The onset of antiferromagnetism in metals: field theory, and Quantum Monte Carlo without the sign problem

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Max Metlitski

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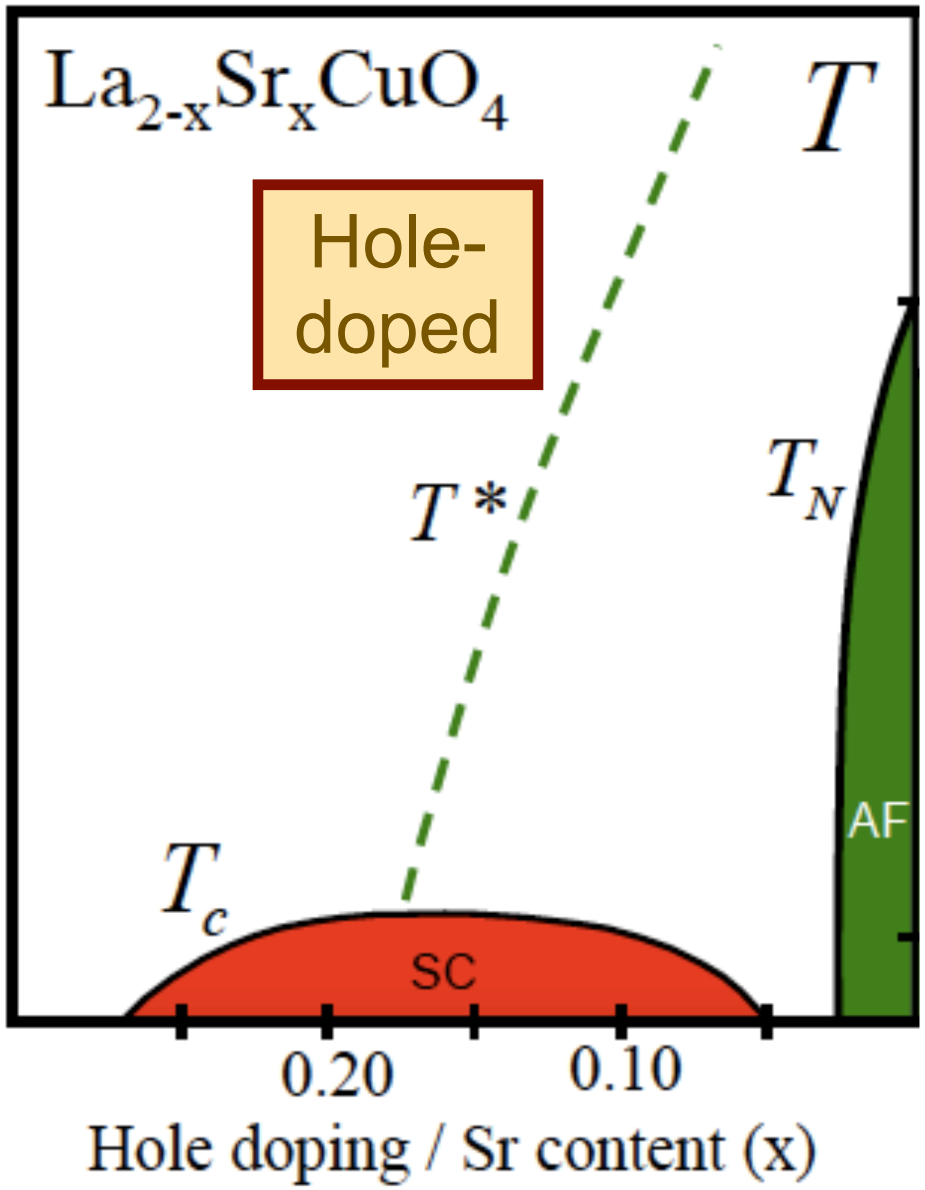
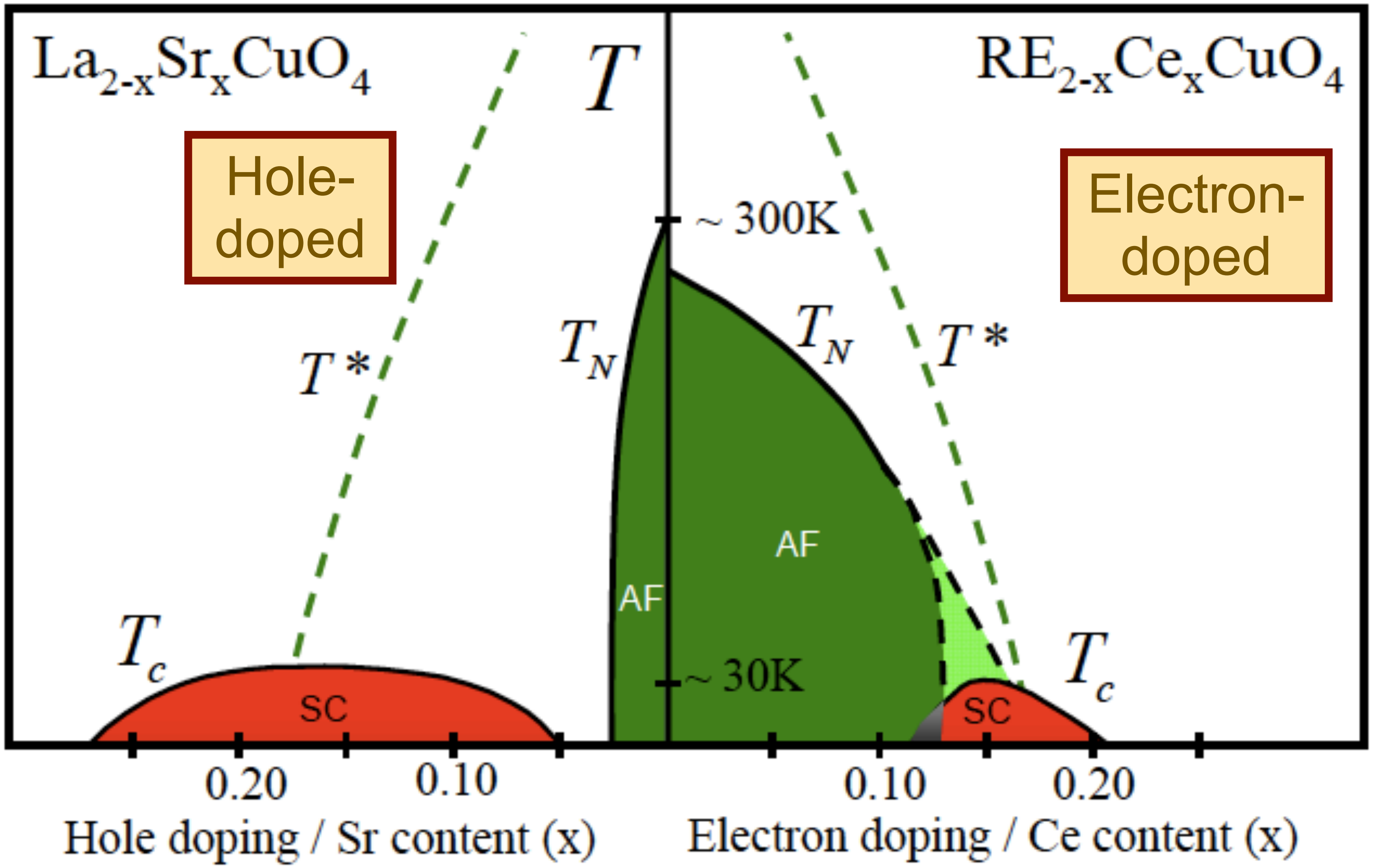


$La_{2-x}Sr_xCuO_4$
T
Hole-
doped
T^*
T_N
AF
T_c
SC
0.20
0.10
Hole doping / Sr content (x)

Electron-doped cuprate superconductors



Electron-doped cuprate superconductors

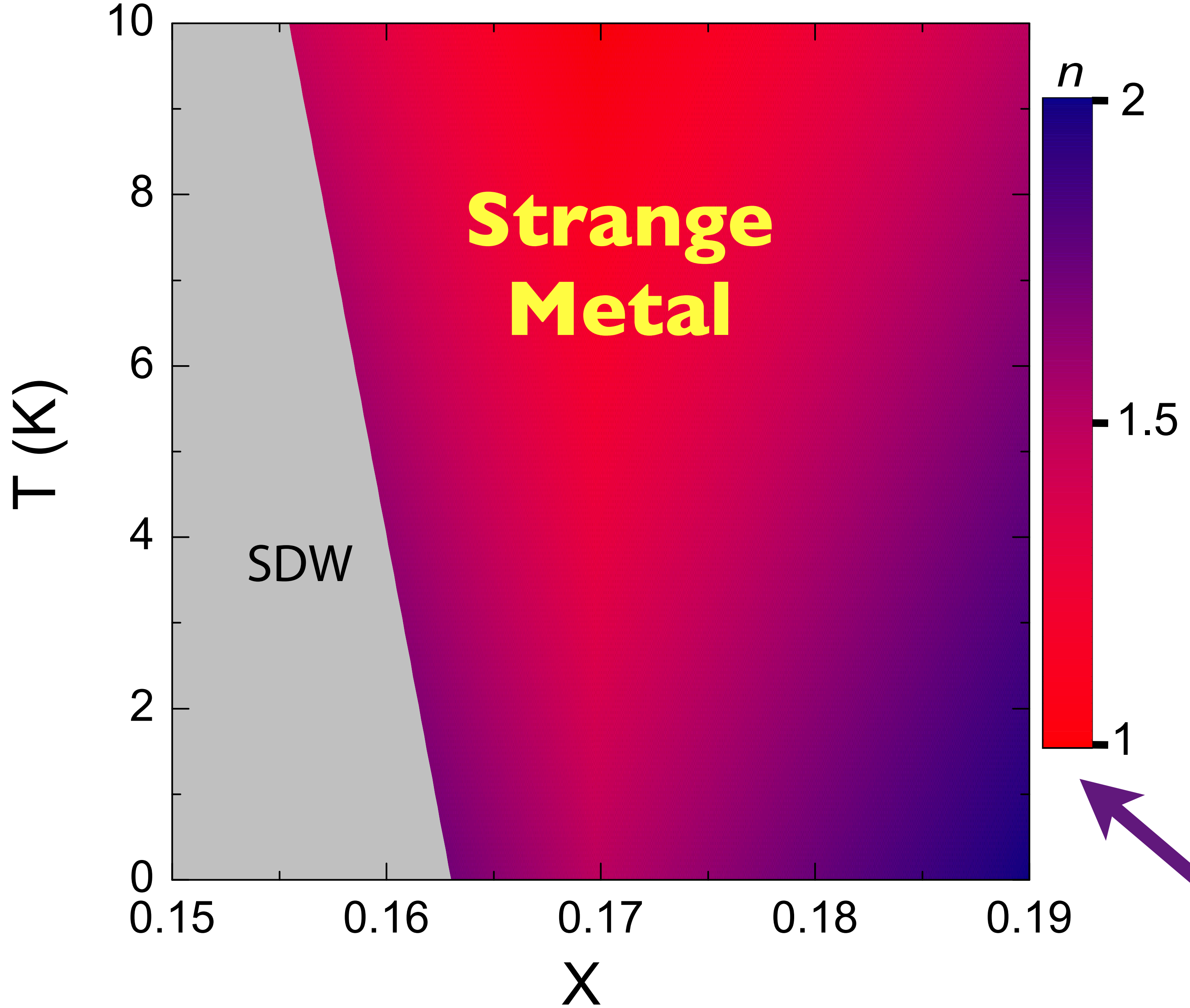
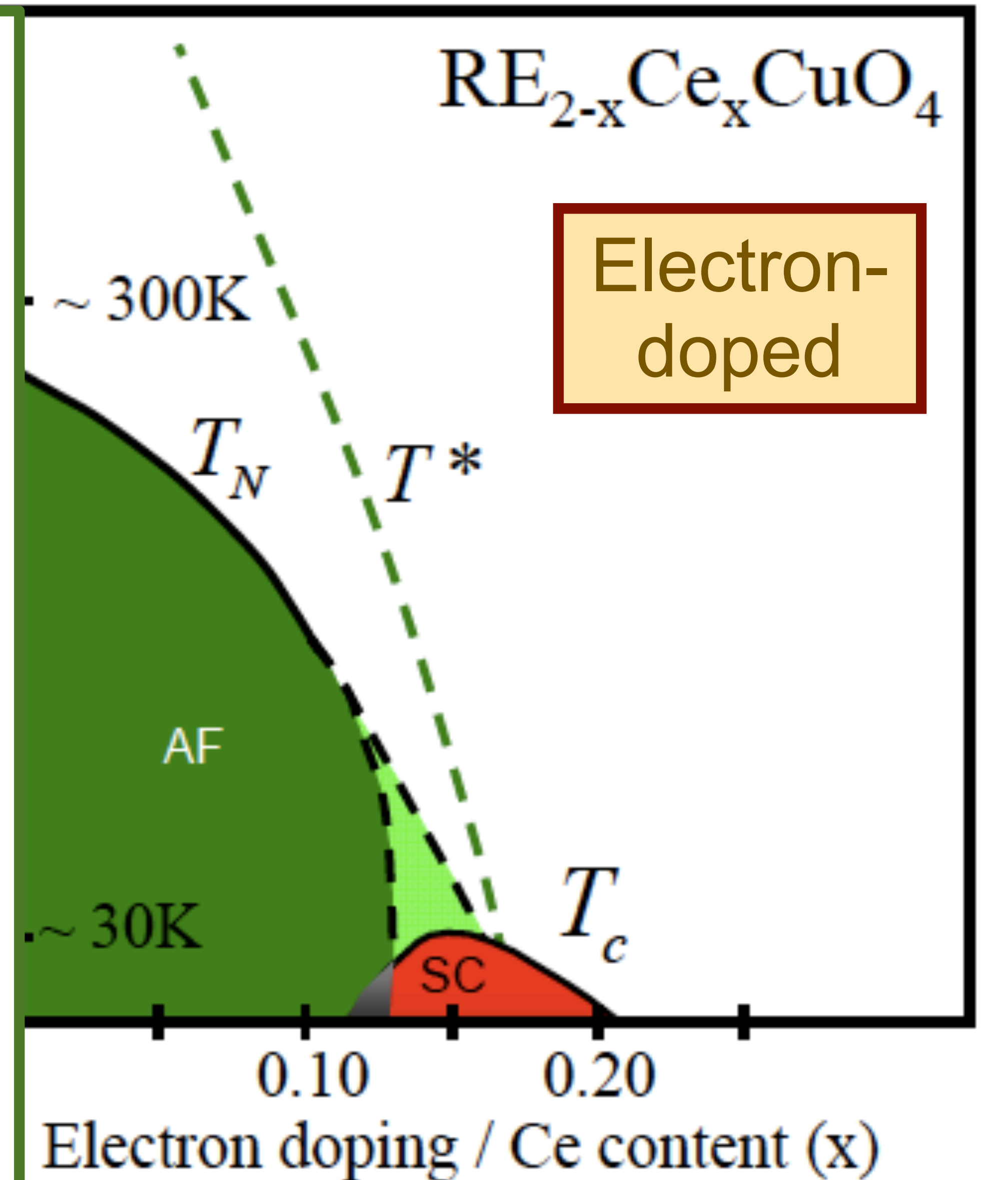
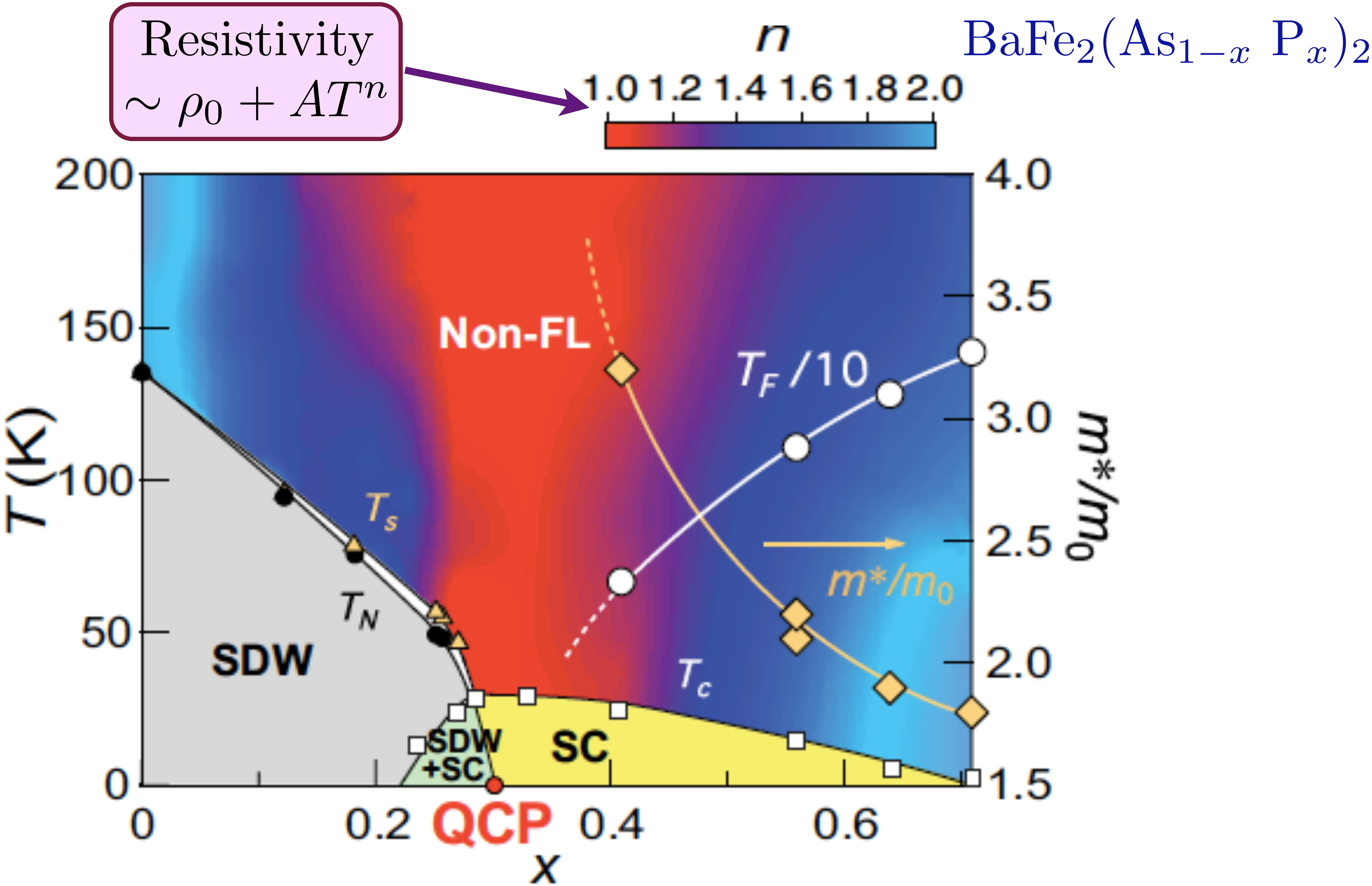


Figure prepared by K. Jin and and R. L. Greene based on N. P. Fournier, P. Armitage, and R. L. Greene, Rev. Mod. Phys. **82**, 2421 (2010).

