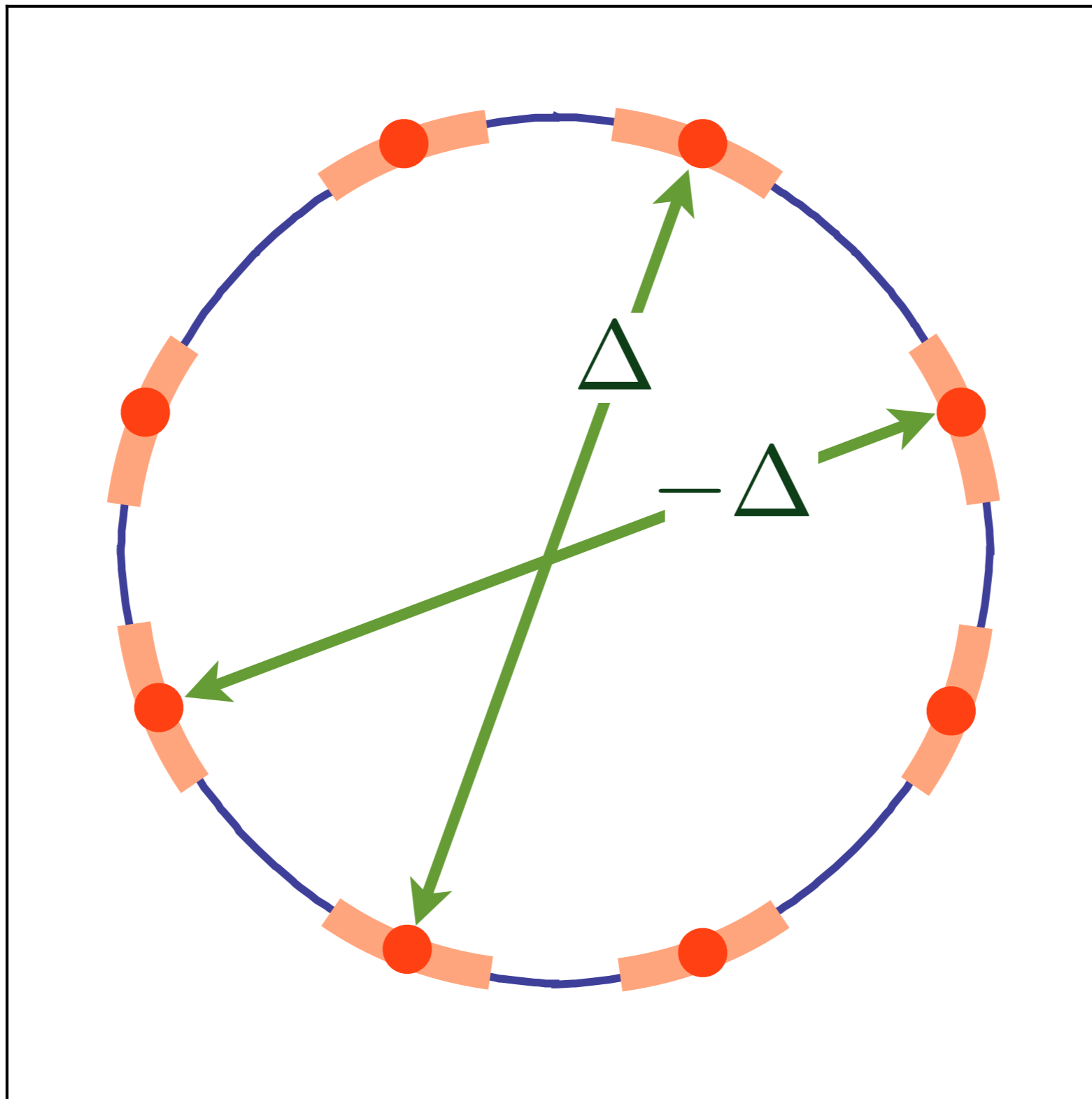
- **Universal** \log^2 singularity arises from Fermi lines; singularity *at* hot spots is weaker.
- Interference between BCS and quantum-critical logs.
- Momentum dependence of self-energy is crucial.
- Not suppressed by $1/N$ factor in $1/N$ expansion.

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

Features of strong coupling

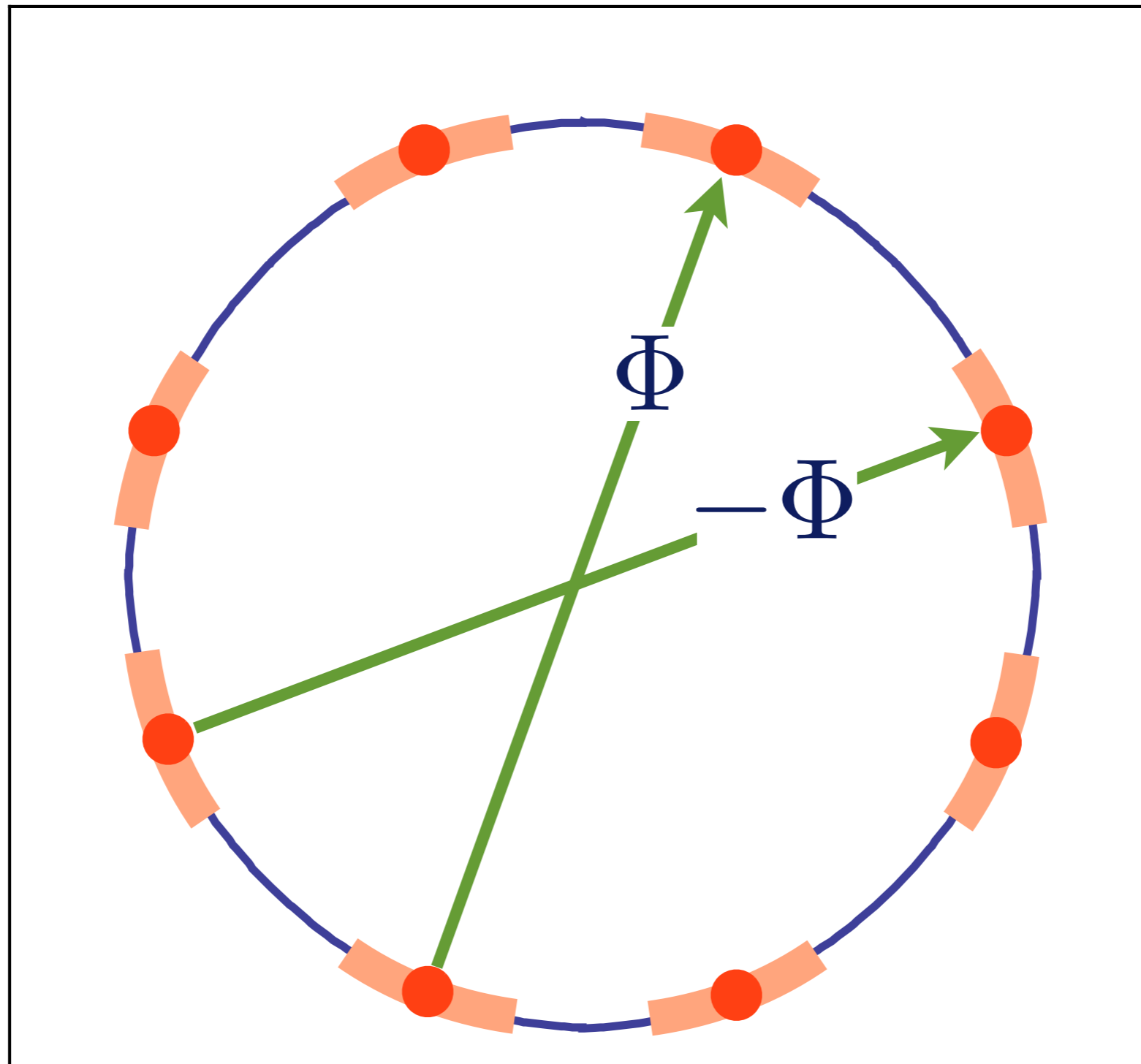
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$$\langle c_{\mathbf{k}\alpha}^\dagger c_{-\mathbf{k}\beta}^\dagger \rangle = \varepsilon_{\alpha\beta} \Delta (\cos k_x - \cos k_y)$$