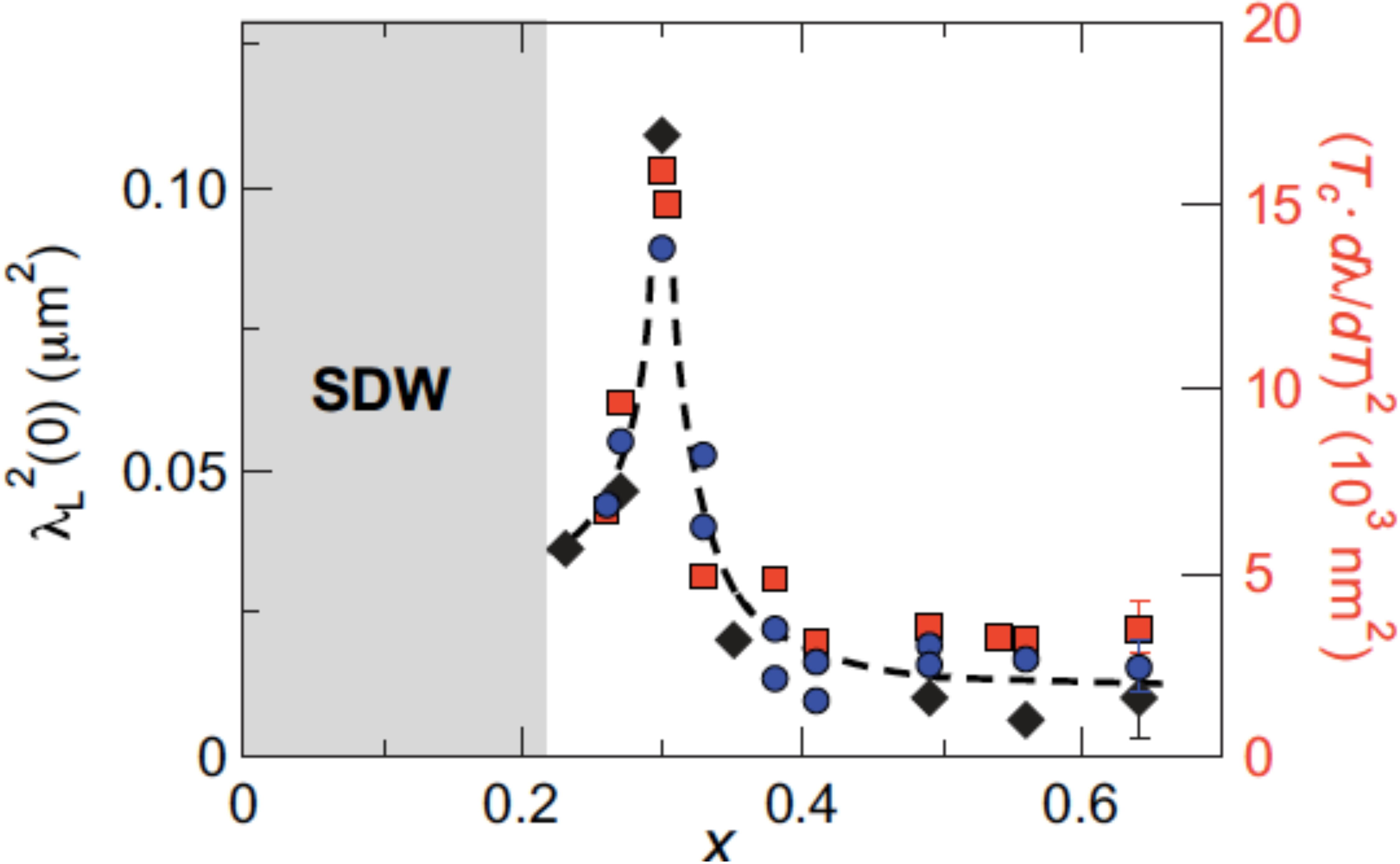


Resistivity $\sim \rho_0 + AT^n$



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 in press

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



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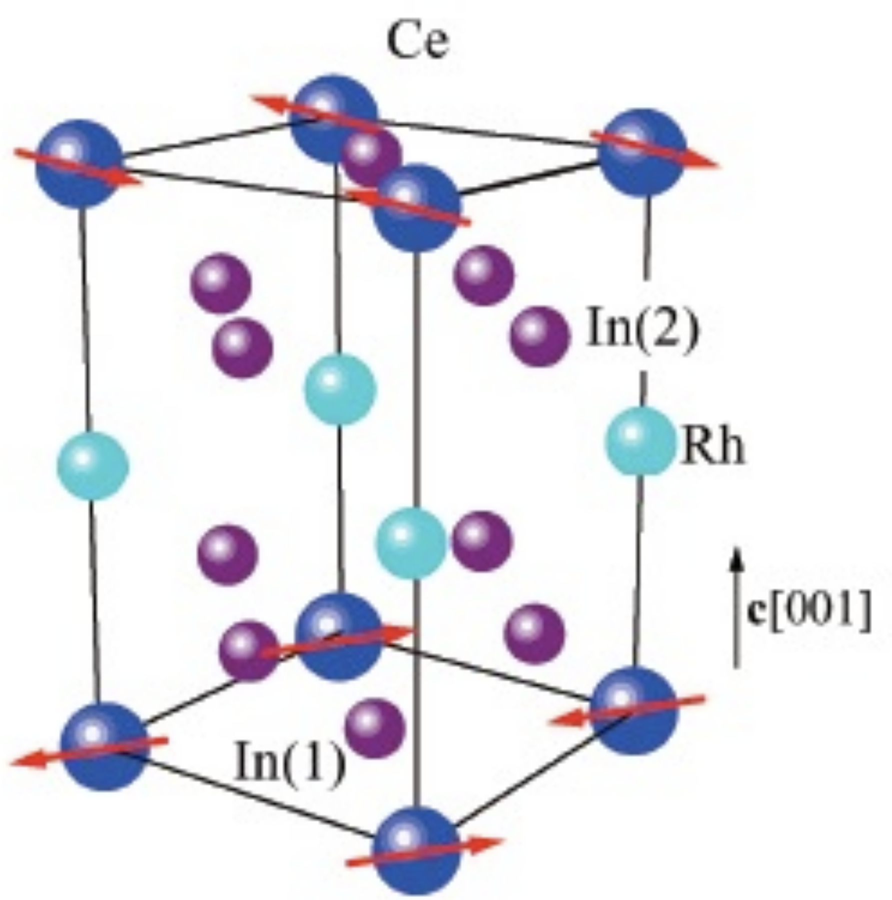
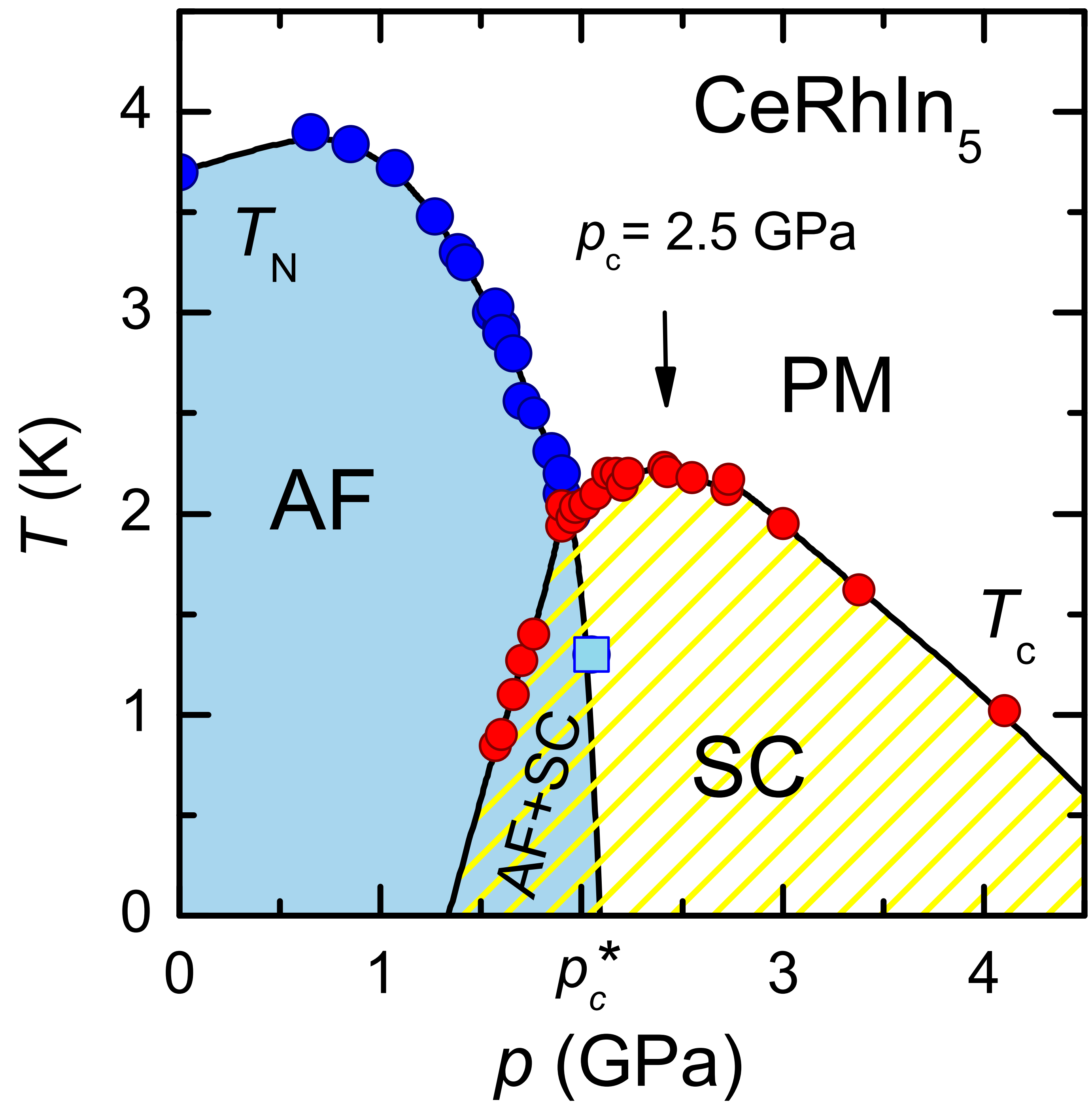
Lower T_c superconductivity in the heavy fermion compounds





G. Knebel, D. Aoki, and J. Flouquet, arXiv:0911.5223

Questions

- *Can quantum fluctuations near the onset of antiferromagnetism induce higher temperature superconductivity ?*

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- *How should such a theory be extended to apply to the hole-doped cuprates ?*

- *What is the physics of the strange metal ?*

Outline

1. Phenomenology of the onset of
   antiferromagnetism in a metal

2. Quantum field theory of the onset of
   antiferromagnetism in a metal

3. Quantum Monte Carlo without the sign problem

4. Fractionalization in metals,
   and the hole-doped cuprates

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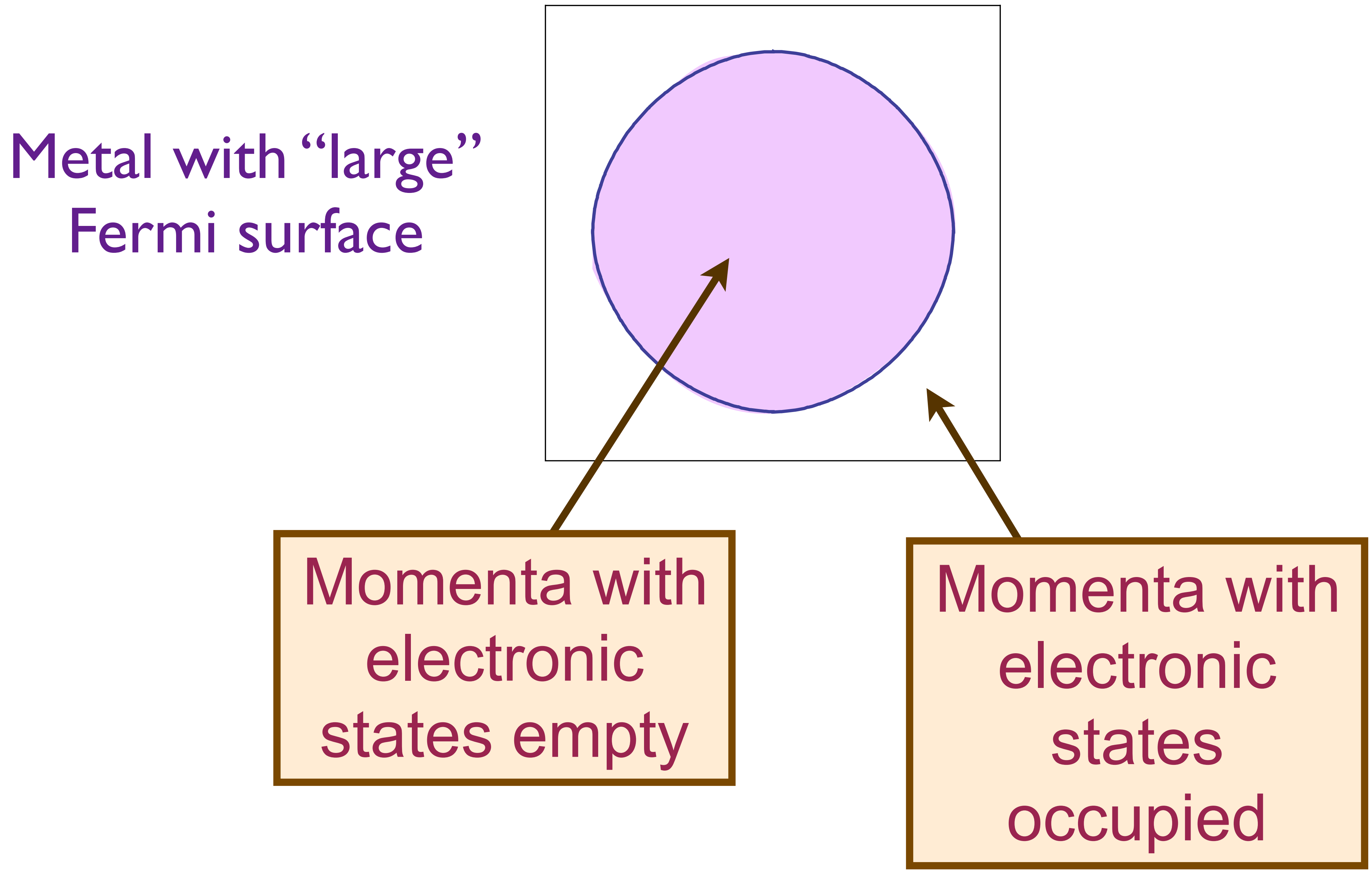
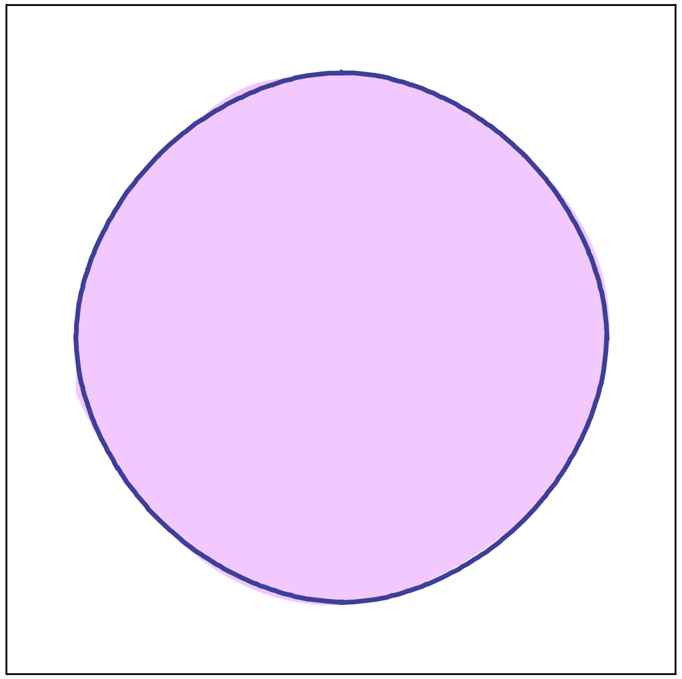
Fermi surface



Fermi surface+antiferromagnetism

Metal with "large"
Fermi surface

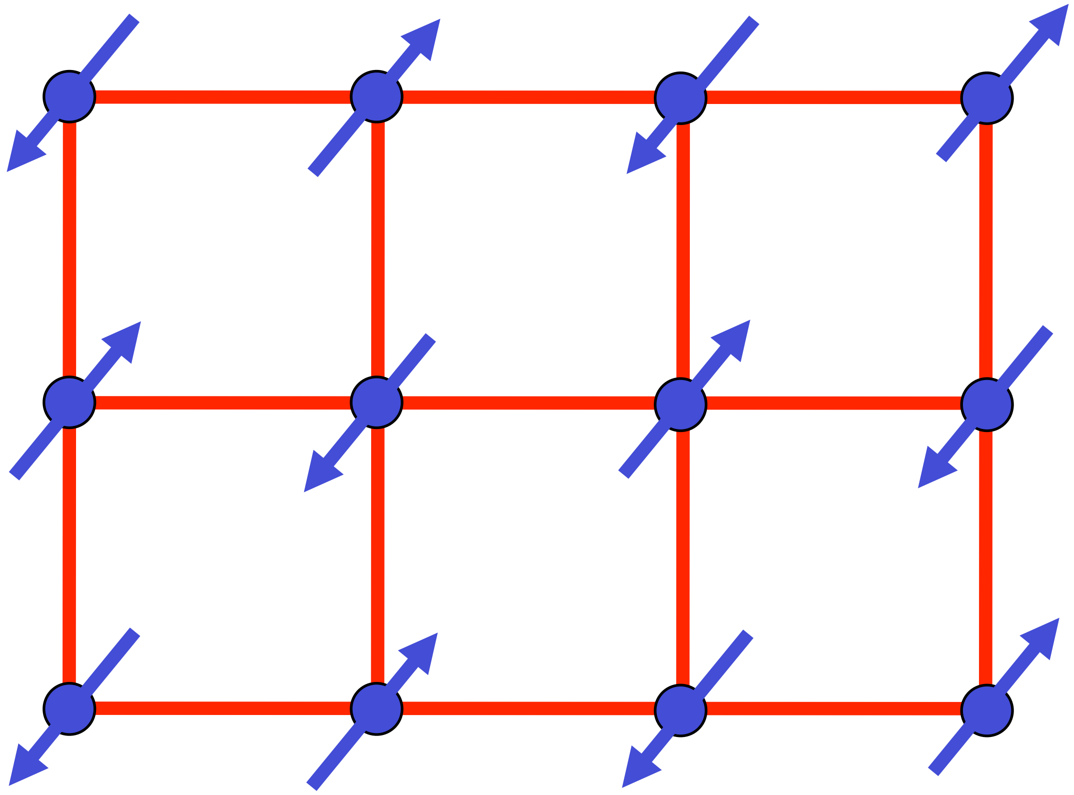


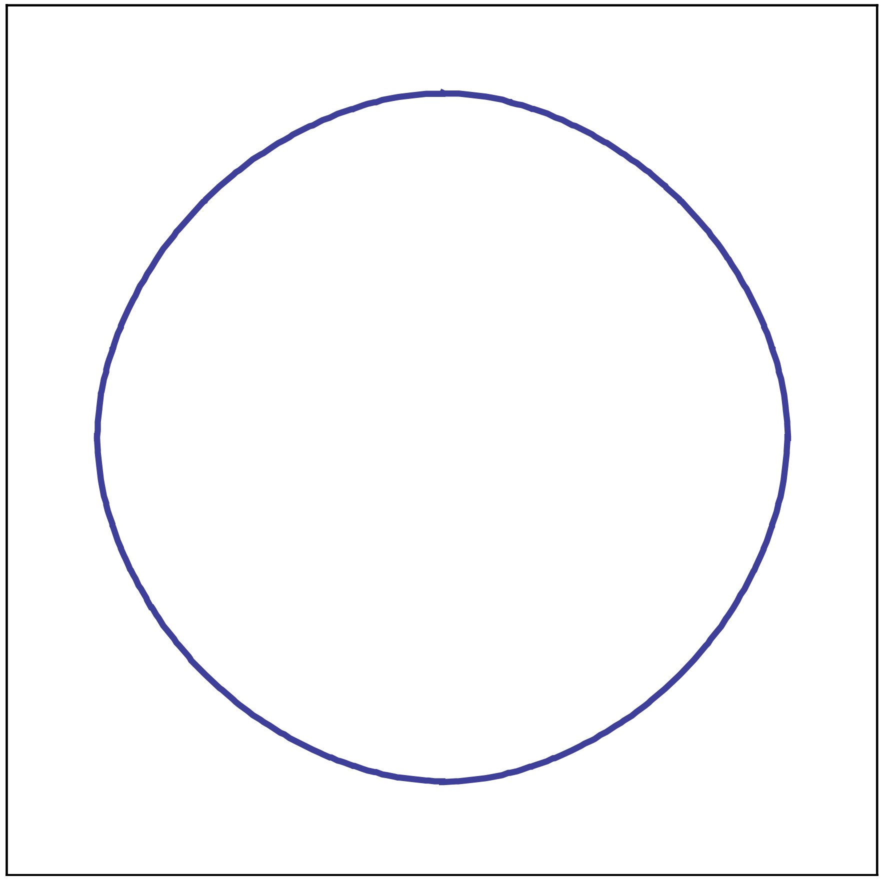
+

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.





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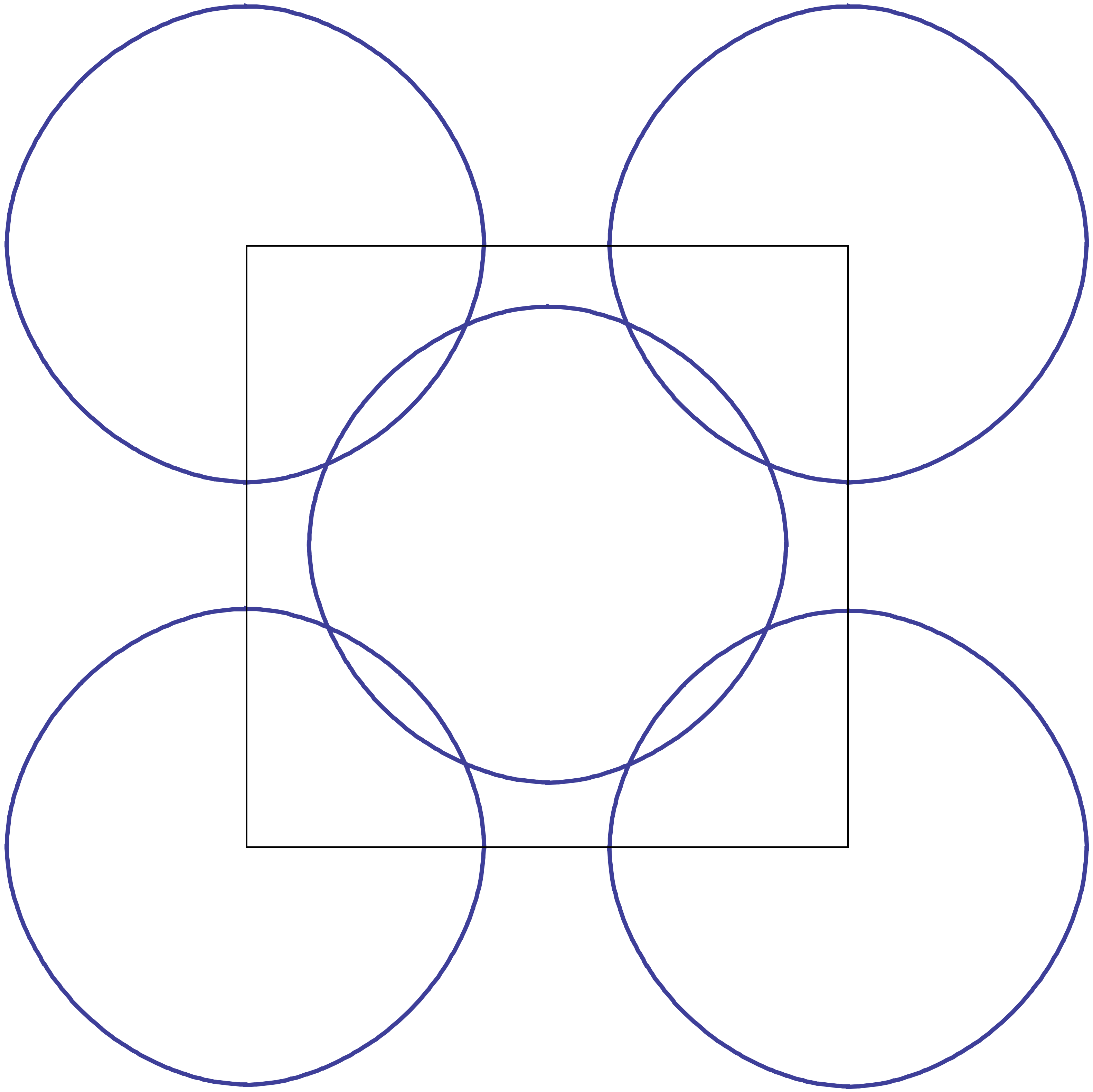

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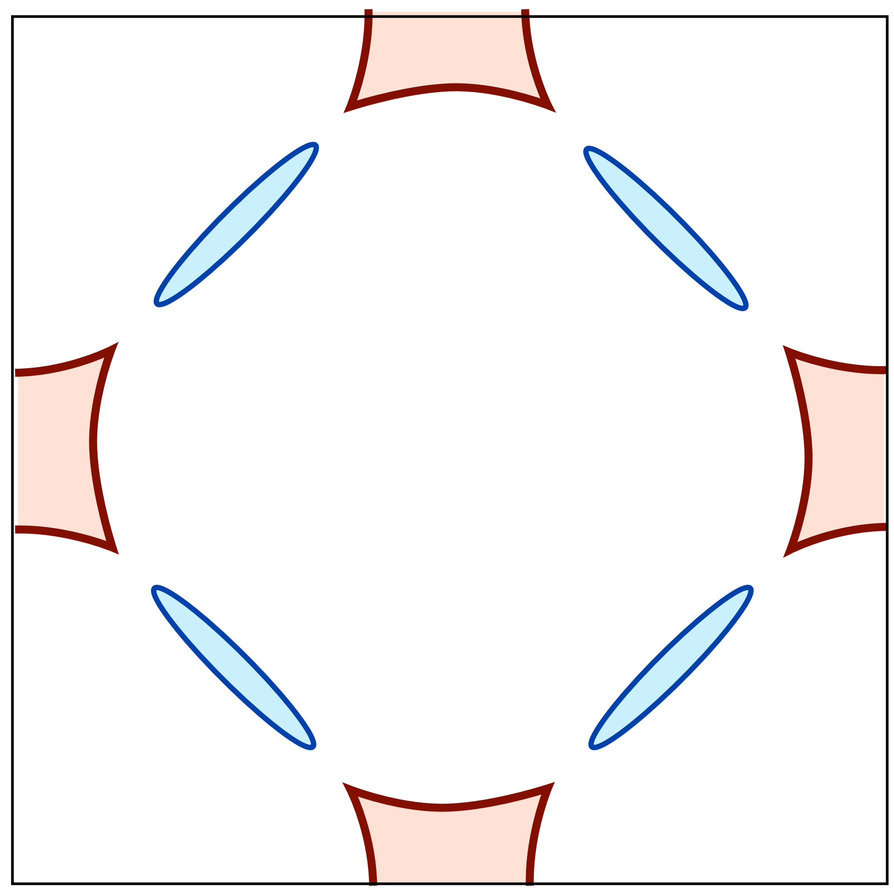
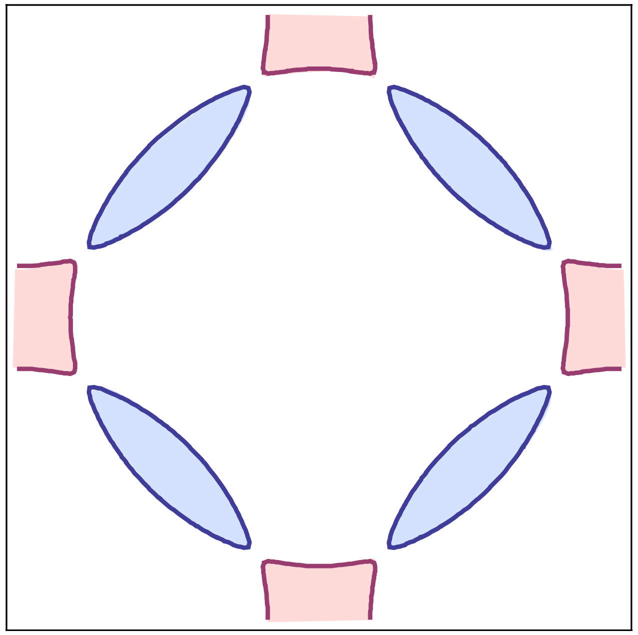
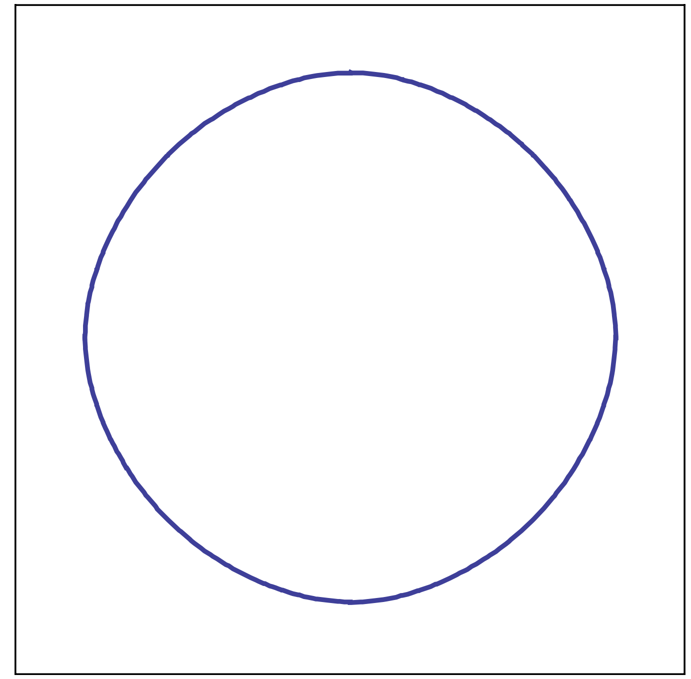