Log-squared instability to d-wave pairing

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

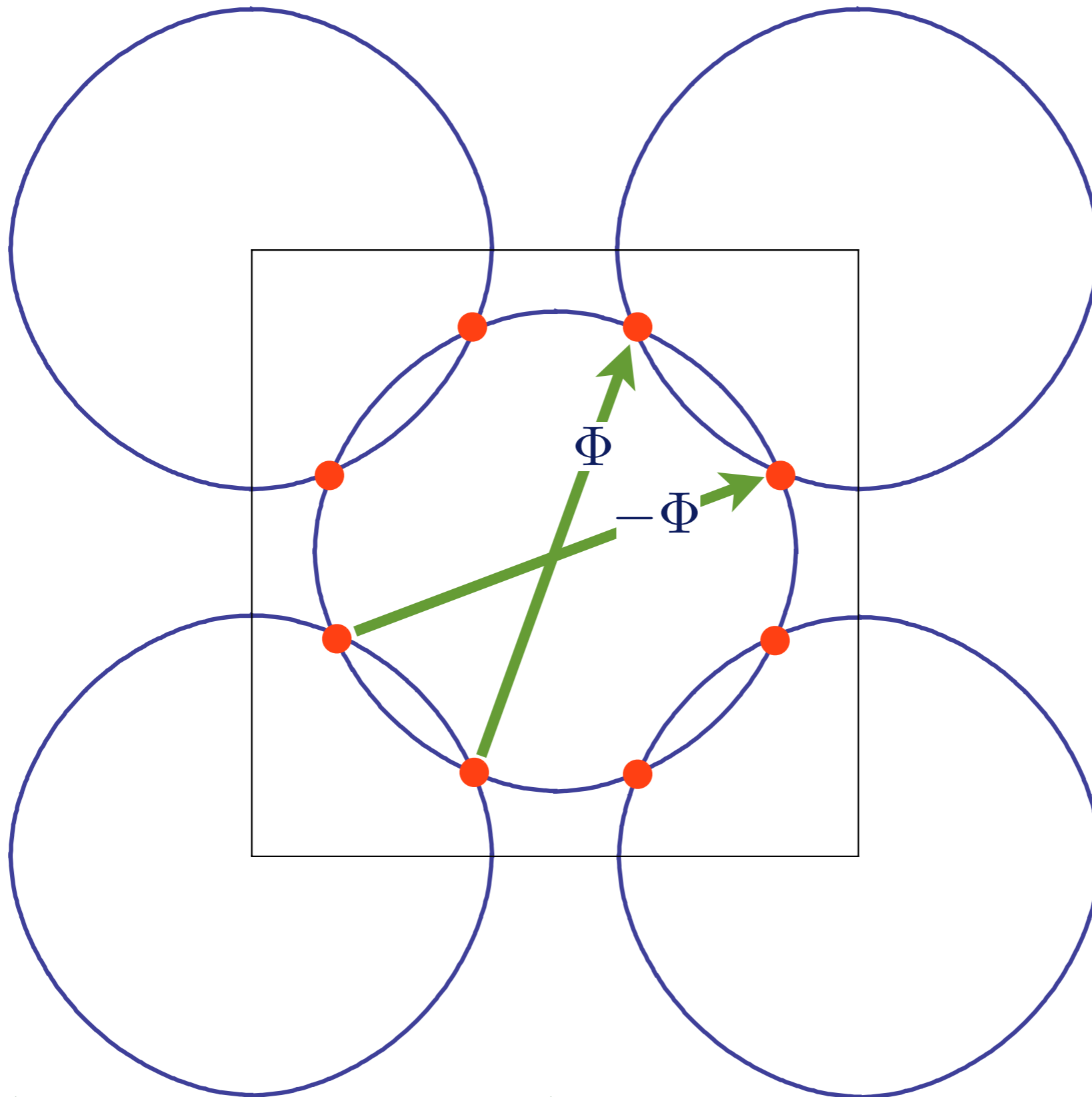


\mathbf{Q} is ' $2k_F$ '
wavevector

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

Bond-modulated charge order

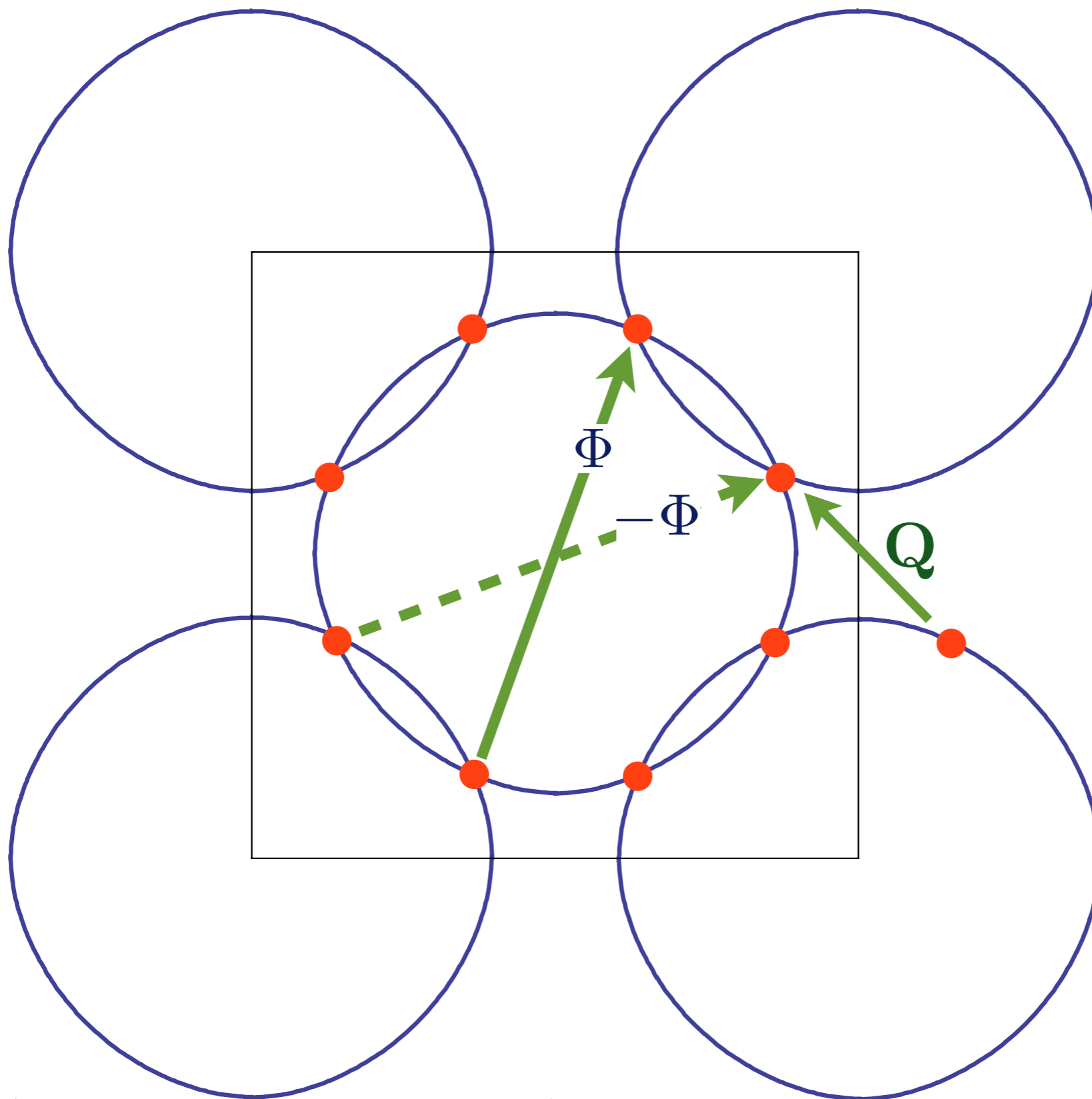