Electron and hole pockets in antiferromagnetic phase with $\langle \vec{\varphi} \rangle \neq 0$

Fermi surface+antiferromagnetism





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

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

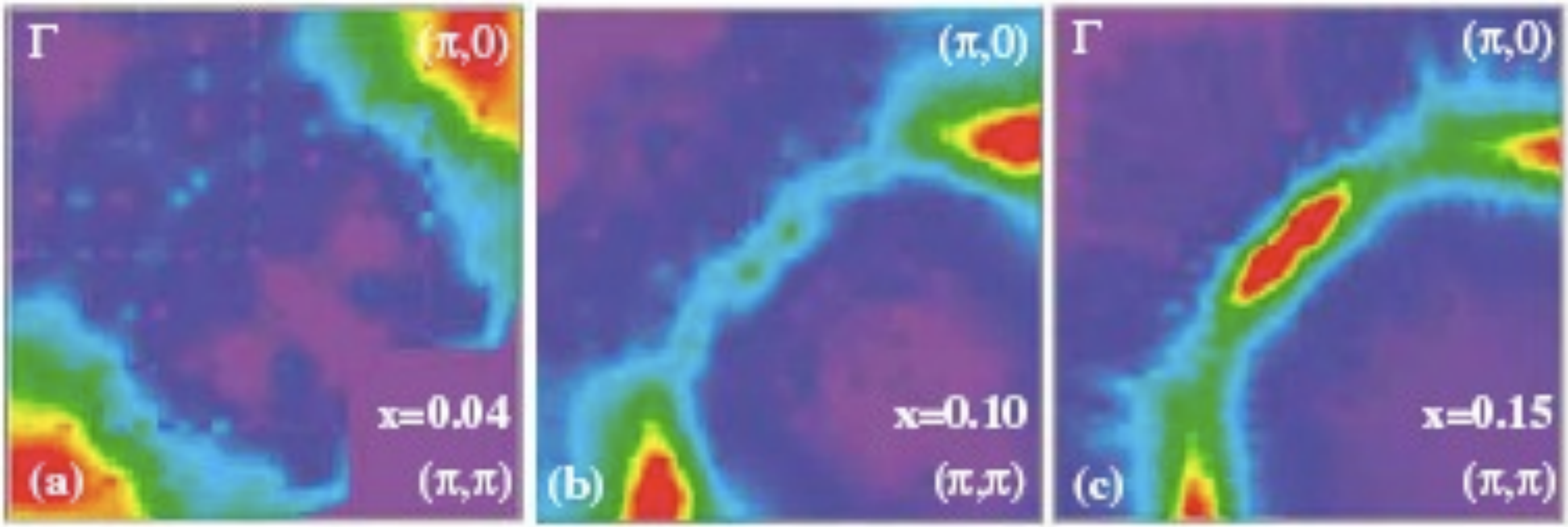
Metal with electron and hole pockets

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).

Photoemission in $Nd_{2-x}Ce_xCuO_4$

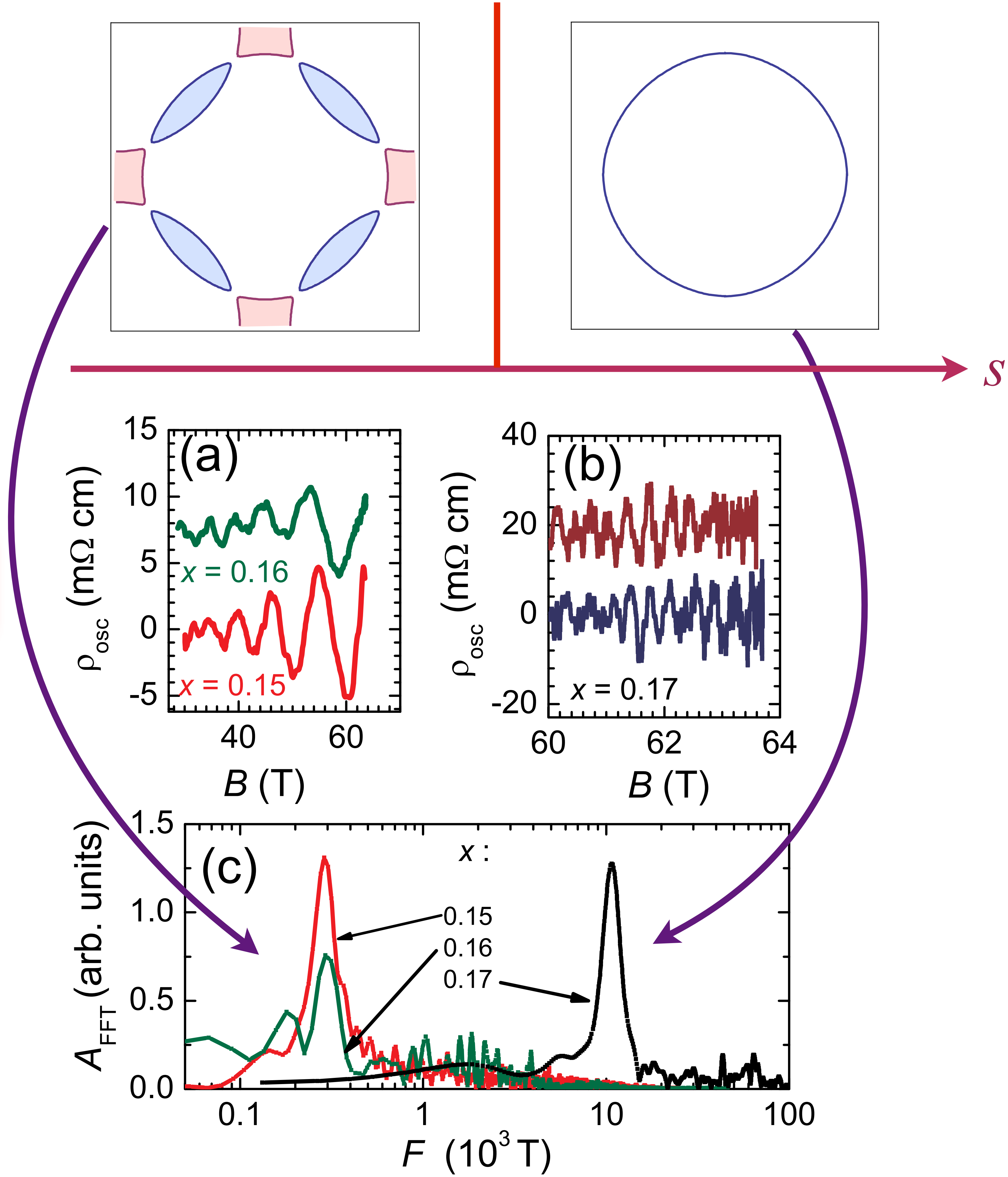


N. P. Armitage *et al.*, Phys. Rev. Lett. **88**, 257001 (2002).

Quantum oscillations

$Nd_{2-x}Ce_xCuO_4$

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



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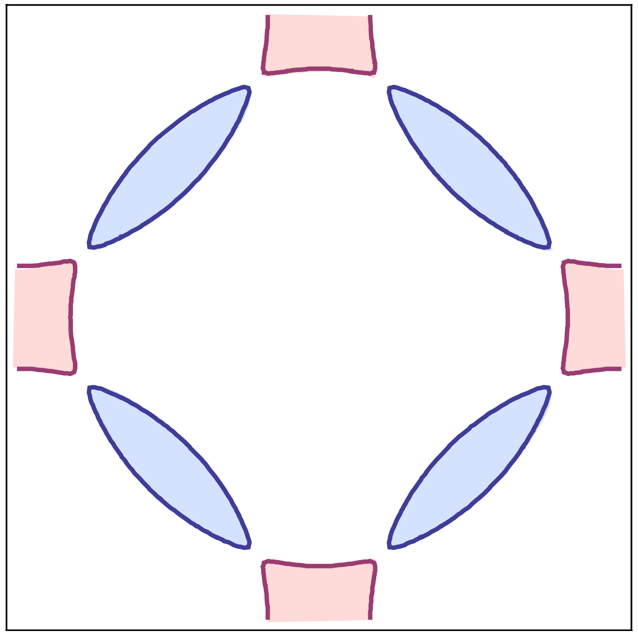

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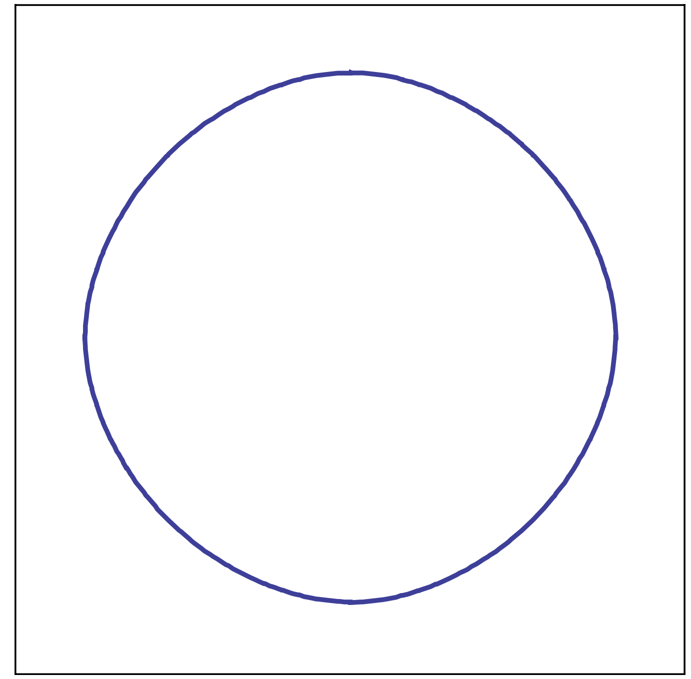

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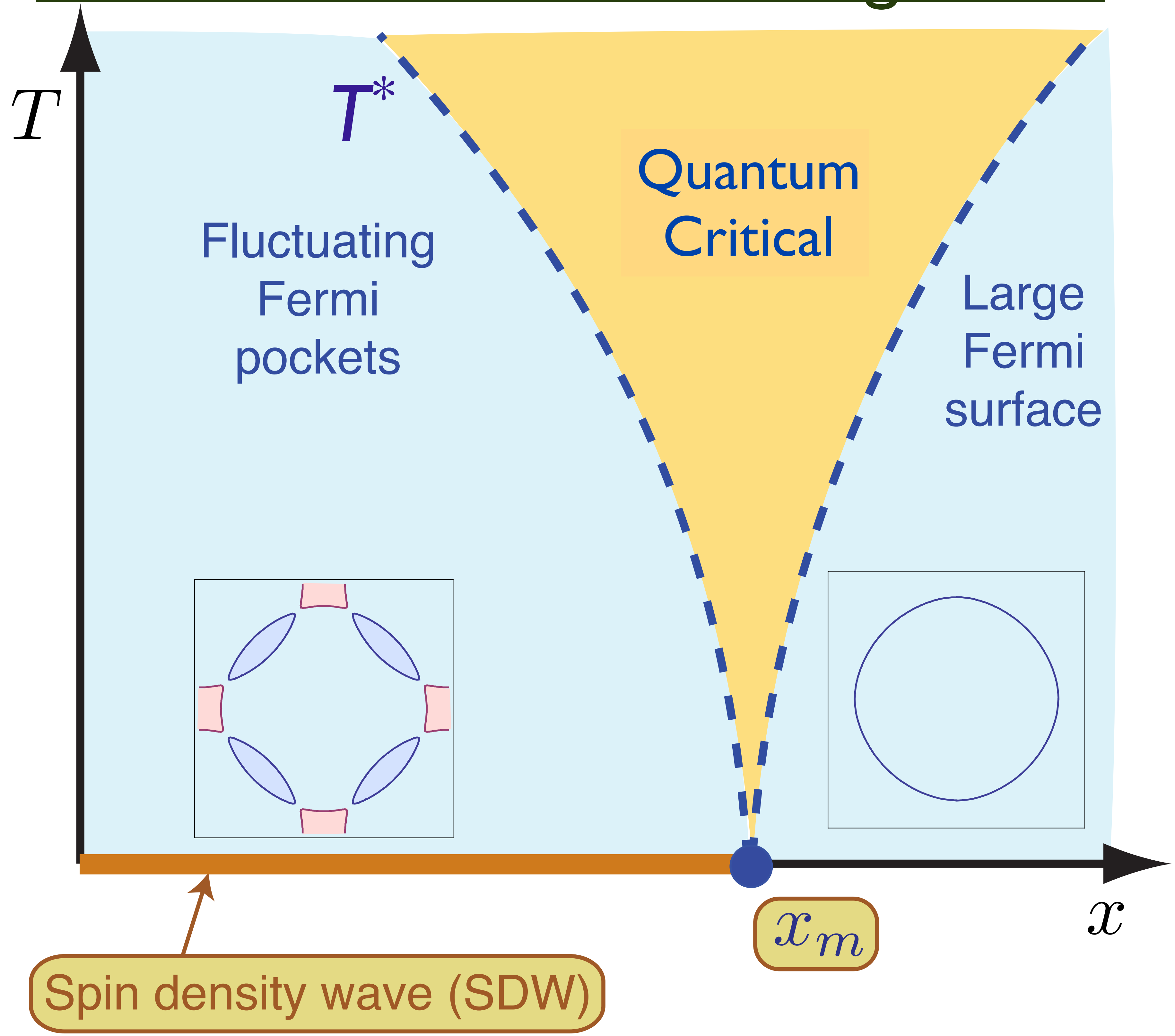
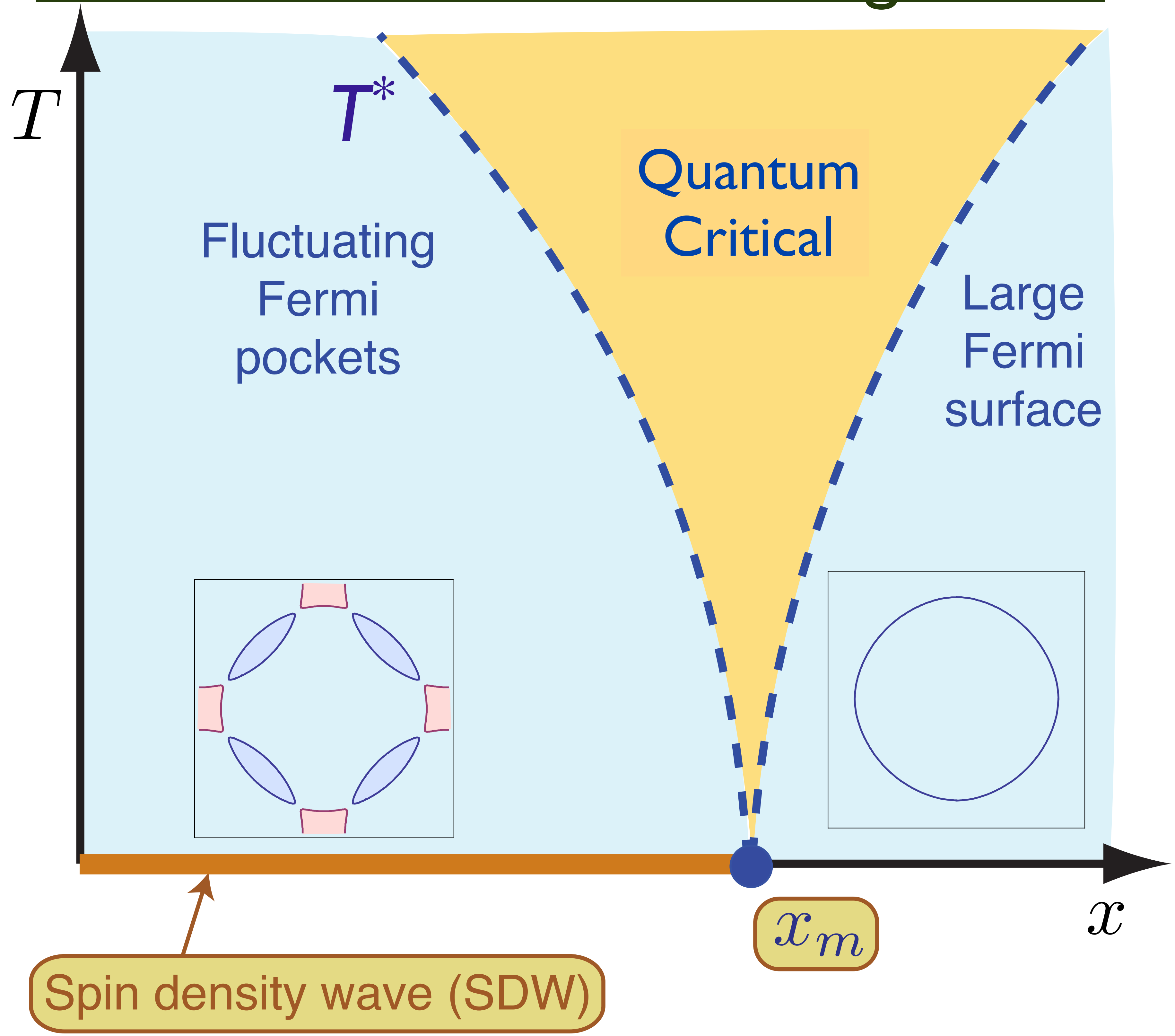


Underlying SDW ordering quantum critical point in **metal** at $x = x_m$

Fermi surface+antiferromagnetism



Relaxation and equilibration times $\sim \hbar/k_B T$ are robust properties of strongly-coupled quantum criticality

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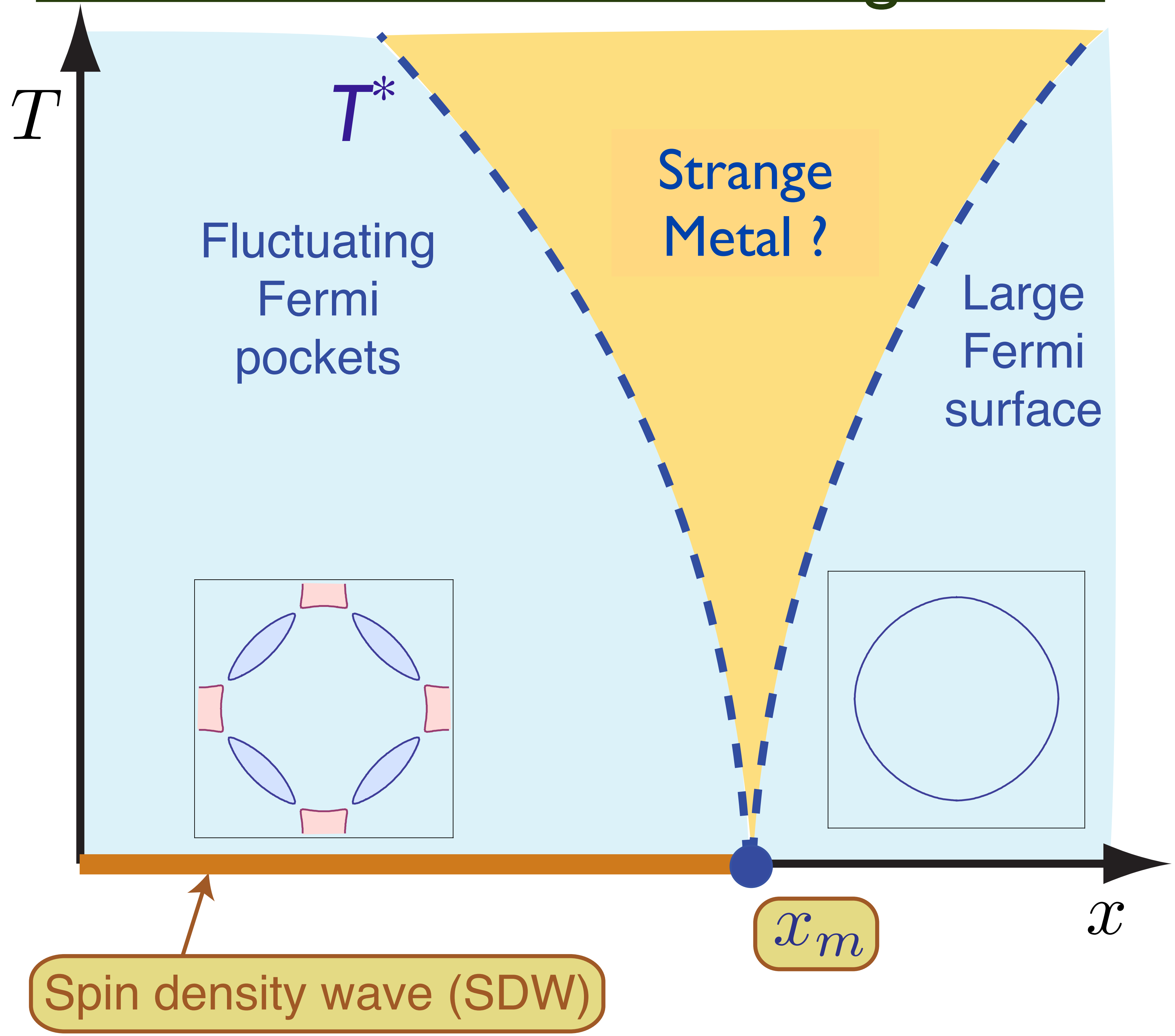

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Boson-fermion theory for both phases

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

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

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

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

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

Hertz-Moriya-Millis theory

- Integrate out Fermi surface quasiparticles and obtain an effective theory for the order parameter $\vec{\varphi}$ alone.

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- This is dangerous, and will lead to non-local in the $\vec{\varphi}$ theory. Hertz focused on only the simplest such non-local term.

- However, there are an infinite number of non-local terms at higher order, and these lead to a breakdown of the Hertz theory in two spatial dimensions.

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

- In $d = 2$, we *must* work in local theores which keeps both the order parameter and the Fermi surface quasiparticles "alive".

Sung-Sik Lee, *Phys. Rev. B* **80**, 165102 (2009)
M. A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)
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- At subleading order, resummation of all "planar" graphics is required (at least): this theory is even more complicated than QCD.

Sung-Sik Lee, *Phys. Rev. B* **80**, 165102 (2009)
M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075127 (2010)
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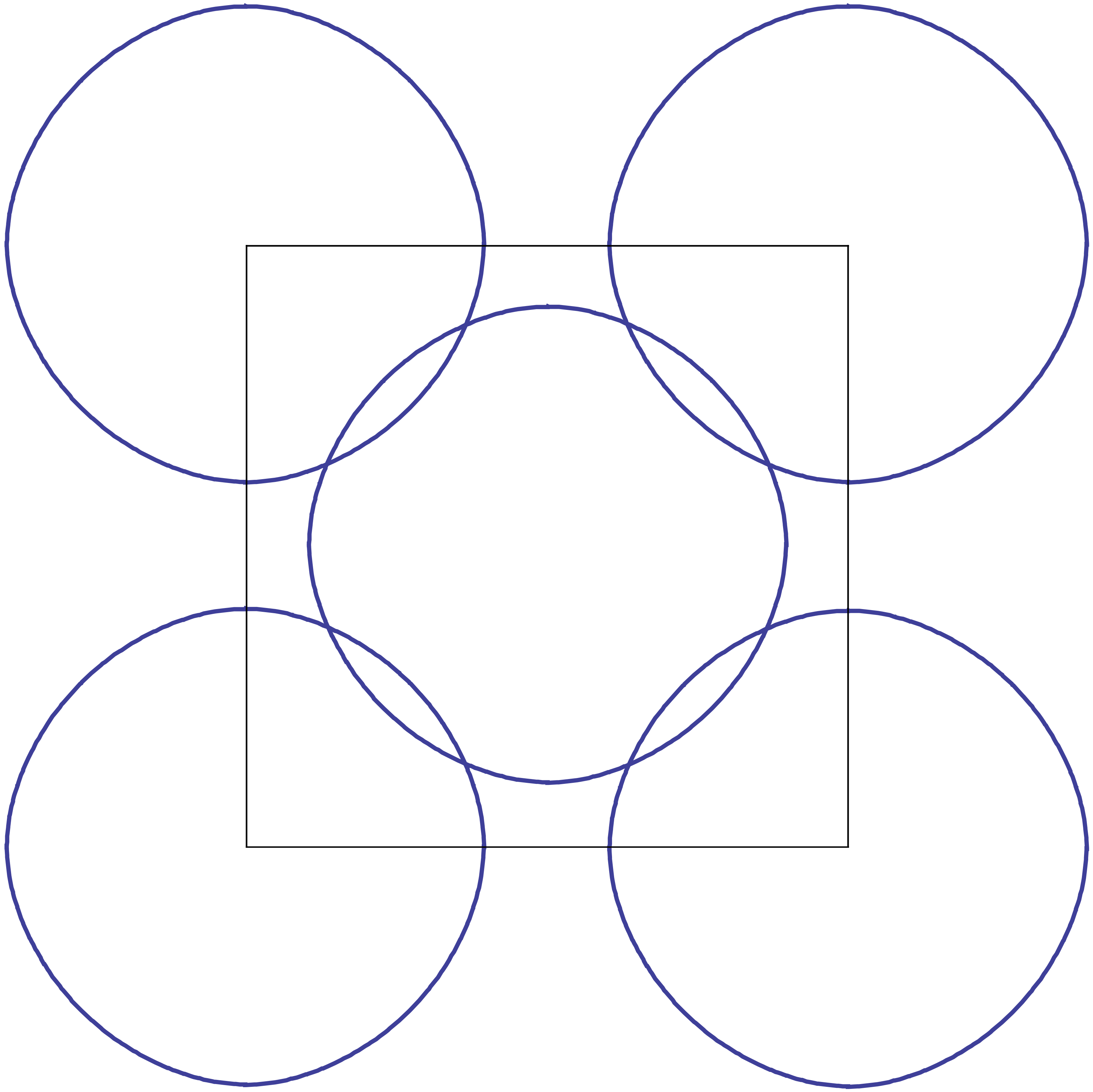

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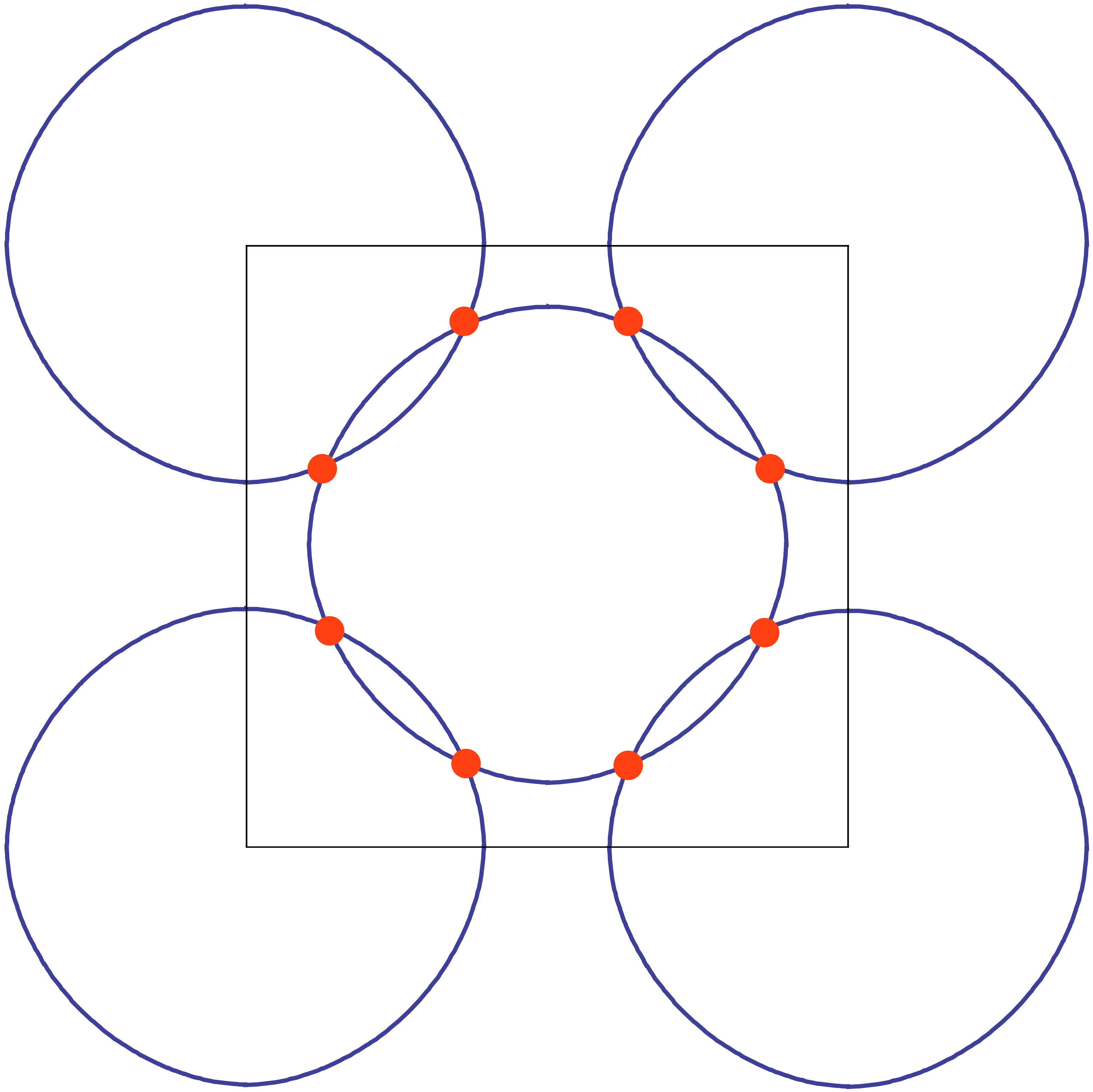
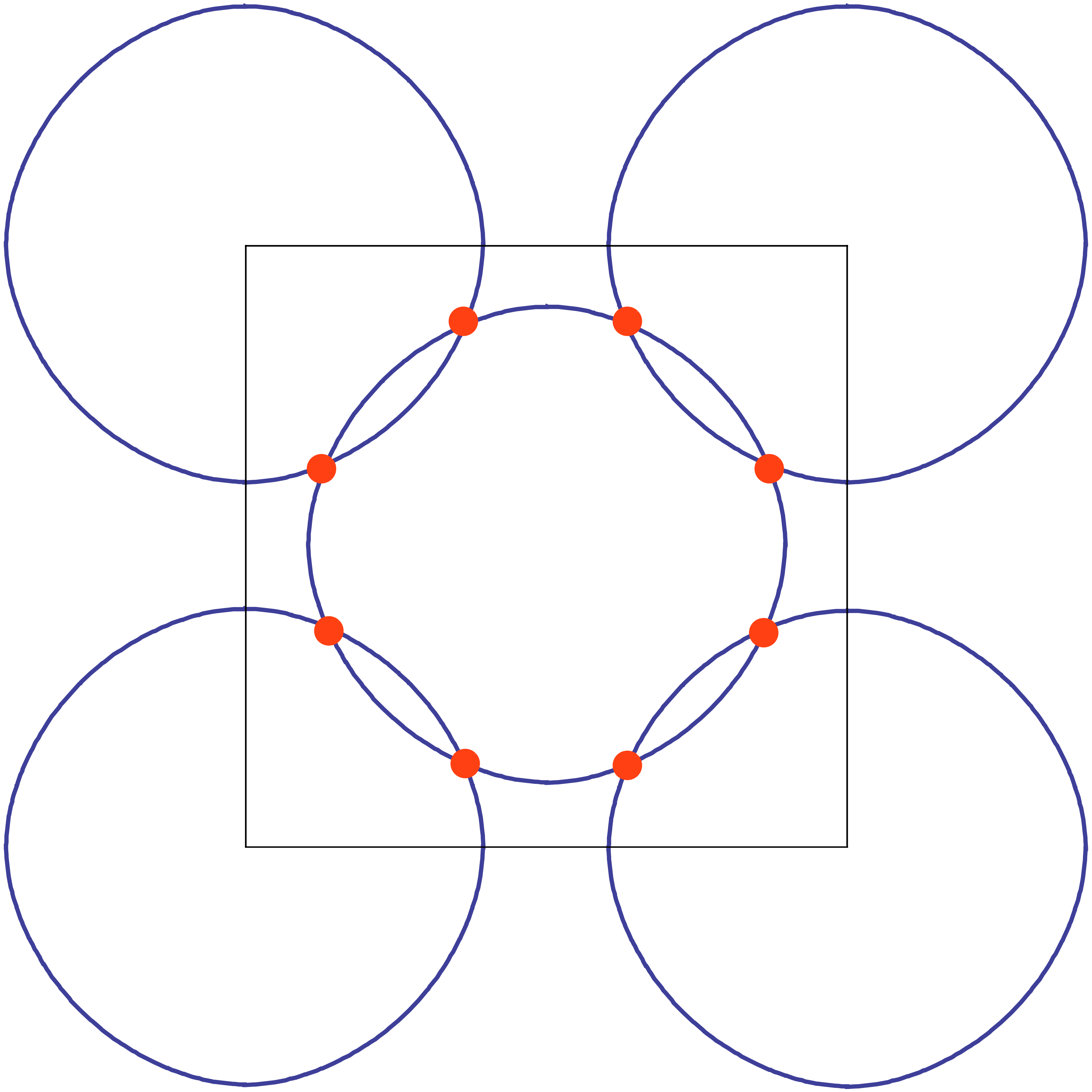
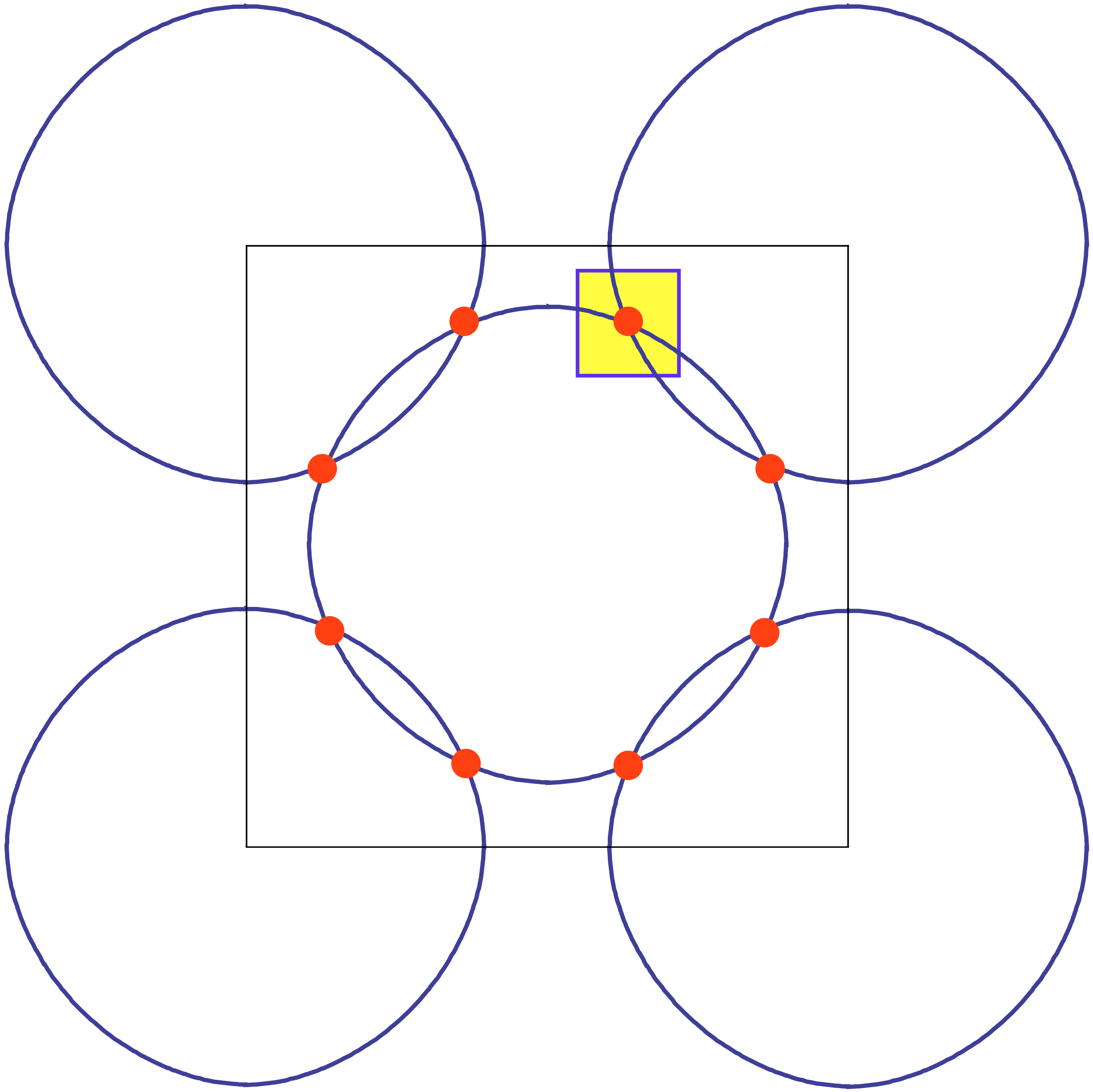


“Hot” spots



Low energy theory for critical point near hot spots



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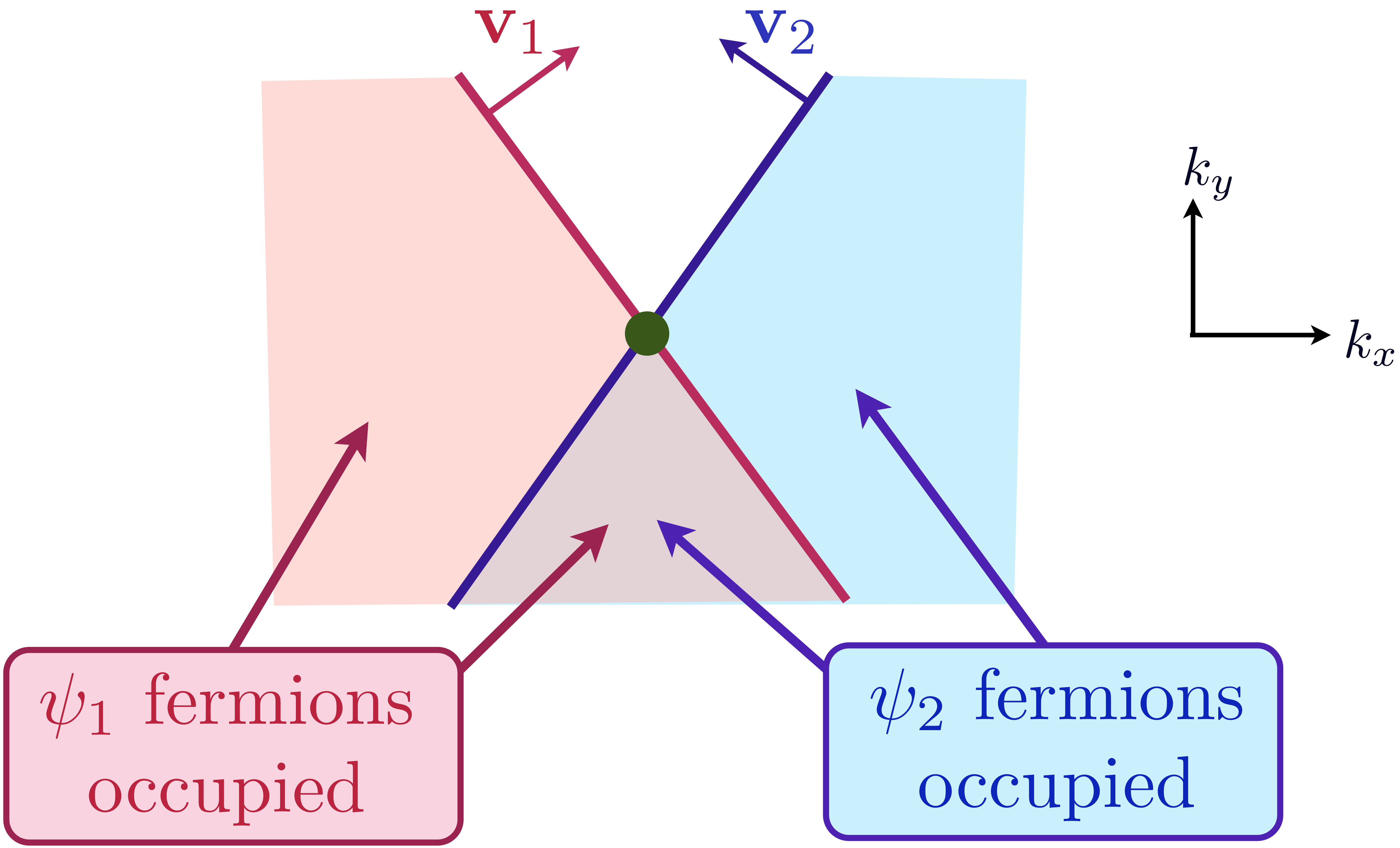
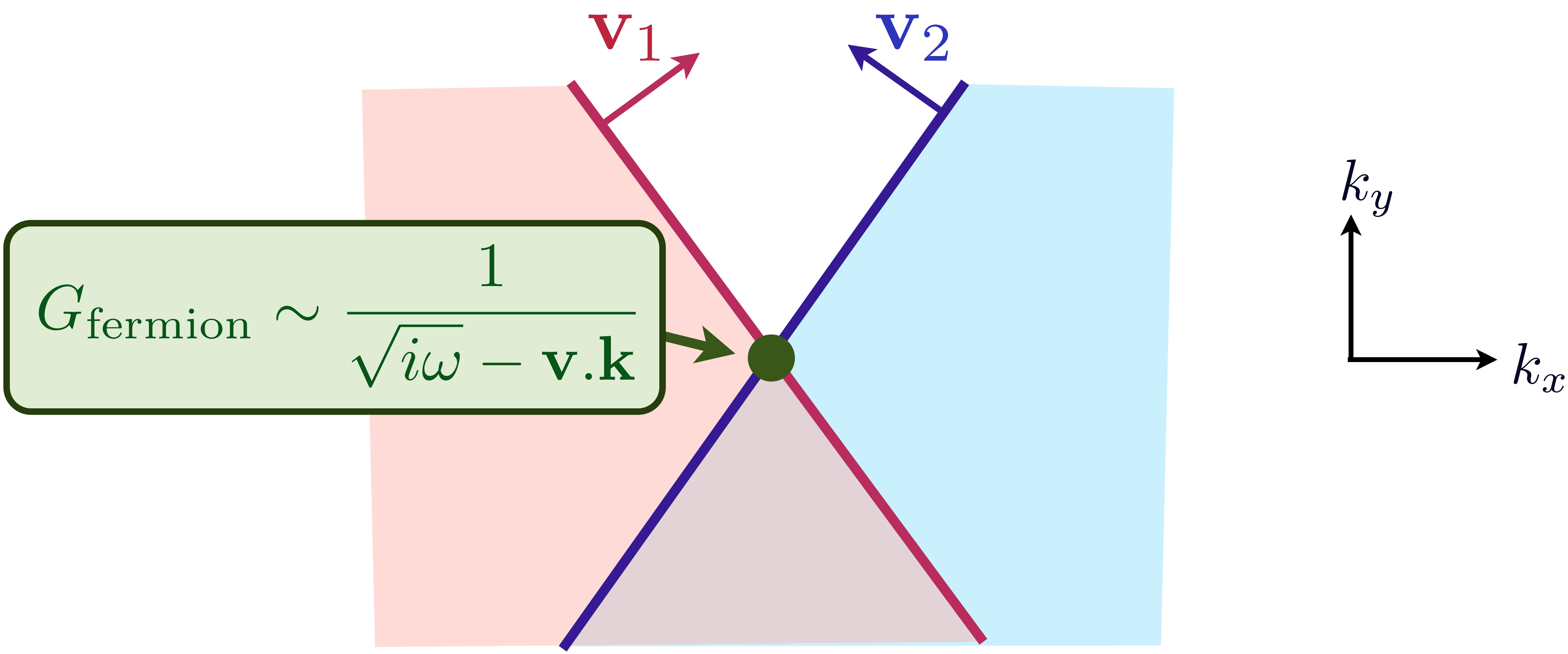


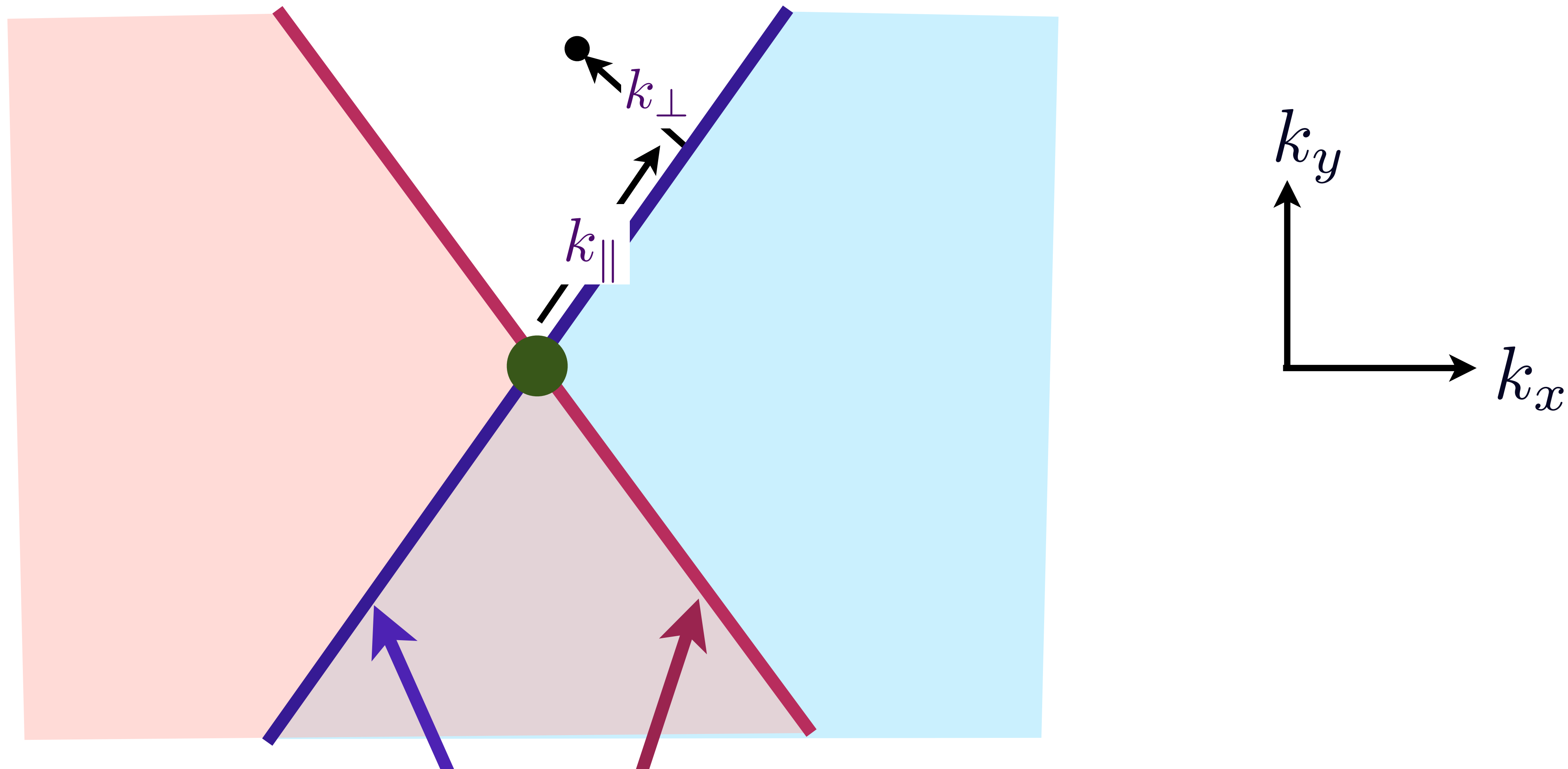
Two loop results: Non-Fermi liquid spectrum at hot spots