M.A. Metlitski and S. Sachdev,
Phys. Rev. B **82**, 075128 (2010)



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

Bond-modulated charge order

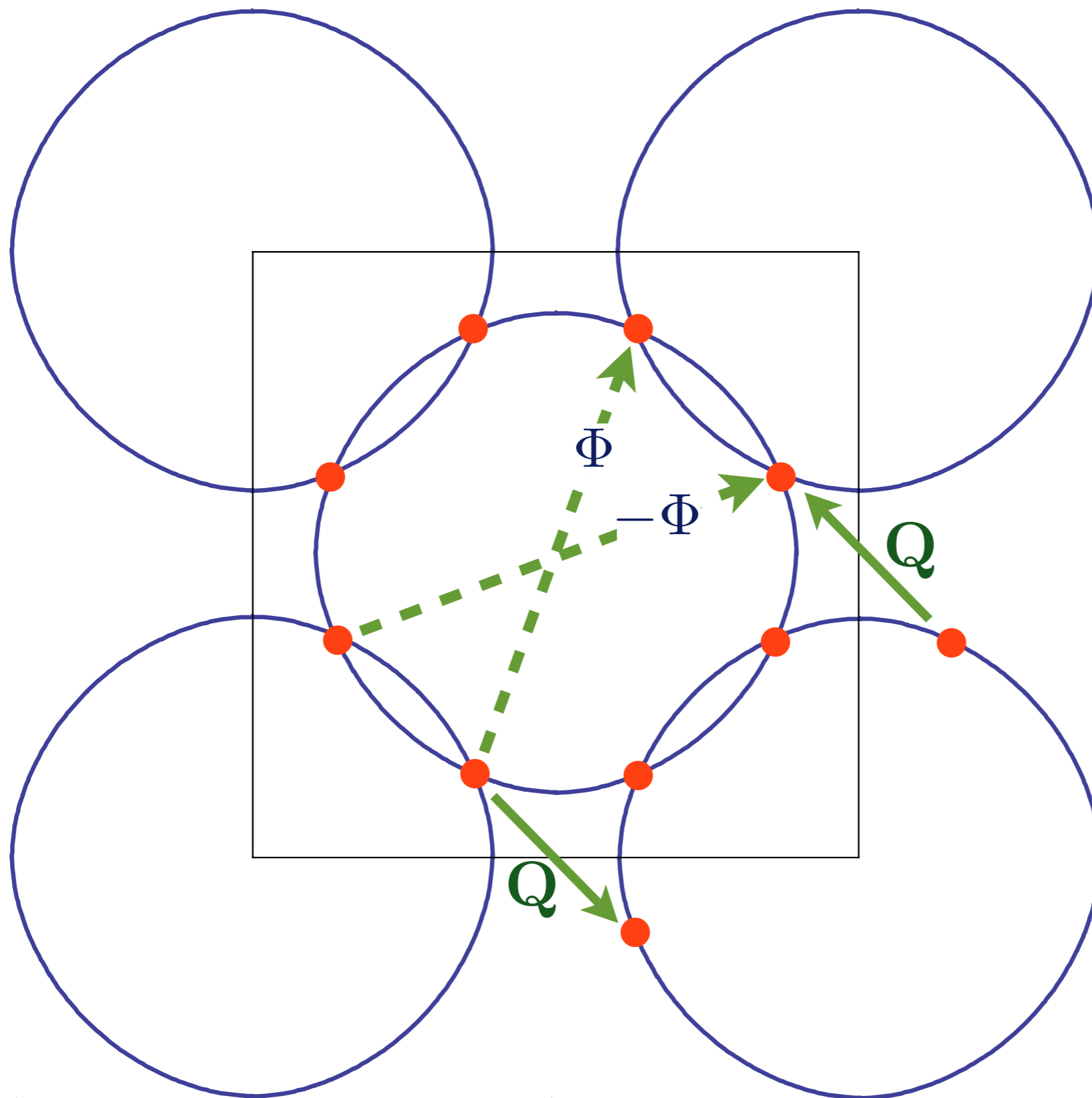
M.A. Metlitski and S. Sachdev,
Phys. Rev. B **82**, 075128 (2010)



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

Bond-modulated charge order

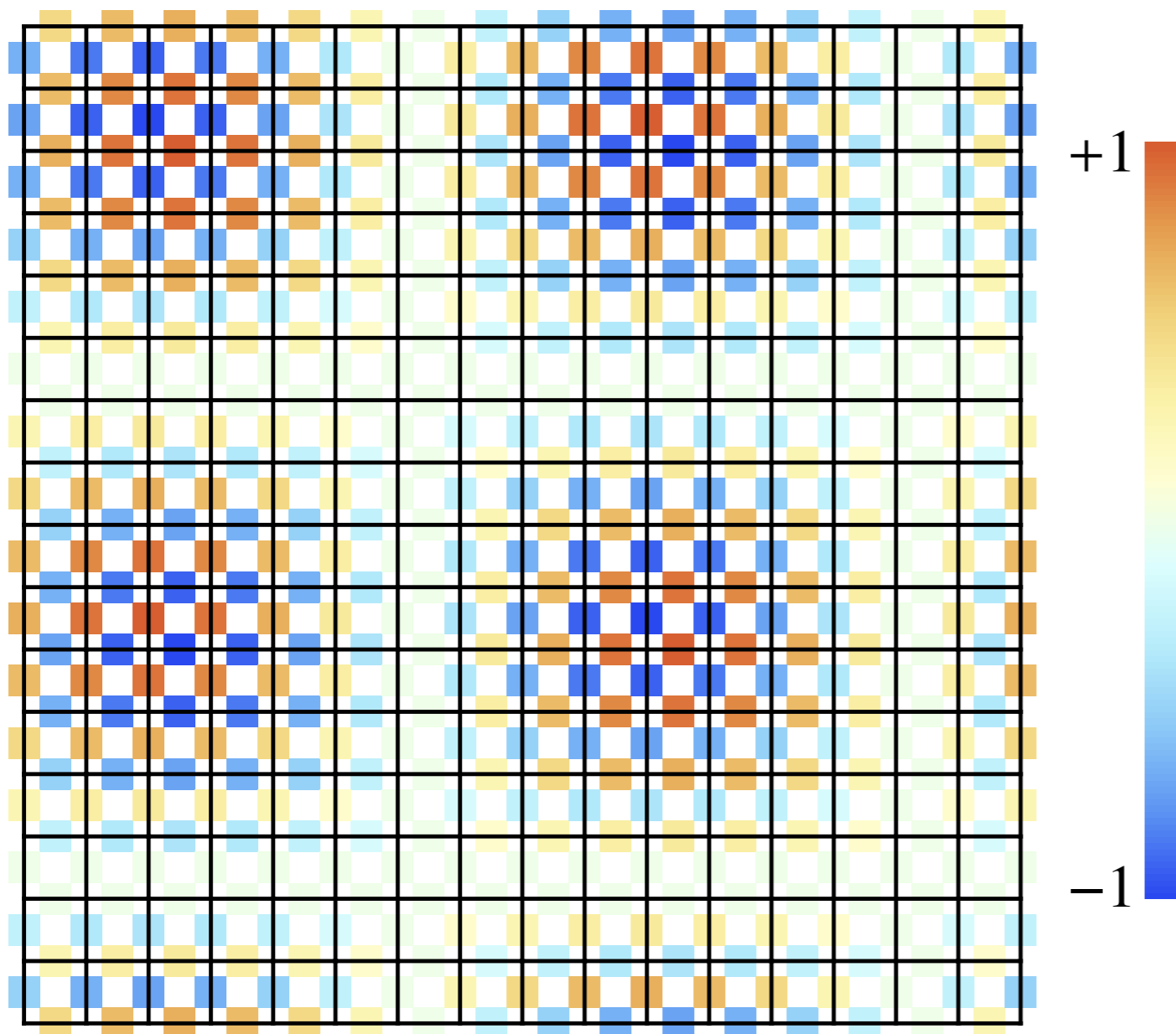
M.A. Metlitski and S. Sachdev,
Phys. Rev. B **82**, 075128 (2010)