A. J. Millis, *Phys. Rev. B* **45**, 13047 (1992)

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

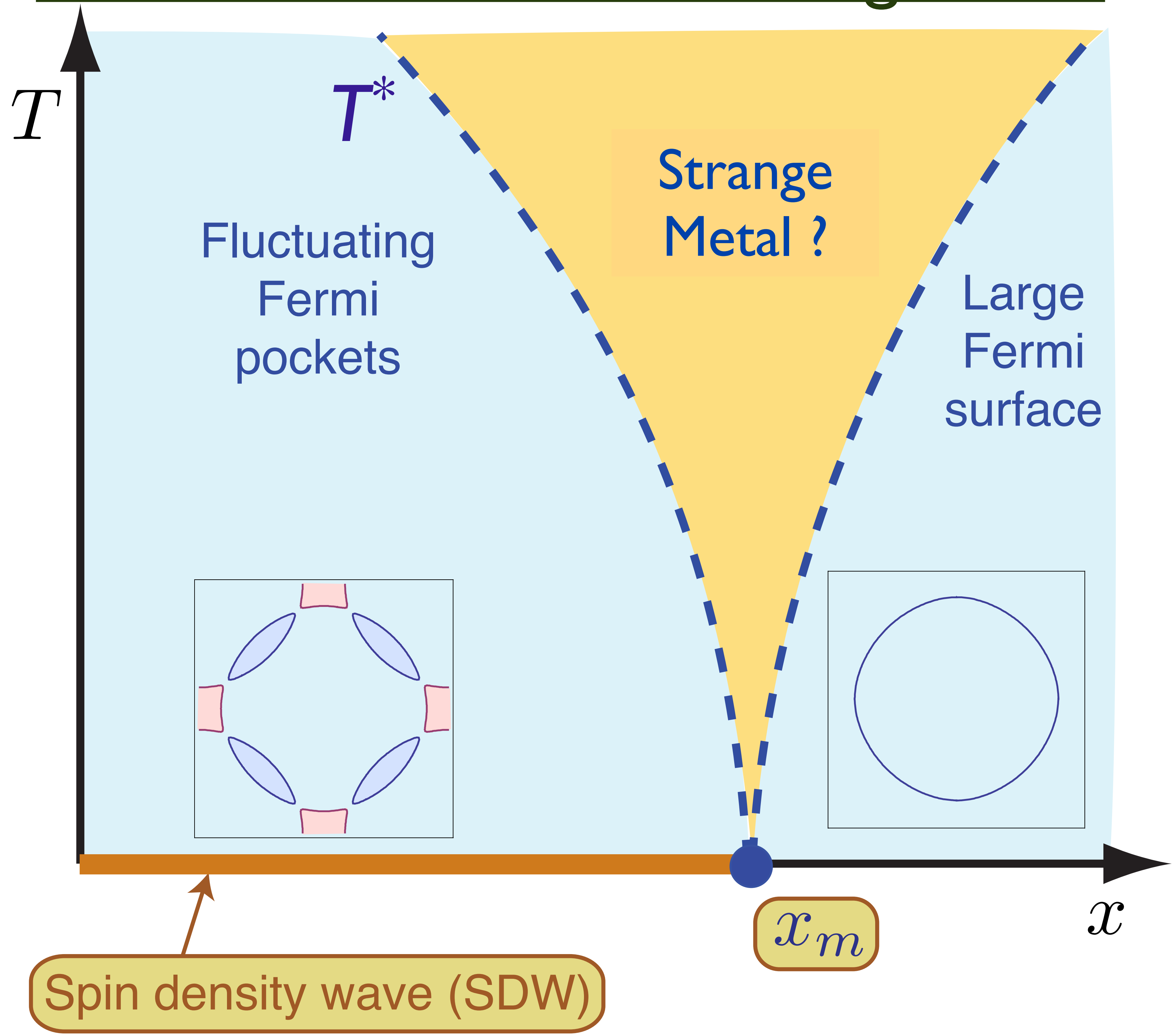
Two loop results: Quasiparticle weight vanishes upon approaching hot spots



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

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

Fermi surface+antiferromagnetism



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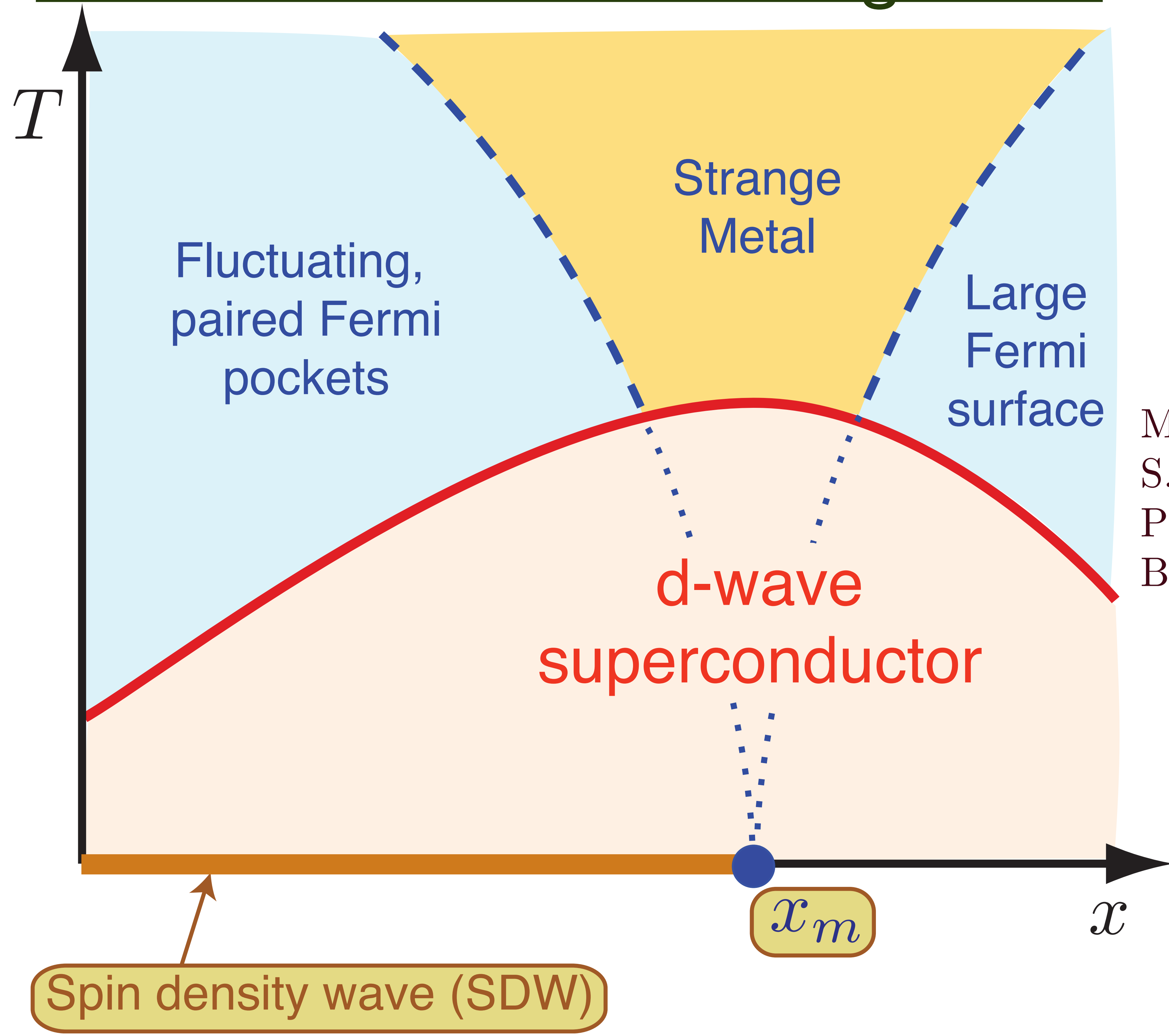

M. A. Metlitski and S. Sachdev, Physical Review B **82**, 075128 (2010)

Pairing "glue" from antiferromagnetic fluctuations

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d-wave pairing near a spin-density-wave instability

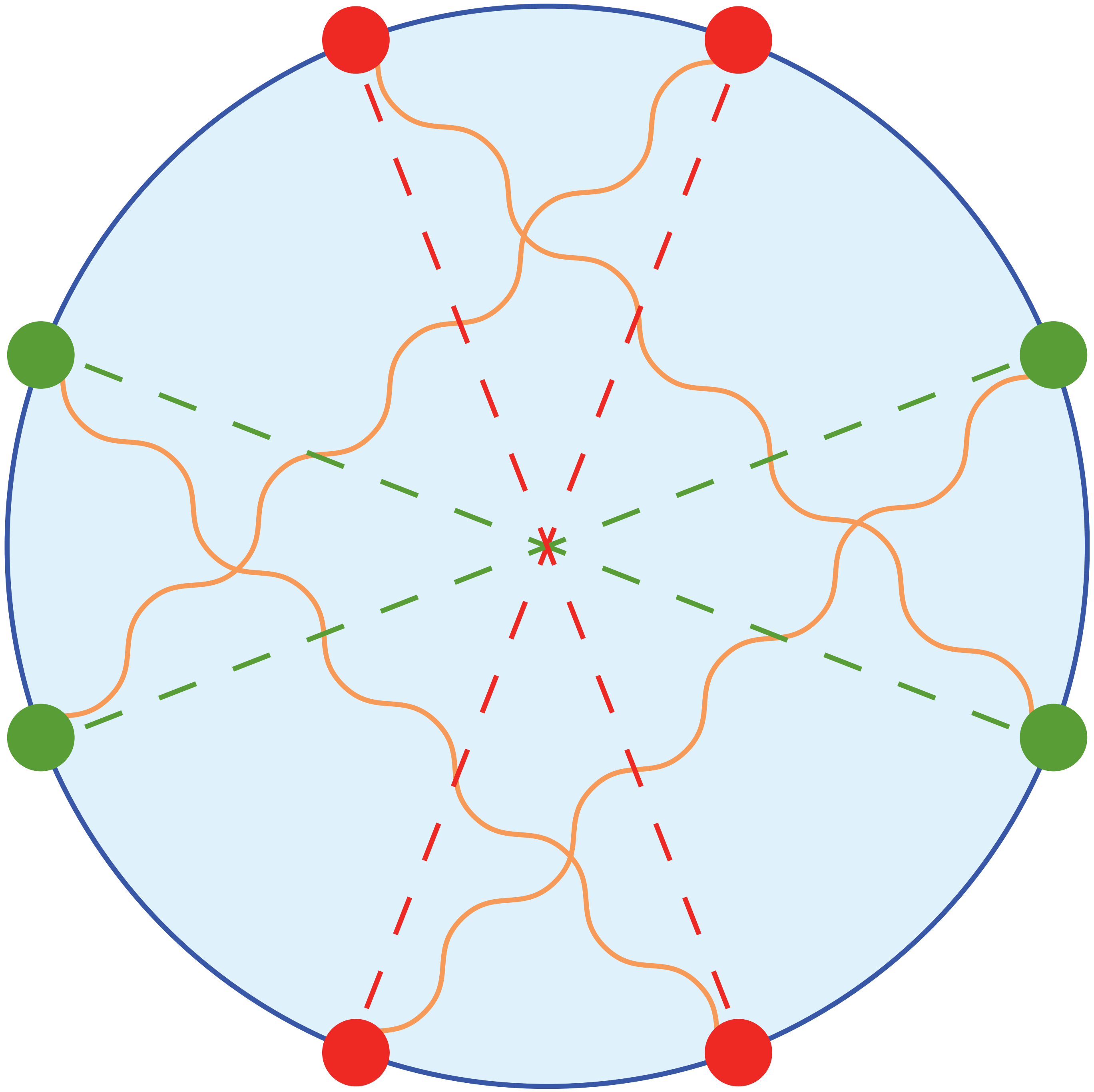
D. J. Scalapino, E. Loh, Jr.,* and J. E. Hirsch†
Institute for Theoretical Physics, University of California, Santa Barbara, California 93106
(Received 23 June 1986)

We investigate the three-dimensional Hubbard model and show that paramagnon exchange near a spin-density-wave instability gives rise to a strong singlet *d*-wave pairing interaction. For a cubic band the singlet ($d_{x^2-y^2}$ and $d_{3z^2-r^2}$) channels are enhanced while the singlet (d_{xy}, d_{xz}, d_{yz}) and triplet *p*-wave channels are suppressed. A unique feature of this pairing mechanism is its sensitivity to band structure and band filling.

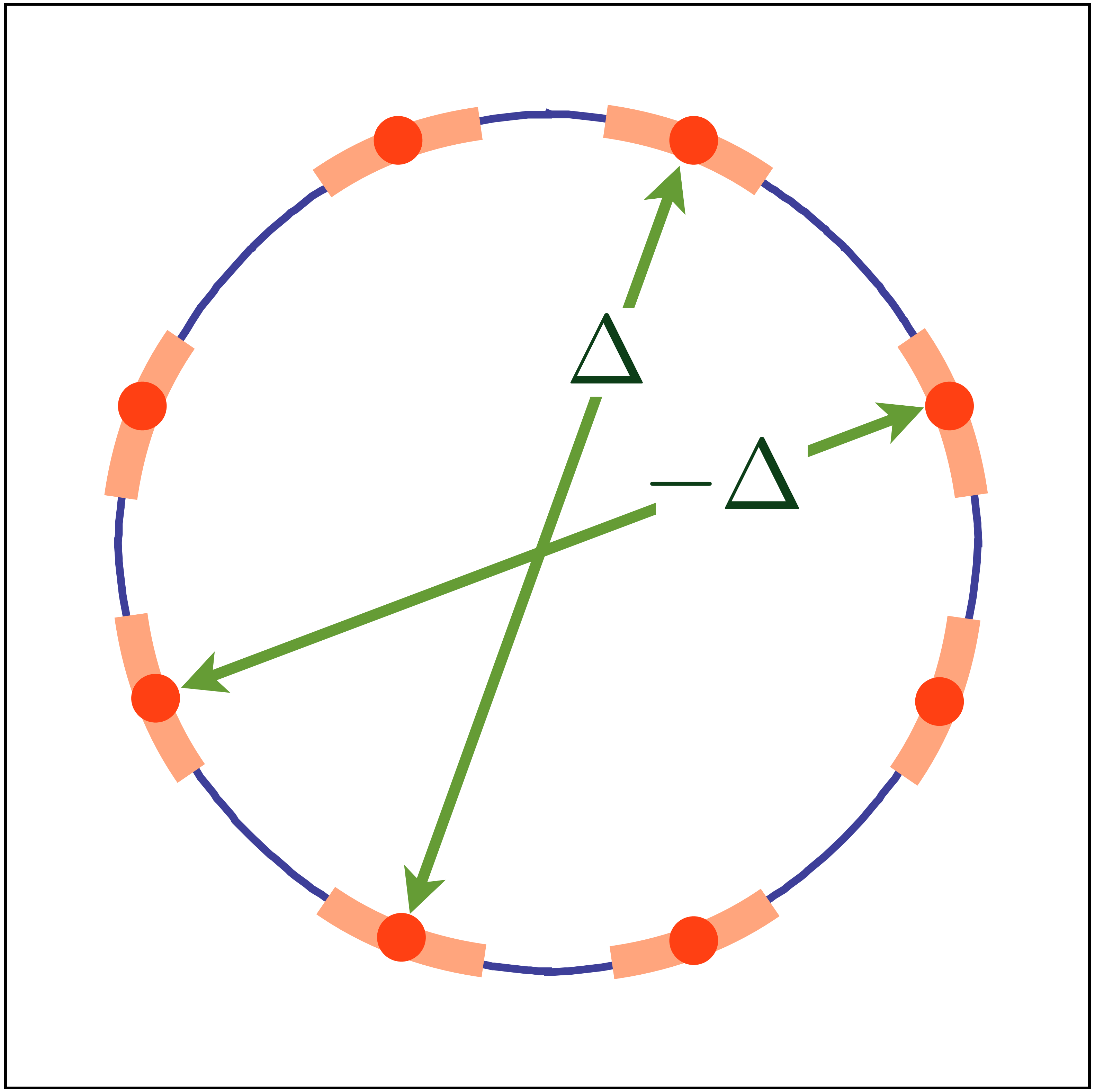
Physical Review B **34**, 8190 (1986)

There is an instability in weak-coupling,
but T_c is low where the theory is reliable:

Pairing "glue" from antiferromagnetic fluctuations



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



Unconventional pairing at ***and near*** hot spots

At stronger coupling, different effects compete:

- Pairing glue becomes stronger.

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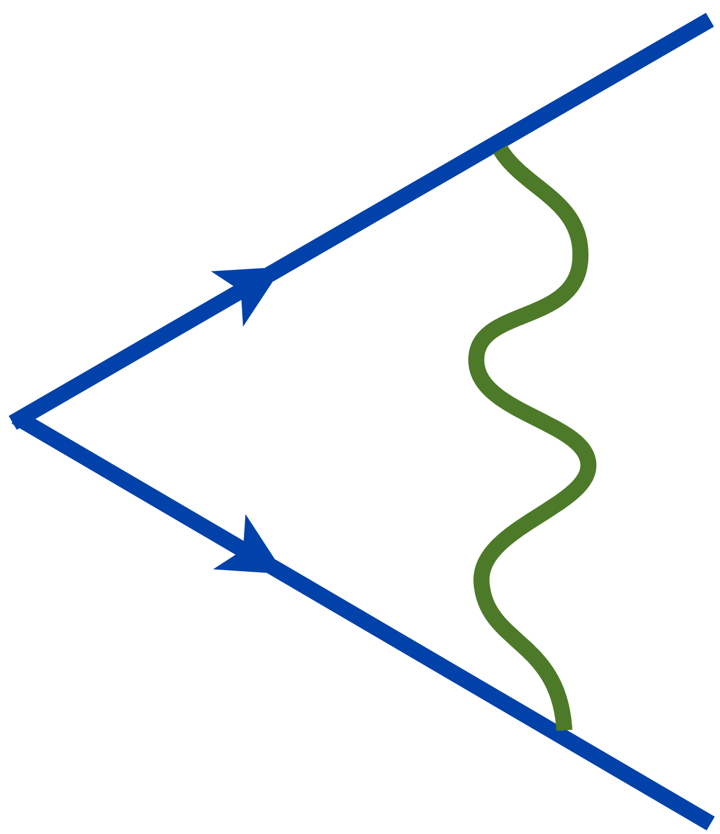
- Other instabilities can appear *e.g.* to charge density waves/stripe order.

BCS theory

Electron-phonon coupling

$$1 + \lambda_{\text{e-ph}} \log\left(\frac{\omega_D}{\omega}\right)$$

Debye frequency



Enhancement of pairing susceptibility by interactions

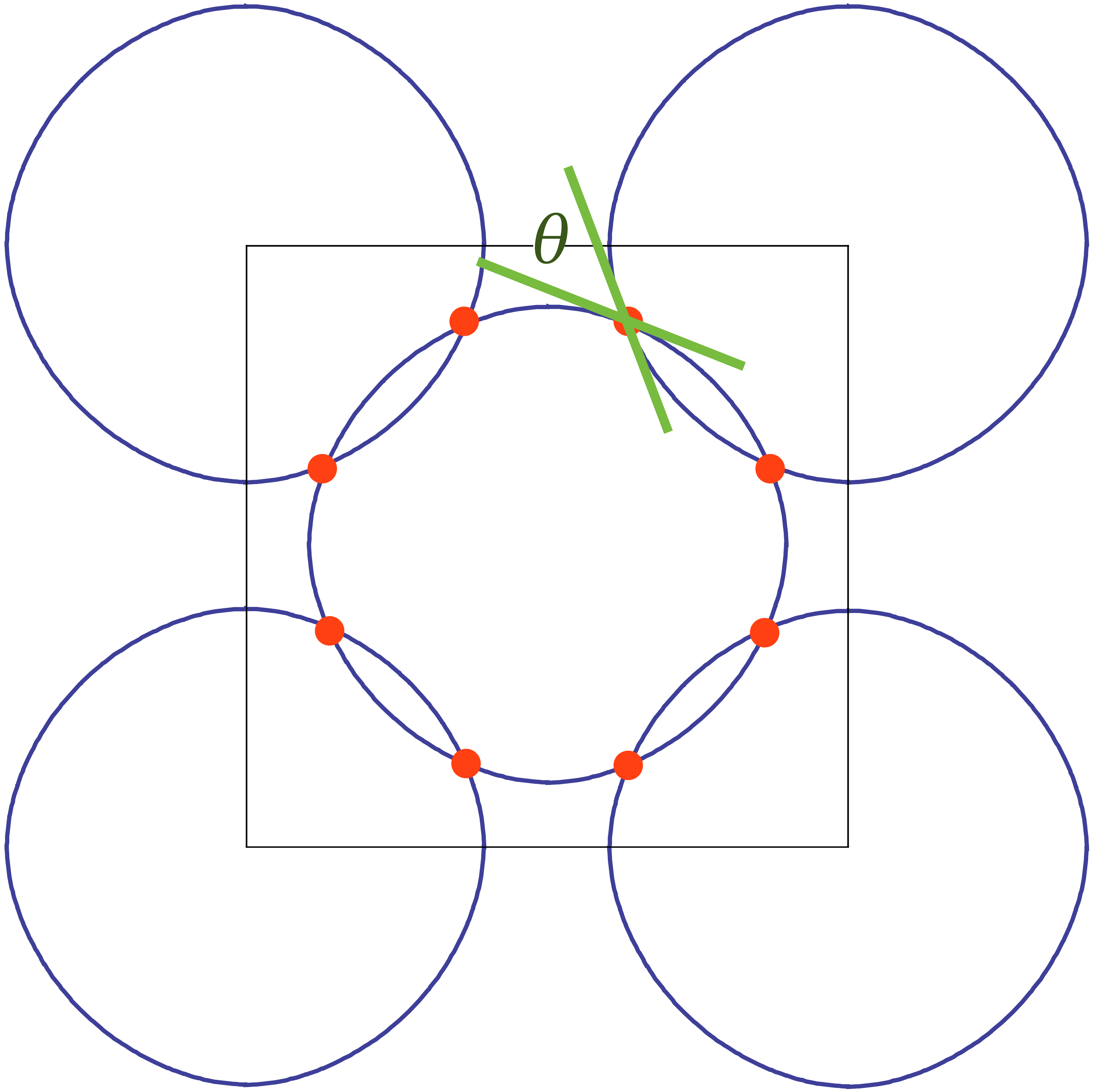
Antiferromagnetic critical point

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

Fermi energy

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* **85**, 075127 (2010)


θ

Enhancement of pairing susceptibility by interactions

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* **85**, 075127 (2010)

Summary:

- Field theory/RG provide strong evidence that there is unconventional ("pairing-amplitude-sign-changing") spin-singlet superconductivity at the antiferromagentic quantum critical point in all two-dimensional metals.