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

Bond-modulated charge order

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



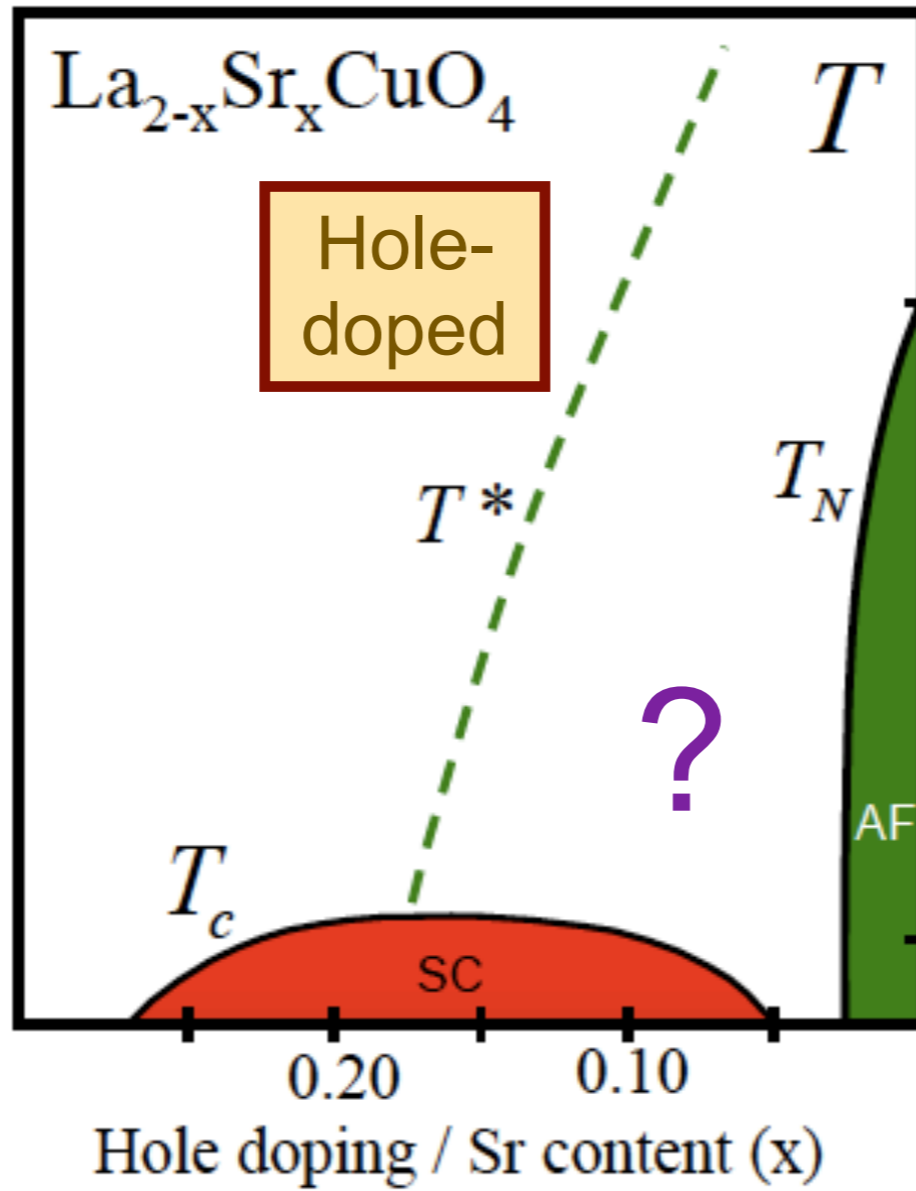
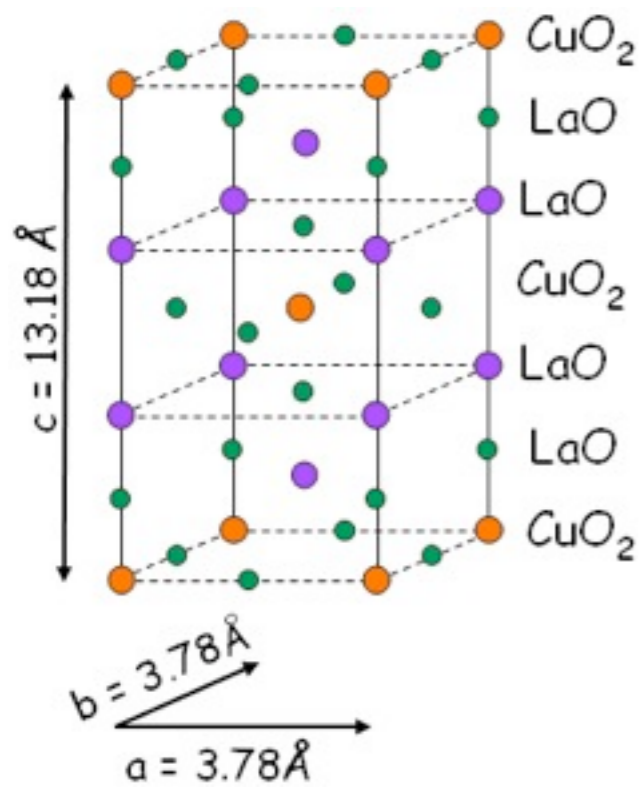
“Bond density”
measures amplitude
for electrons to be
in spin-singlet
valence bond.

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

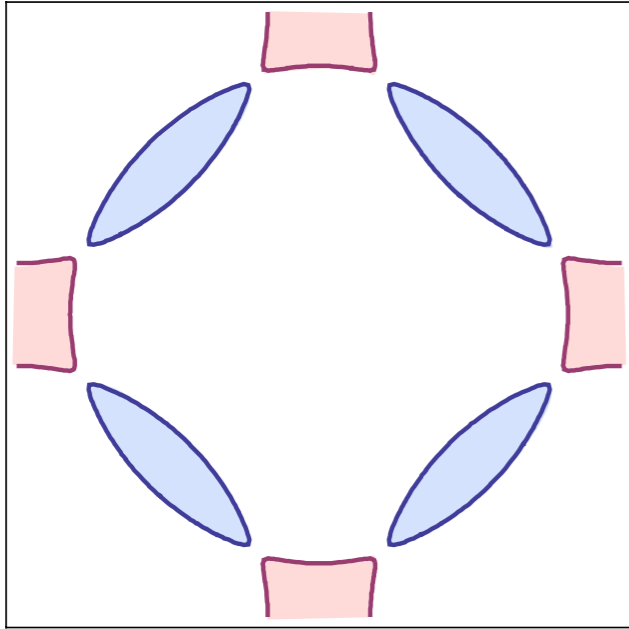
$$\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \rangle = \Phi(\cos k_x - \cos k_y)$$

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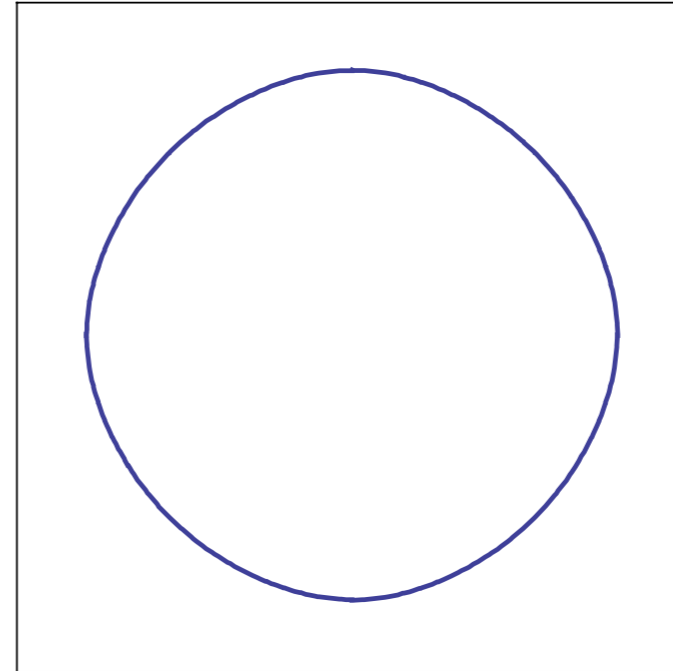