- The flow to strong-coupling indicates that Feynman graph/field theory/RG methods have reached their limits, and we have reached an impasse........

For the future........

- Use 1/(ego) as an expansion parameter (R. Shankar)

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- Solve on a computer: sign problem.........

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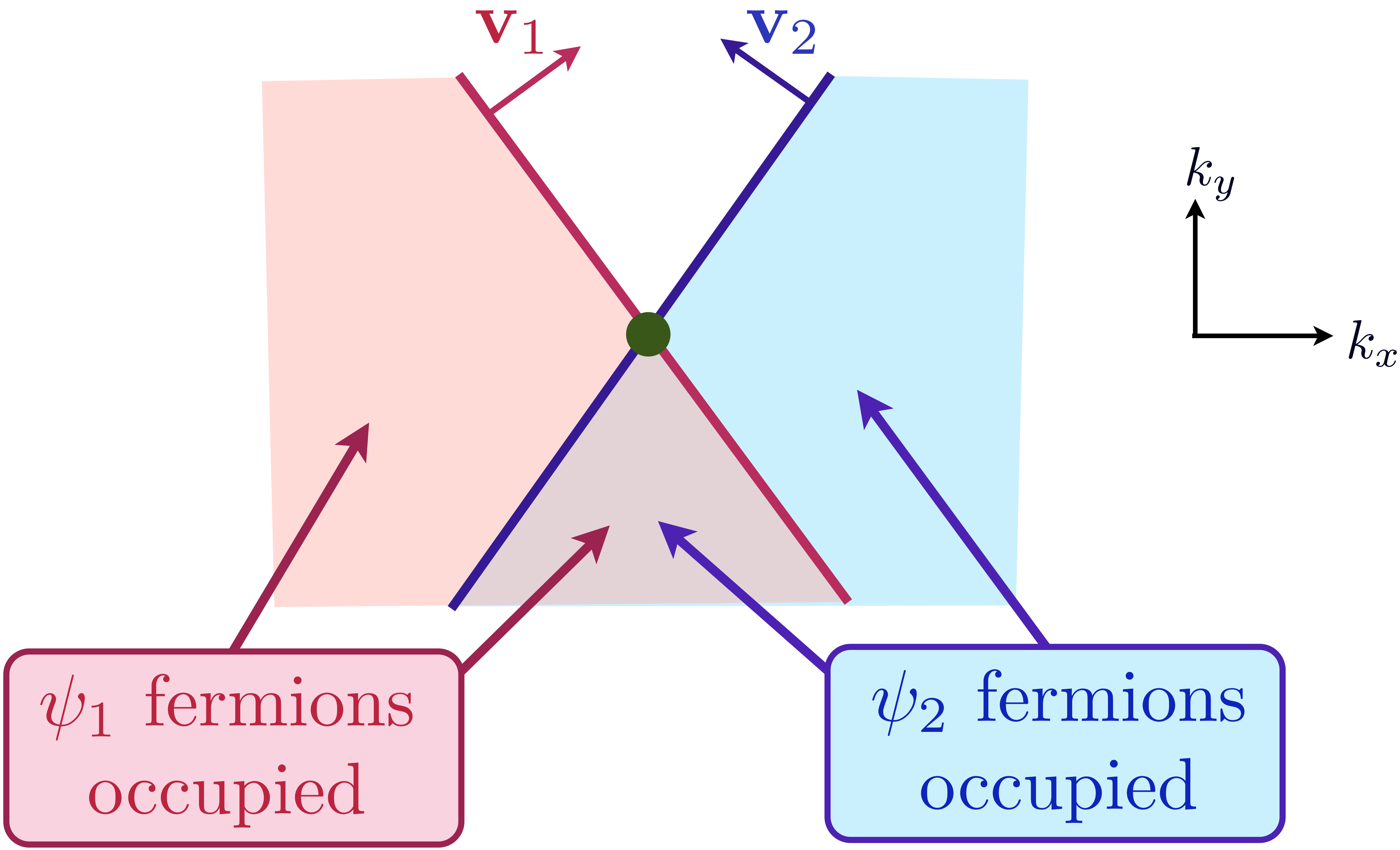

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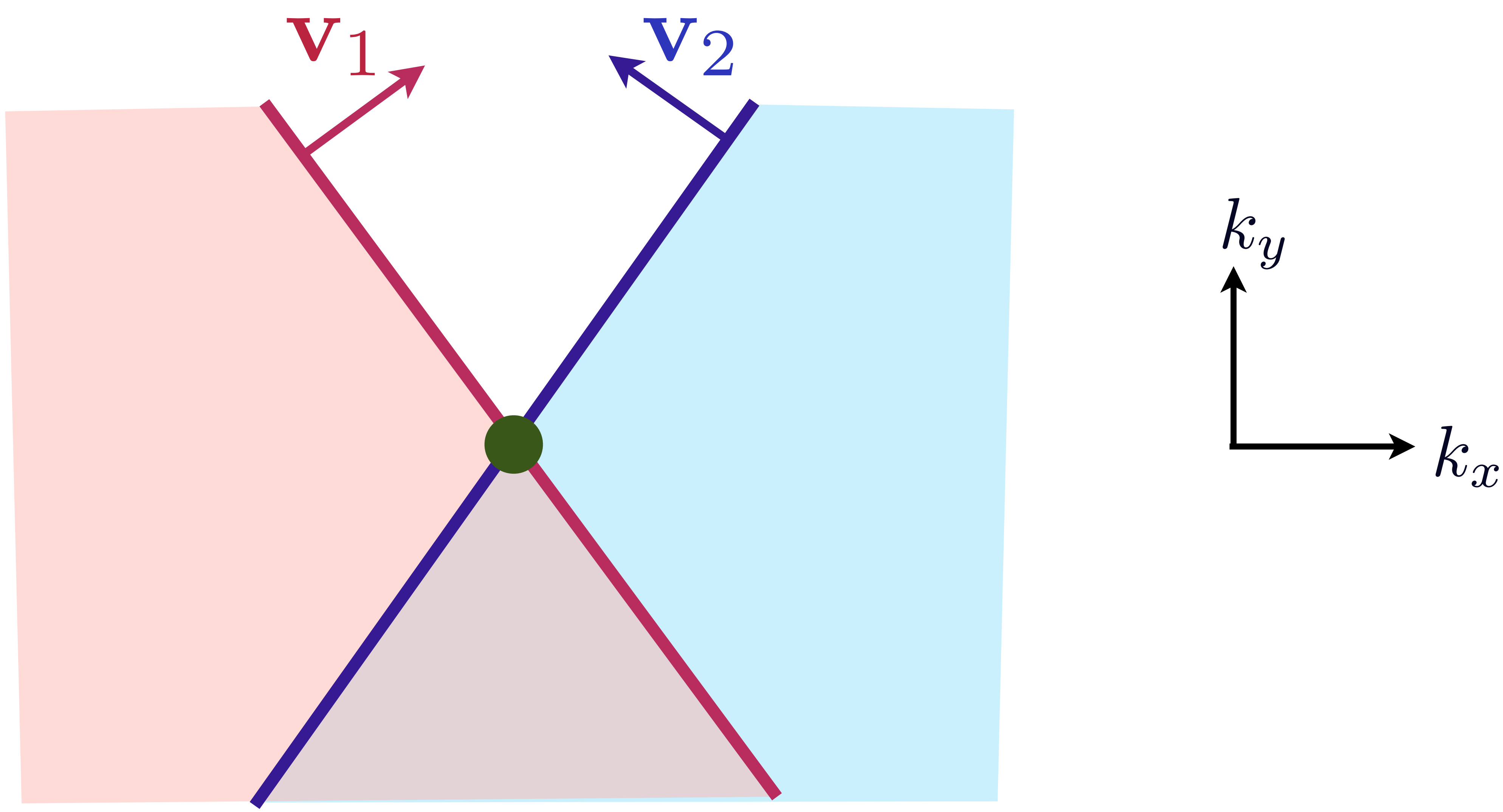
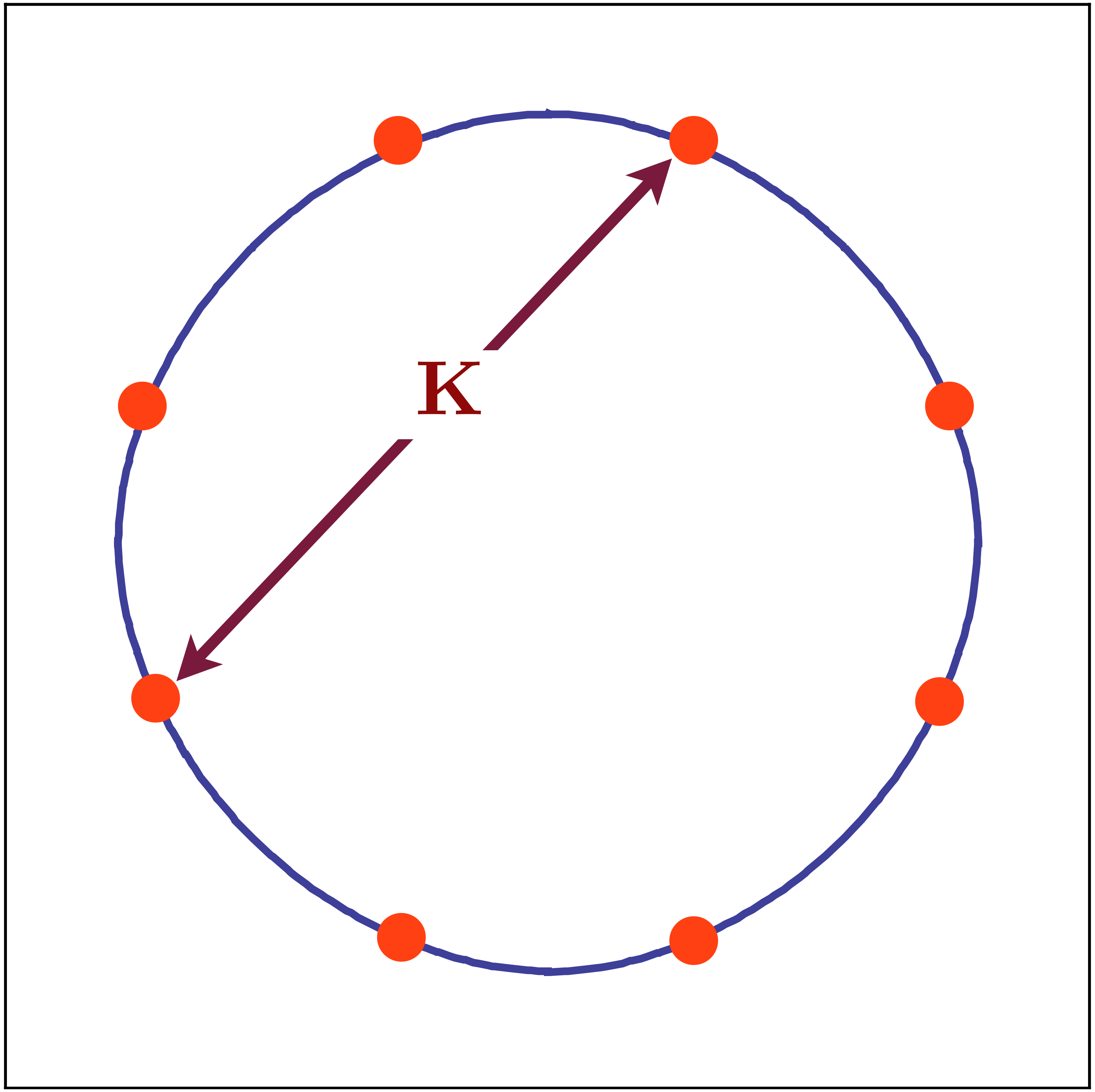


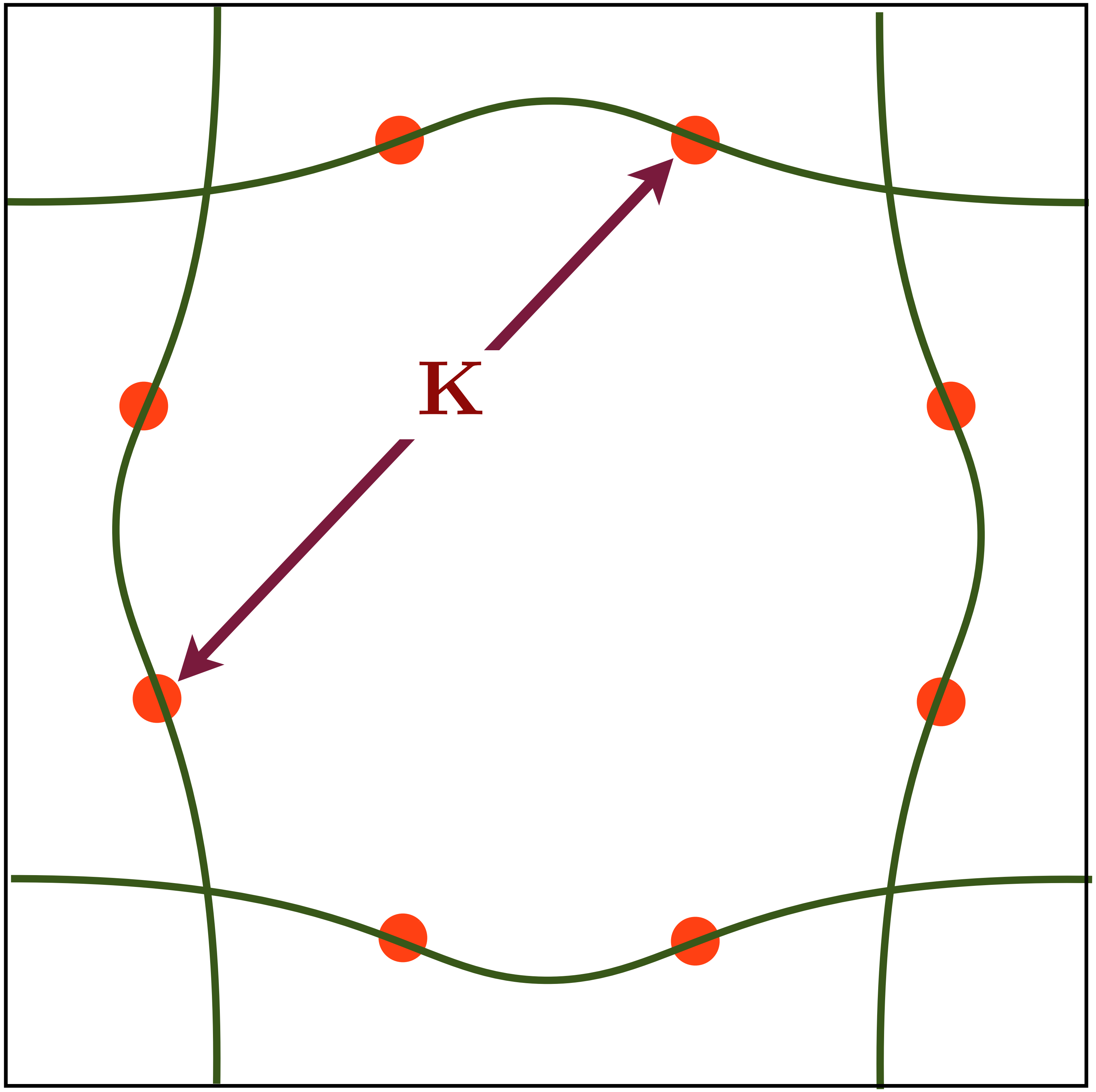
To faithfully realize low energy theory in quantum Monte Carlo, we need a UV completion in which Fermi lines don't end and all weights are positive.

QMC for the onset of antiferromagnetism



Hot spots in a single band model

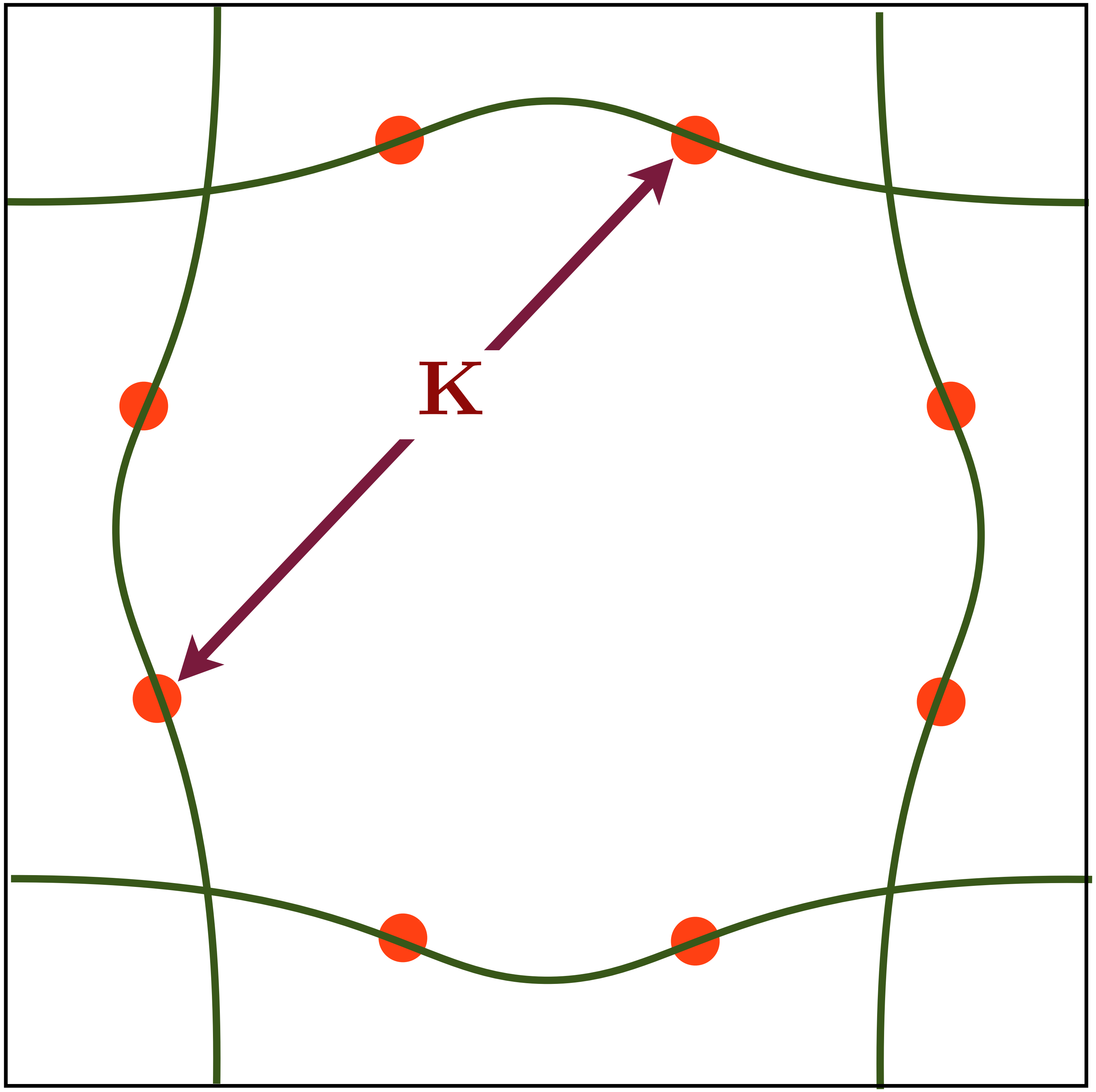
QMC for the onset of antiferromagnetism



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

Hot spots in a two band model

QMC for the onset of antiferromagnetism



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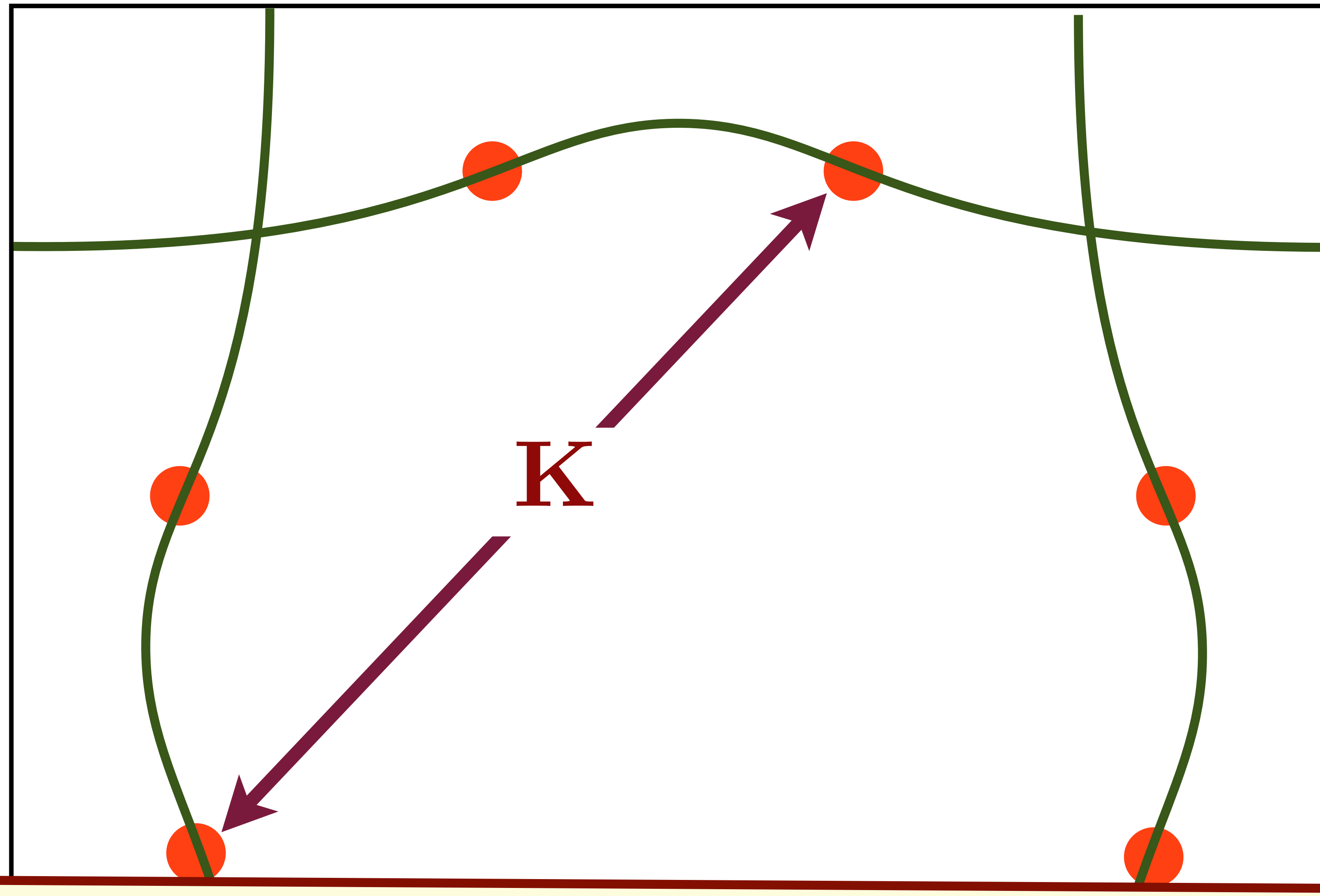

E. Berg,
M. Metlitski, and
S. Sachdev,
arXiv:1206.0742

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 $\vec{\varphi}$.