Quantum phase transition with Fermi surface reconstruction



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

Metal with electron
and hole pockets

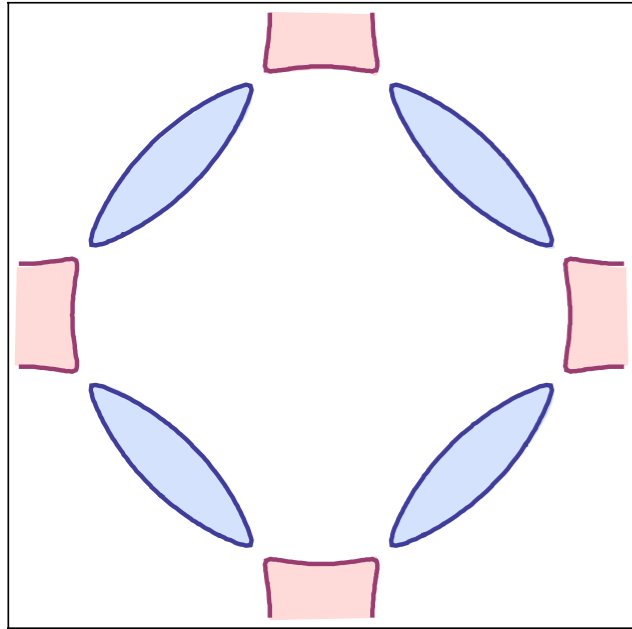


$$\langle \vec{\varphi} \rangle = 0$$

Metal with "large"
Fermi surface

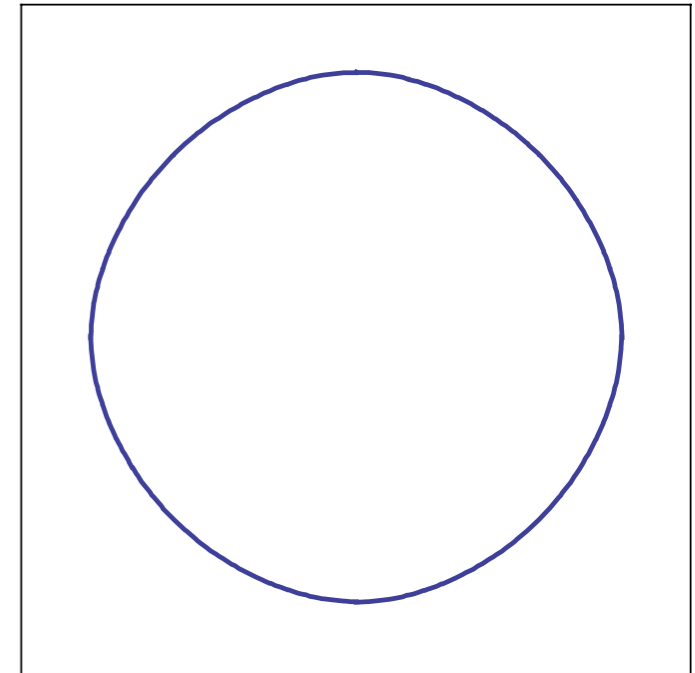


Separating onset of SDW order and Fermi surface reconstruction



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

Metal with electron
and hole pockets

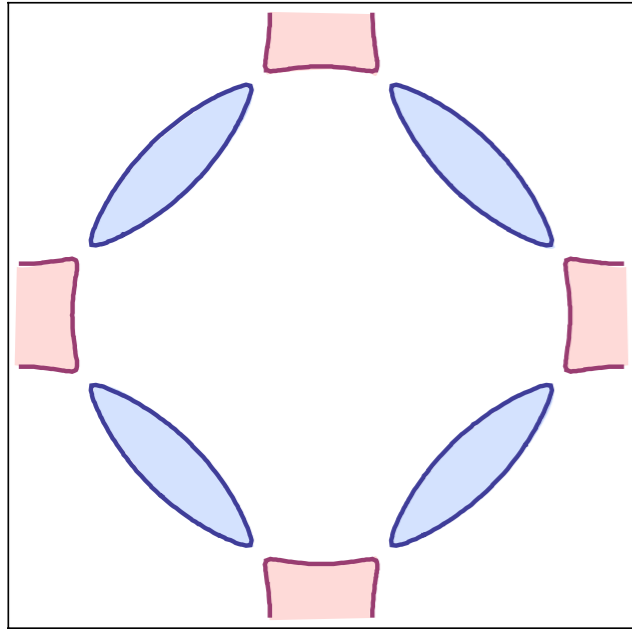


$$\langle \vec{\varphi} \rangle = 0$$

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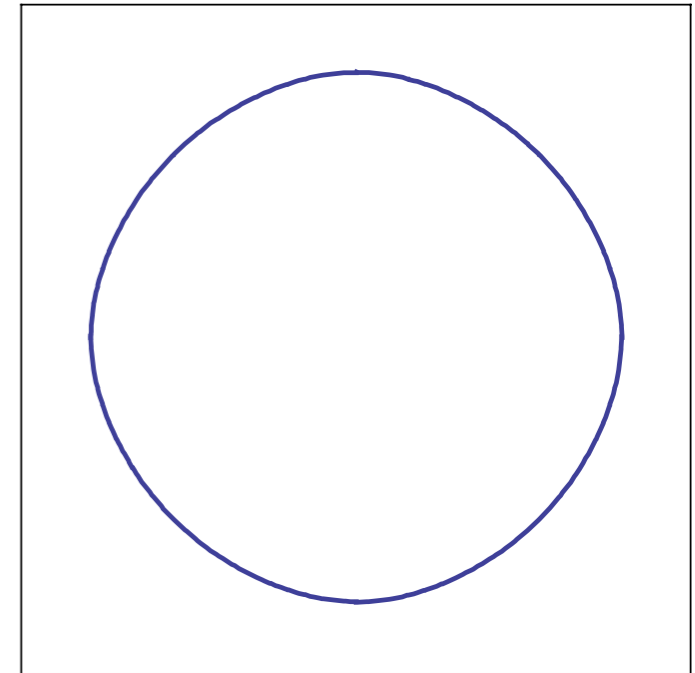
$$\langle \vec{\varphi} \rangle \neq 0$$

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

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

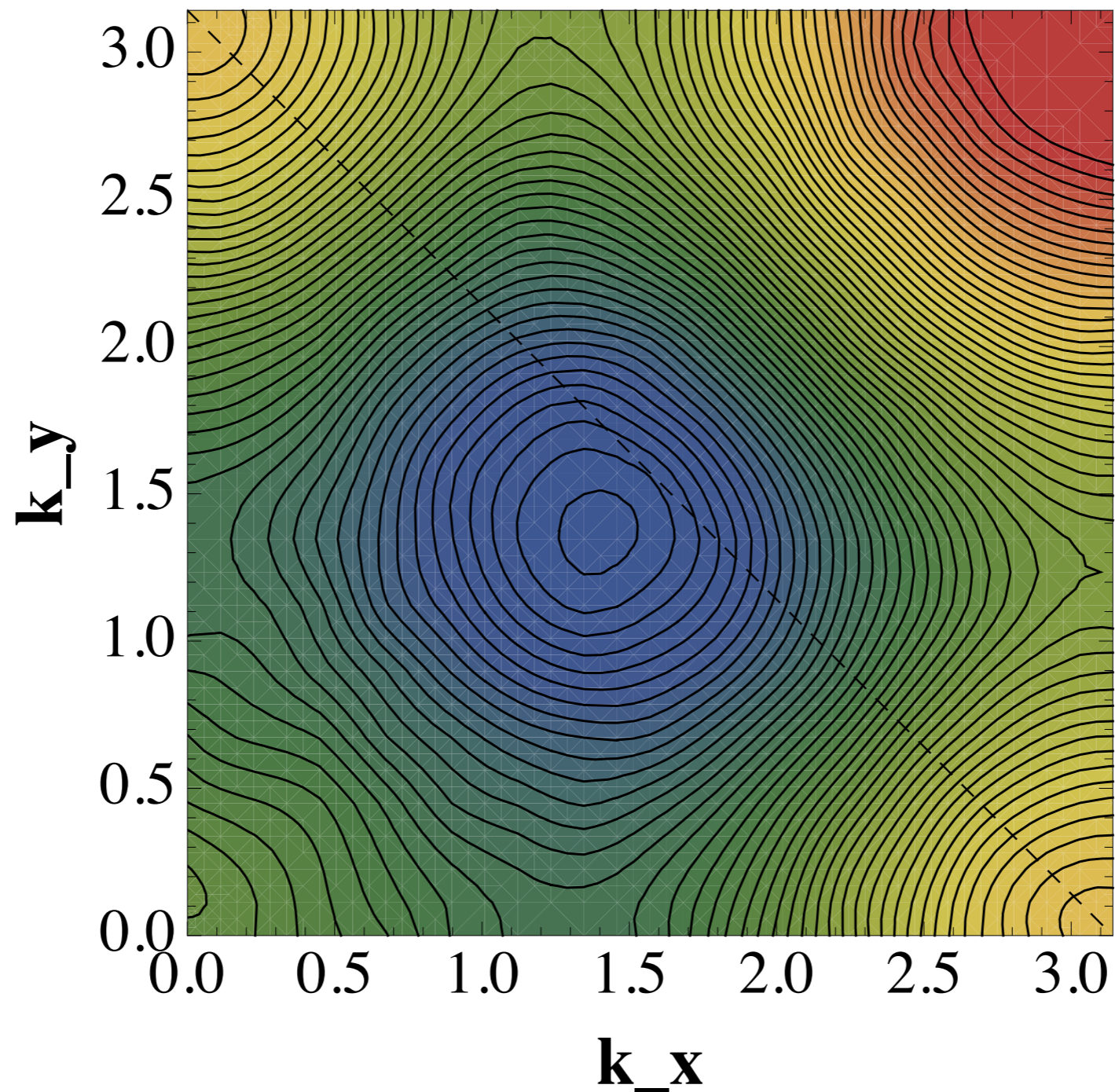
Fractionalized Fermi
liquid (FL*) phase
with no symmetry
breaking and “small”
Fermi surface



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

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)