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

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

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

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

QMC for the onset of antiferromagnetism

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
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E. Berg,
M. Metlitski, and
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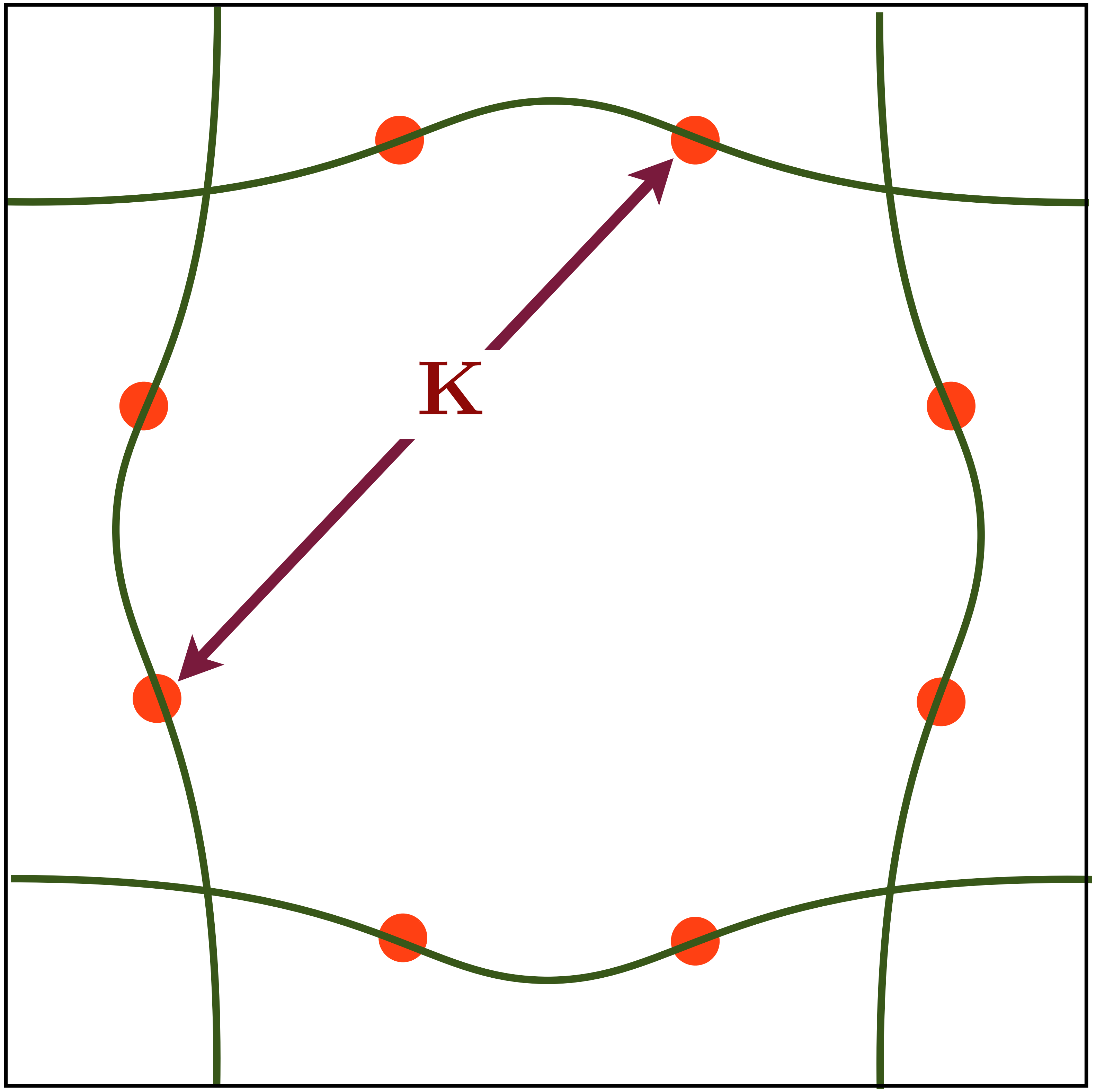
No sign problem !

QMC for the onset of antiferromagnetism



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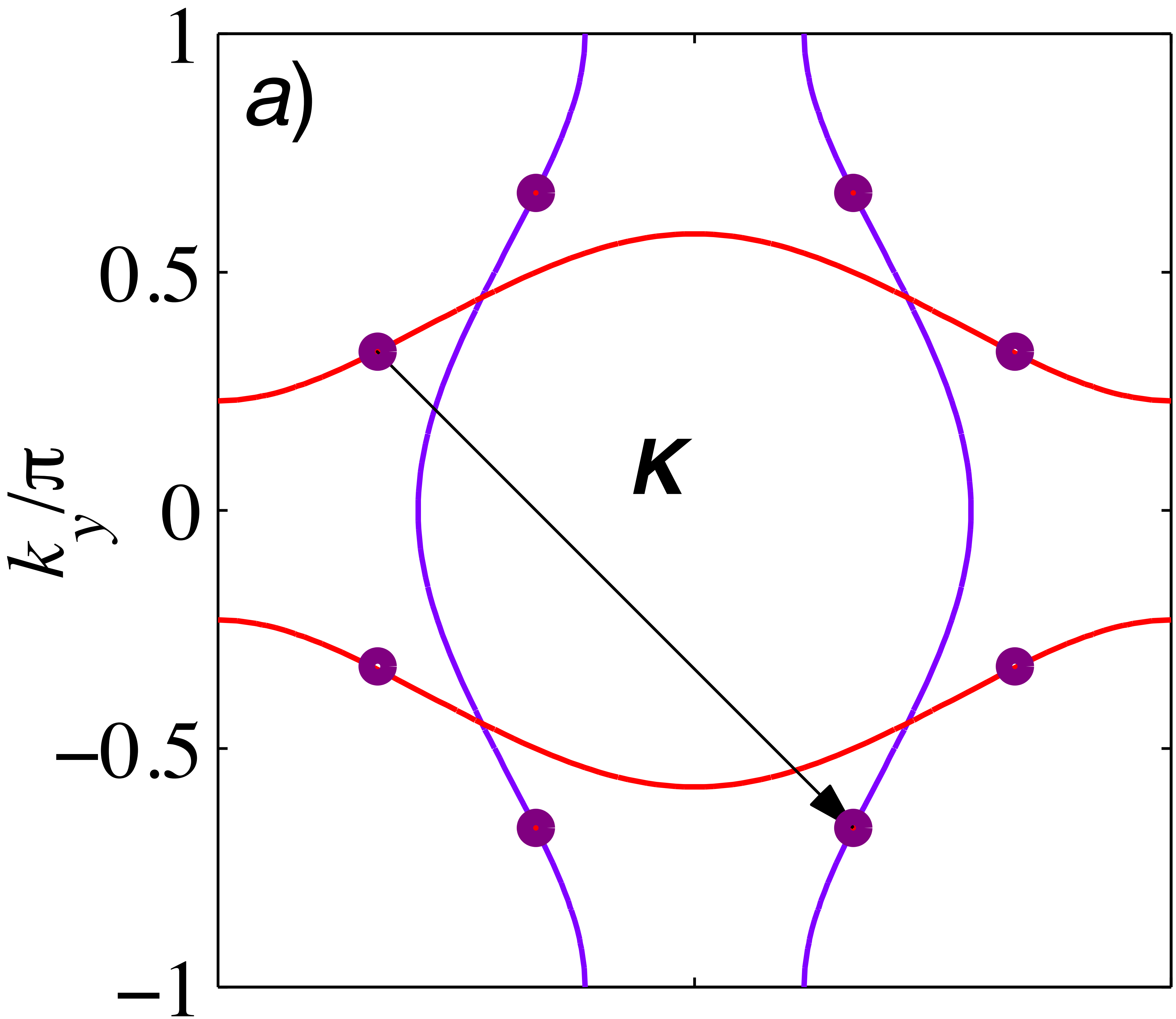
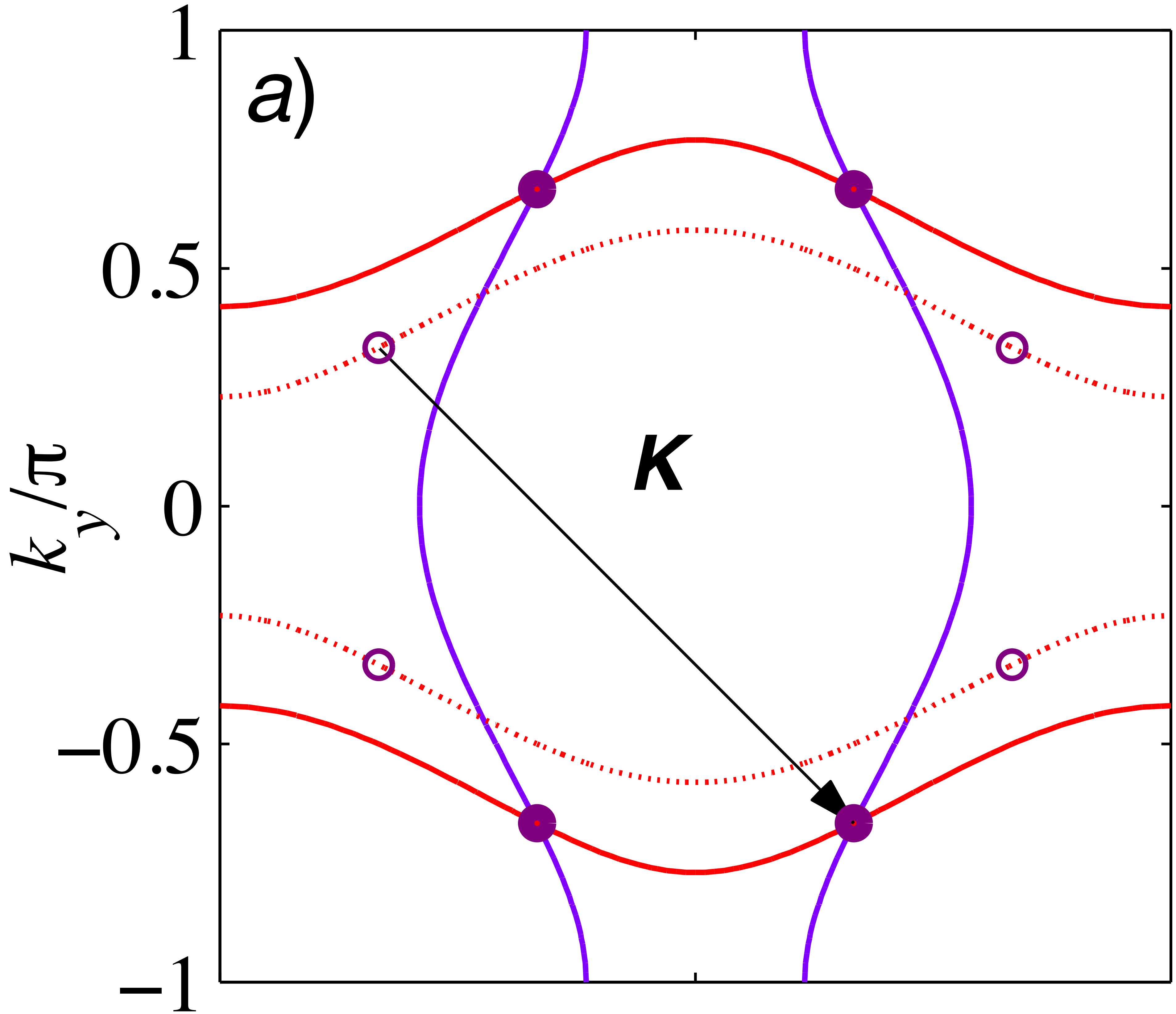


Center Brillouin zone at (π,π,)

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

QMC for the onset of antiferromagnetism

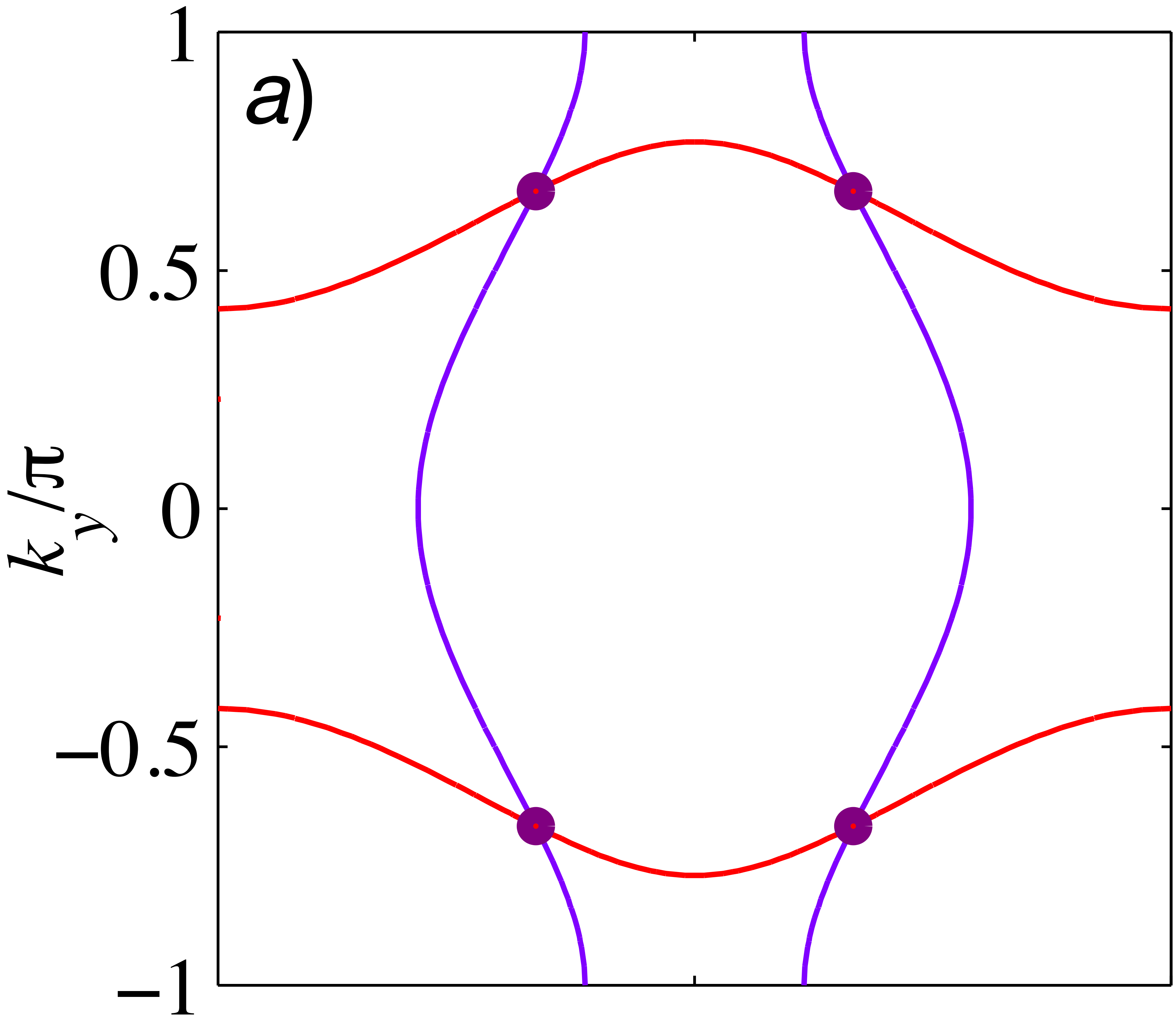


Move one of the Fermi surface by (π,π,)

E. Berg,
M. Metlitski, and
S. Sachdev,

arXiv:1206.0742

QMC for the onset of antiferromagnetism



E. Berg,
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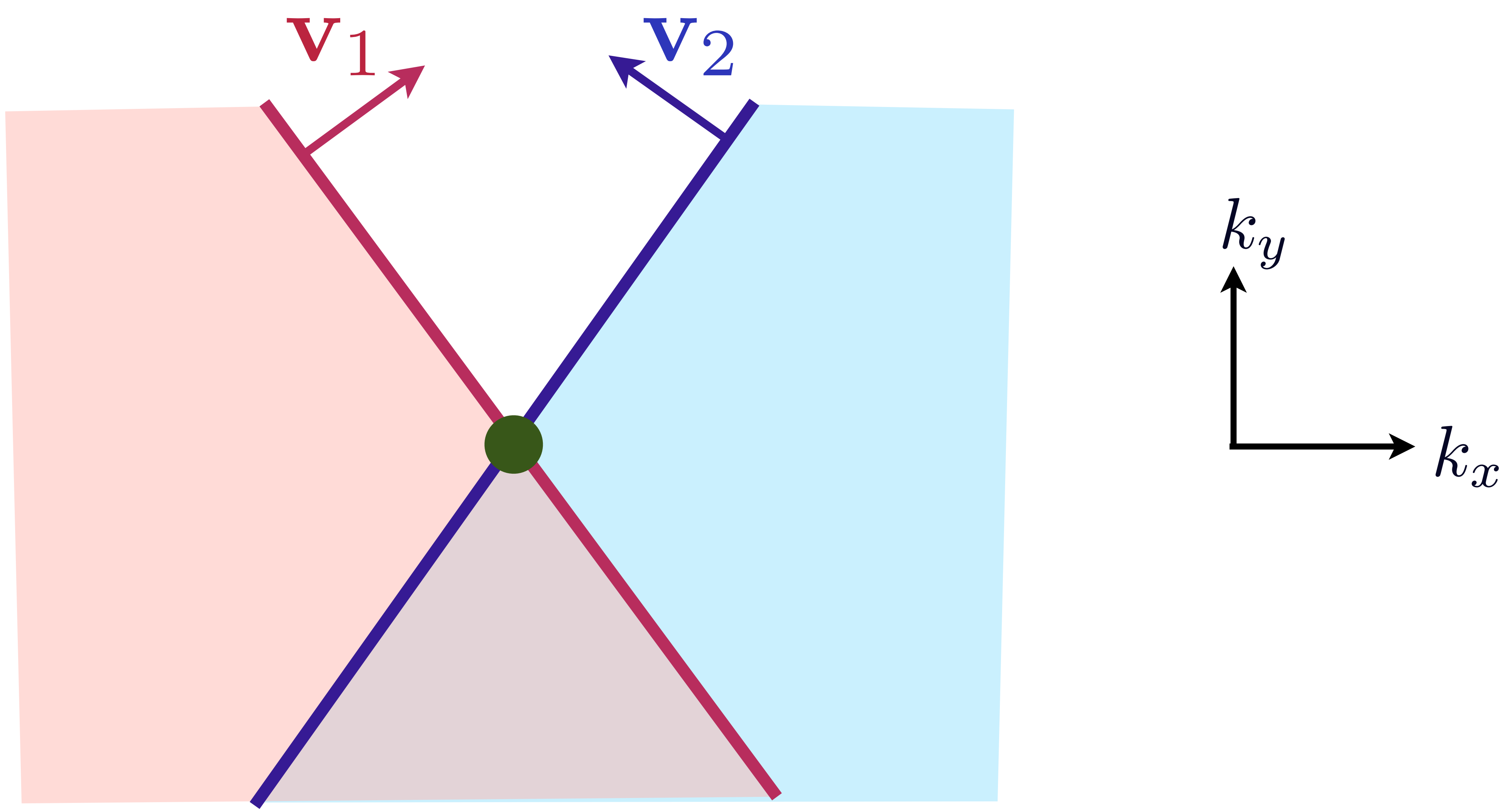
arXiv:1206.0742

Now hot spots are at Fermi surface intersections

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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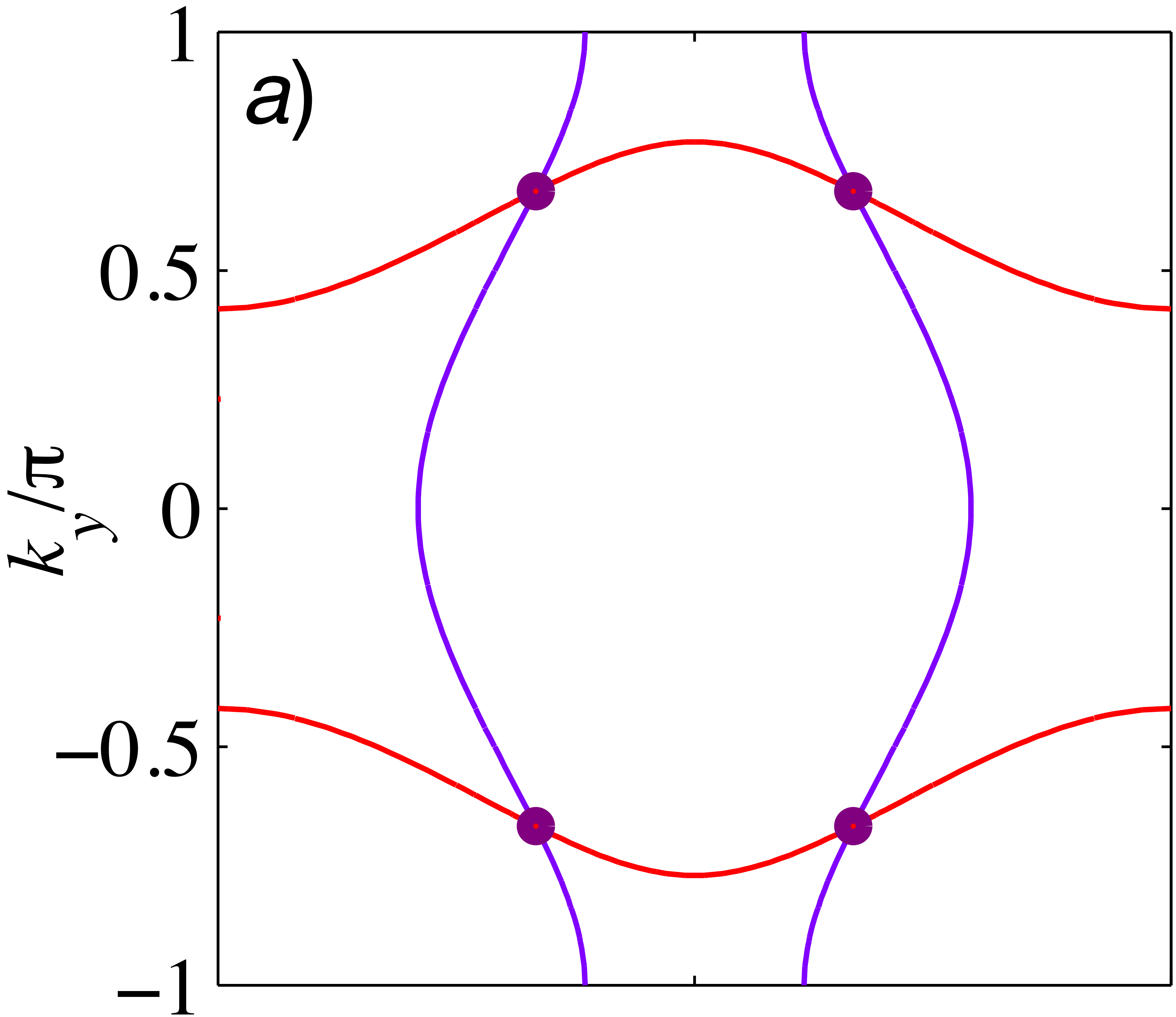