Characteristics of FL* phase

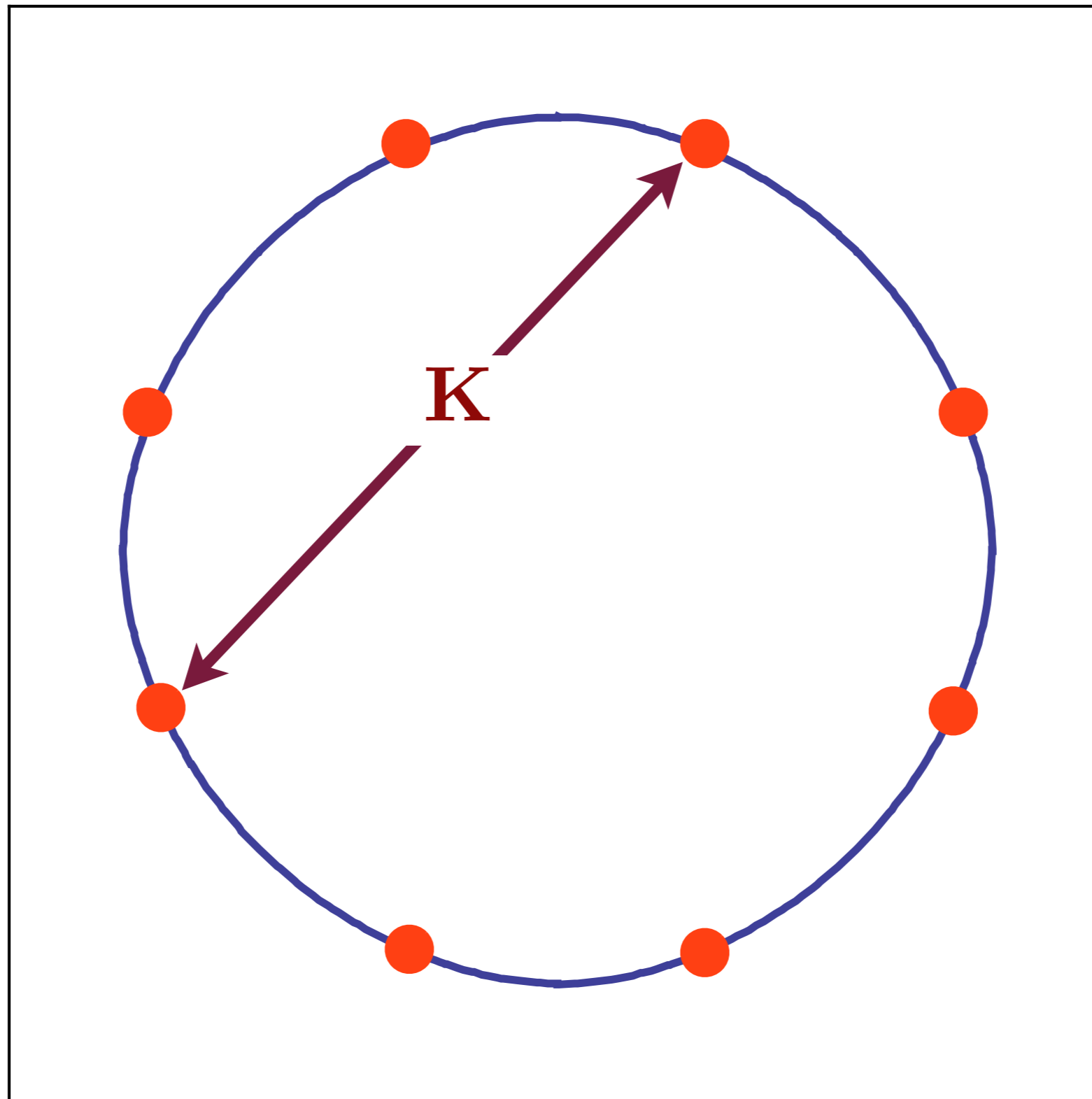
- Fermi surface volume does not count all electrons.
- Such a phase *must* have neutral $S = 1/2$ excitations (“spinons”), and collective spinless gauge excitations (“topological” order).
- These topological excitations are needed to account for the deficit in the Fermi surface volume, in M. Oshikawa’s proof of the Luttinger theorem.

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

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without the sign problem
4. Features of strong coupling

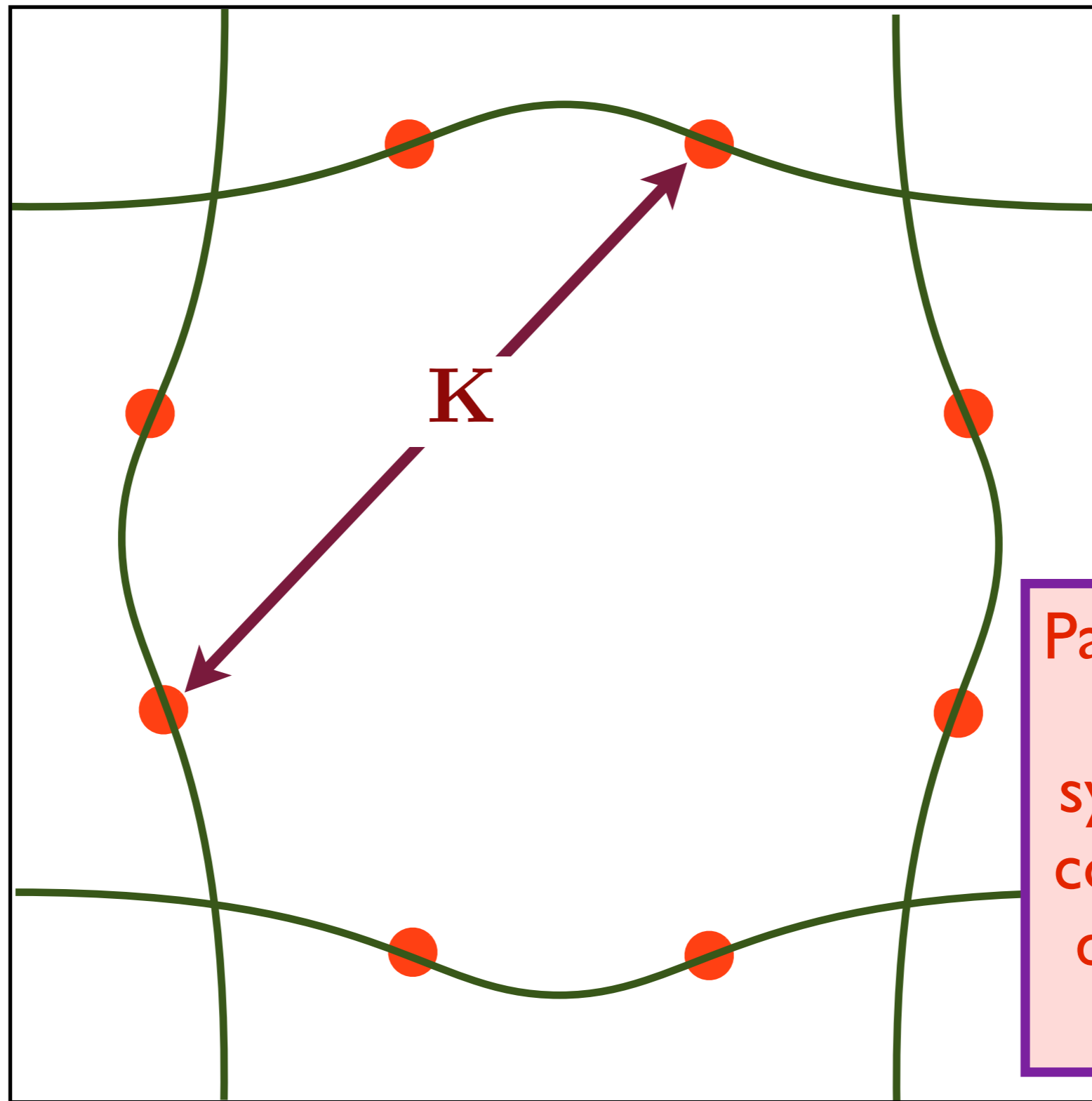
QMC for the onset of antiferromagnetism



Hot spots in a single band model

QMC for the onset of antiferromagnetism

Faithful realization of low energy theory. Sign problem is absent as long as K connects hotspots in distinct bands



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

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

Hot spots in a two band model