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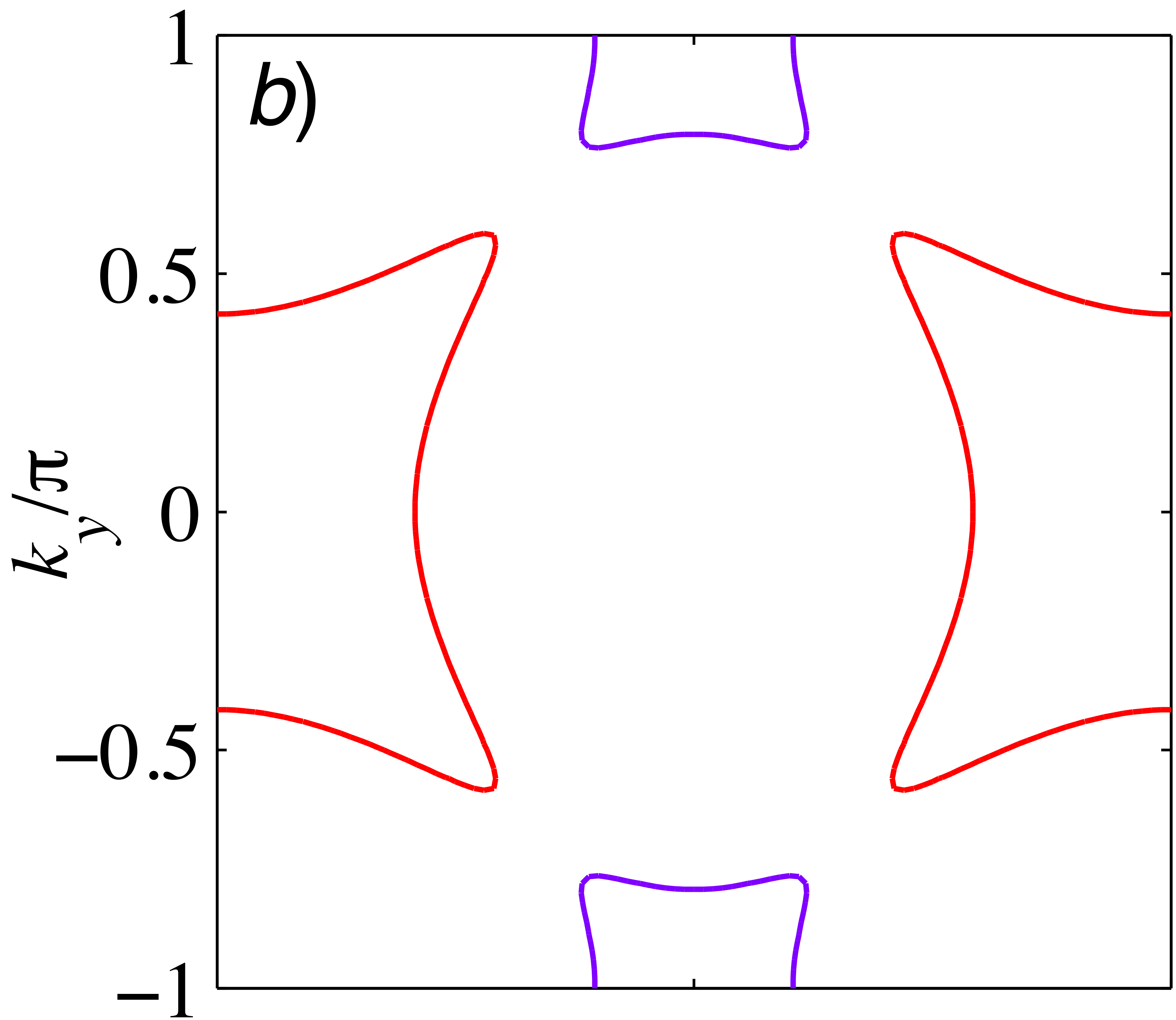
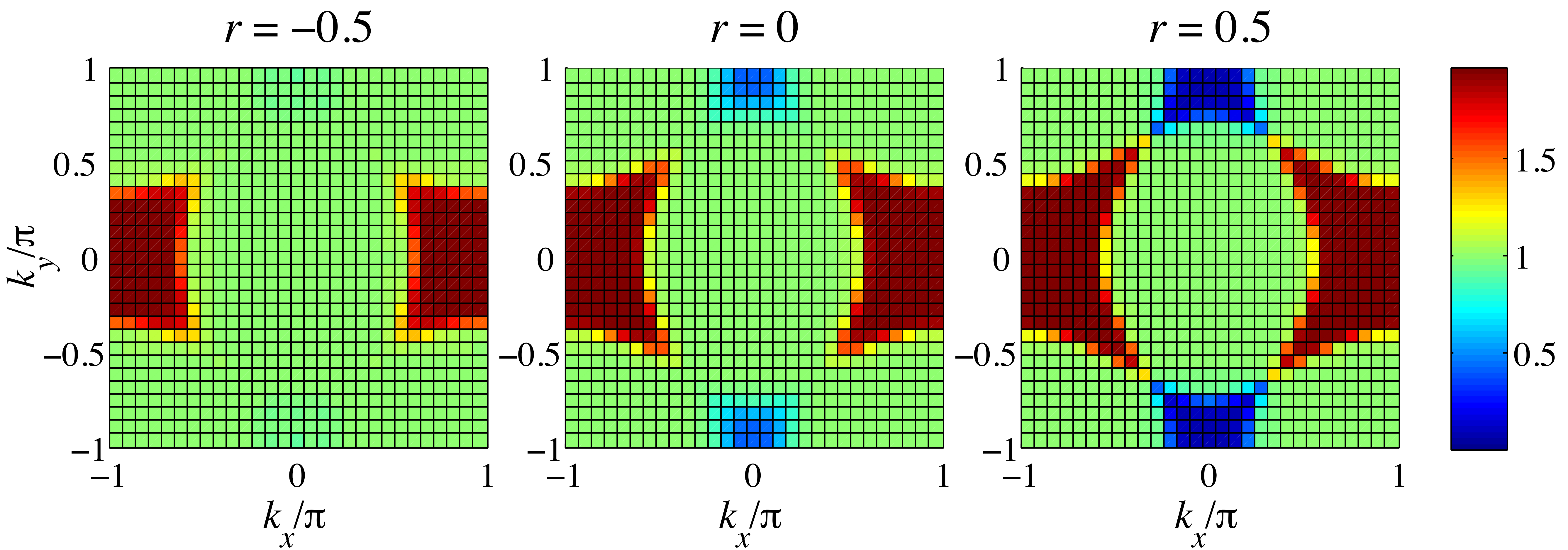


E. Berg,
M. Metlitski, and
S. Sachdev,
arXiv:1206.0742

Expected Fermi surfaces in the AFM ordered phase

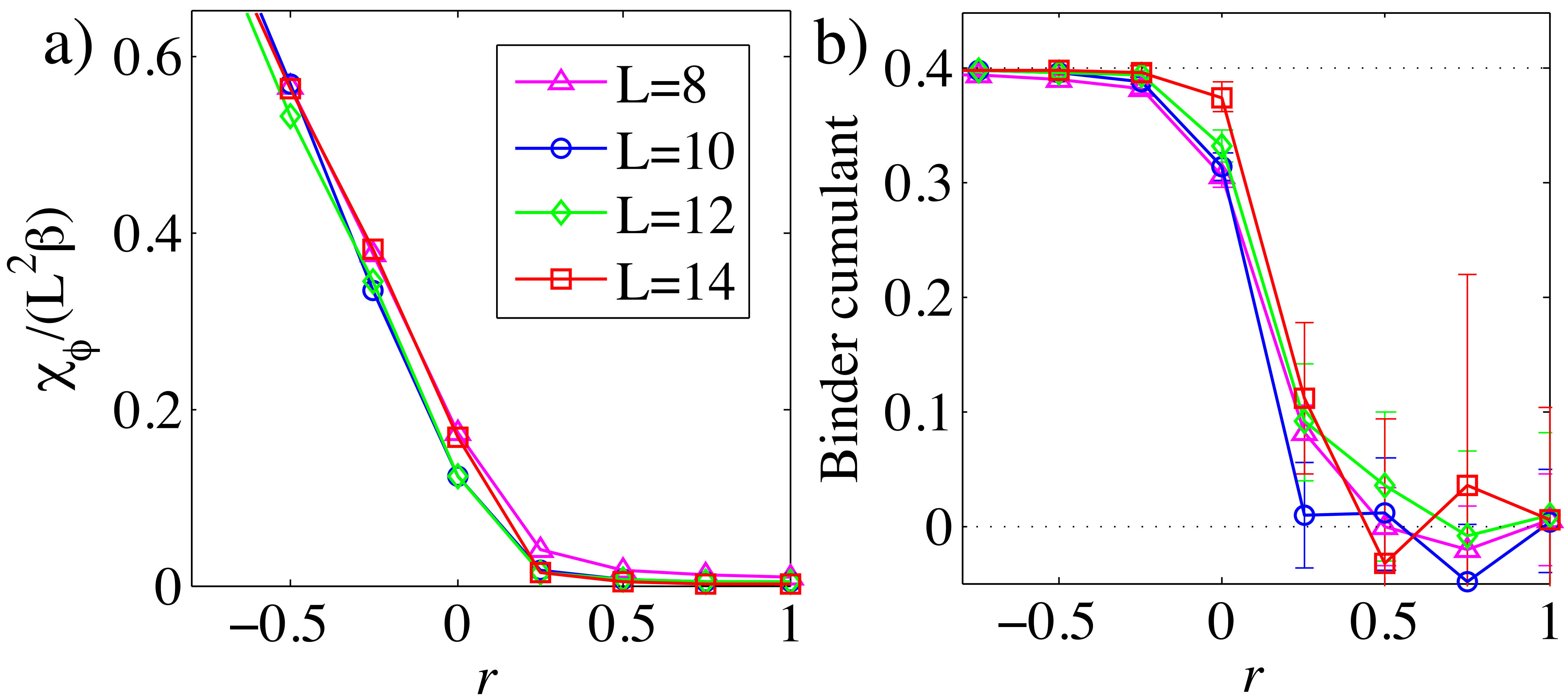
QMC for the onset of antiferromagnetism



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

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

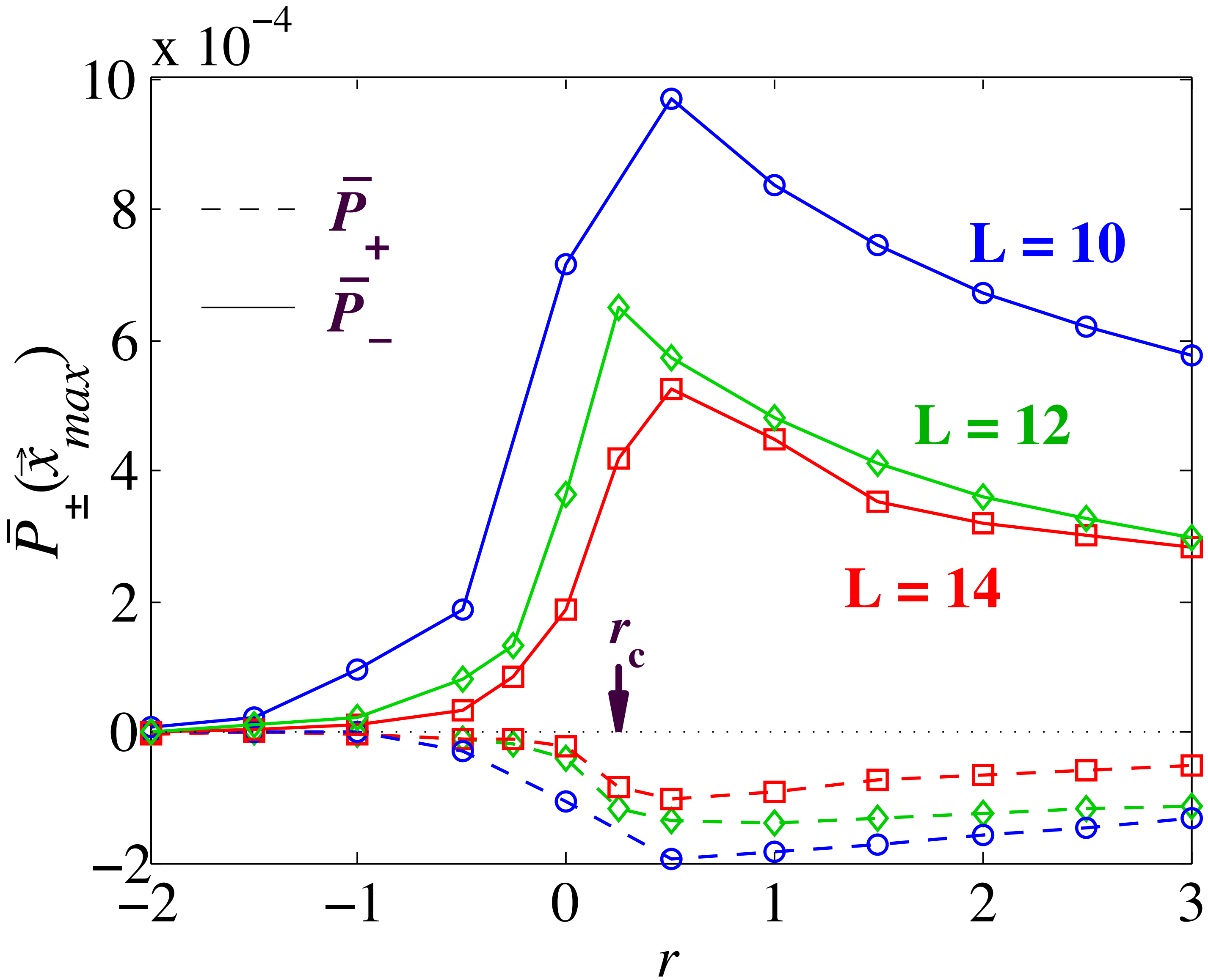
QMC for the onset of antiferromagnetism



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

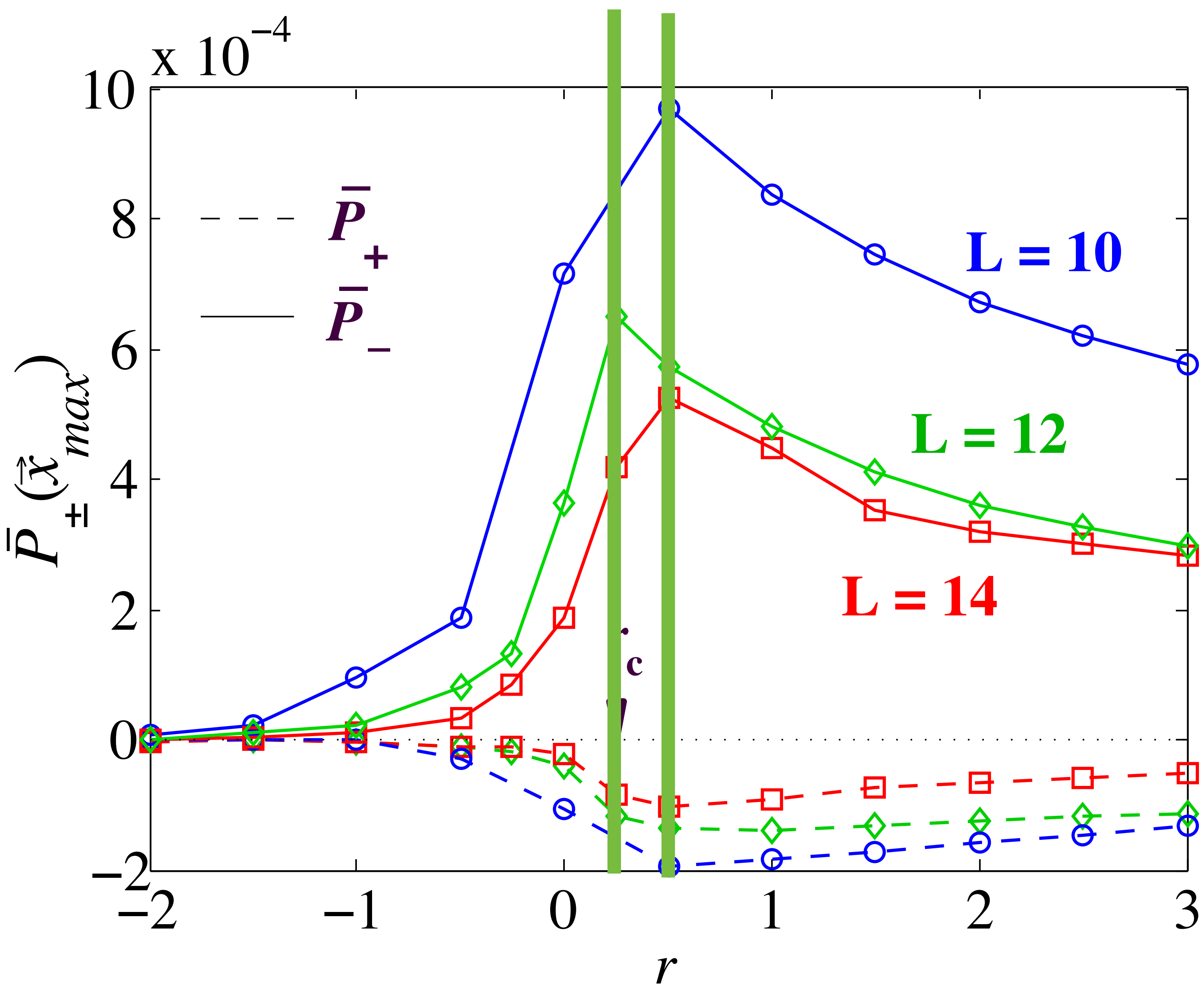
QMC for the onset of antiferromagnetism



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

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

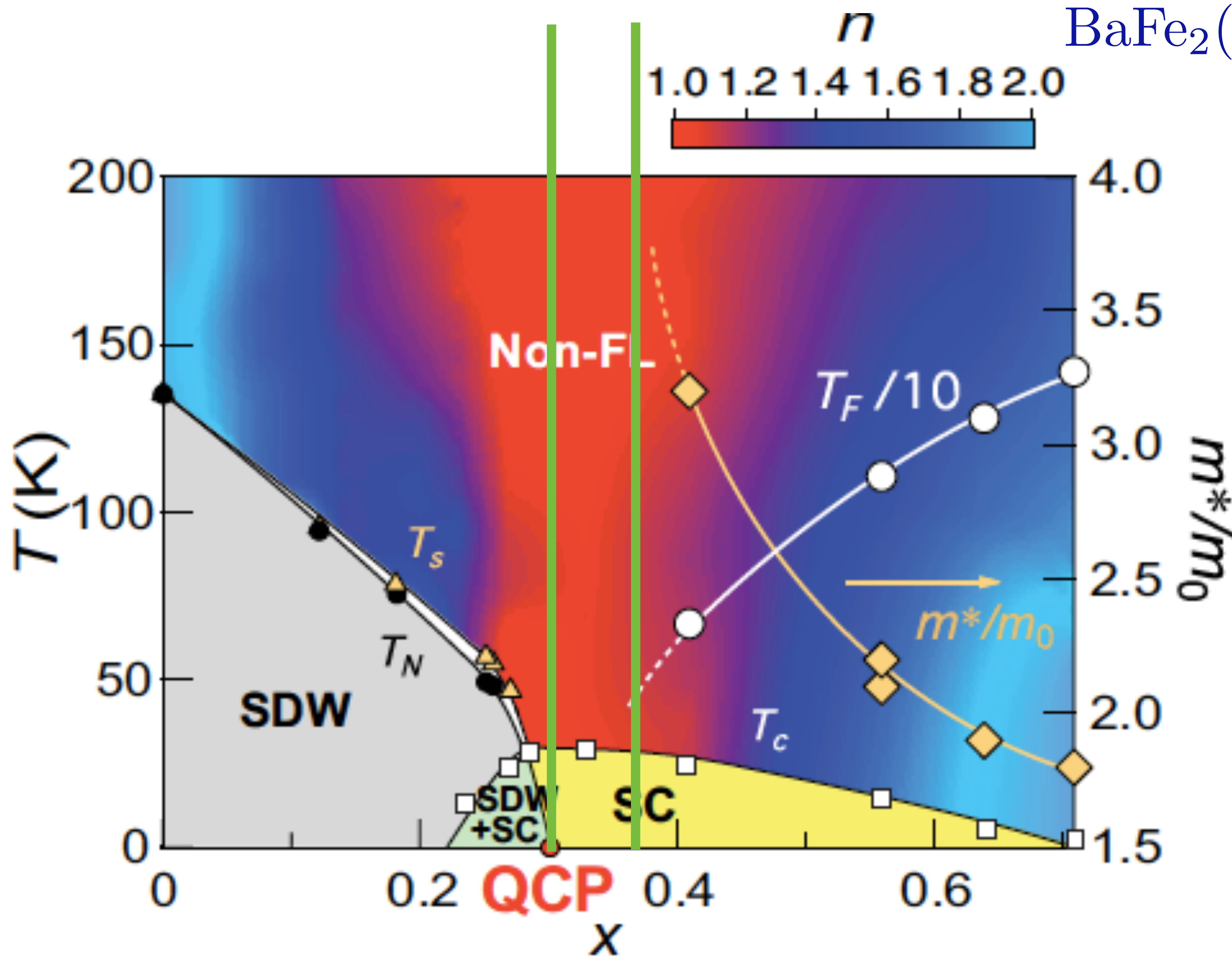
QMC for the onset of antiferromagnetism



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

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

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



Notice shift between the position of the QCP in the superconductor, and the divergence in effective mass in the metal measured at high magnetic fields

Outline

1. Phenomenology of the onset of antiferromagnetism in a metal

2. Quantum field theory of the onset of antiferromagnetism in a metal

3. Quantum Monte Carlo without the sign problem

4. Fractionalization in metals, and the hole-doped cuprates

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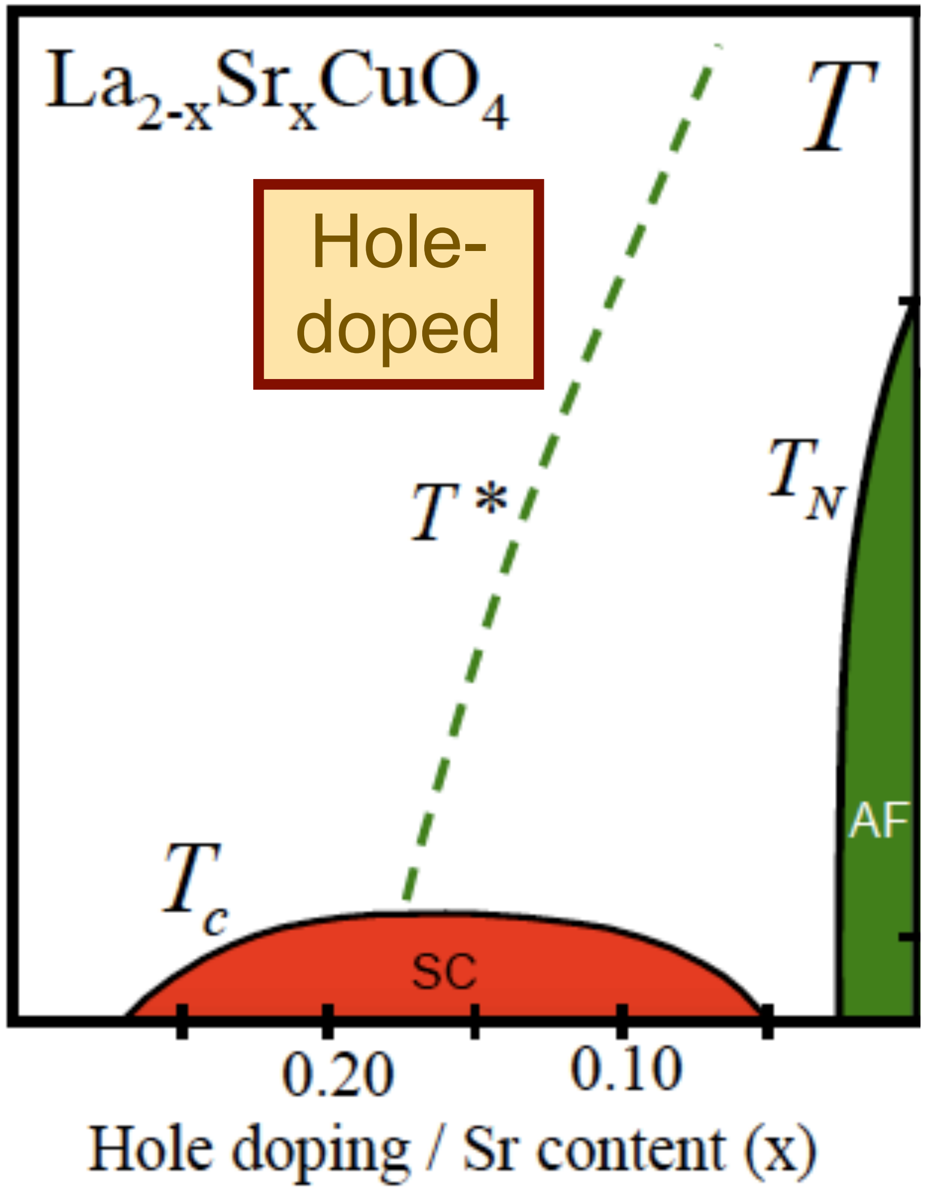
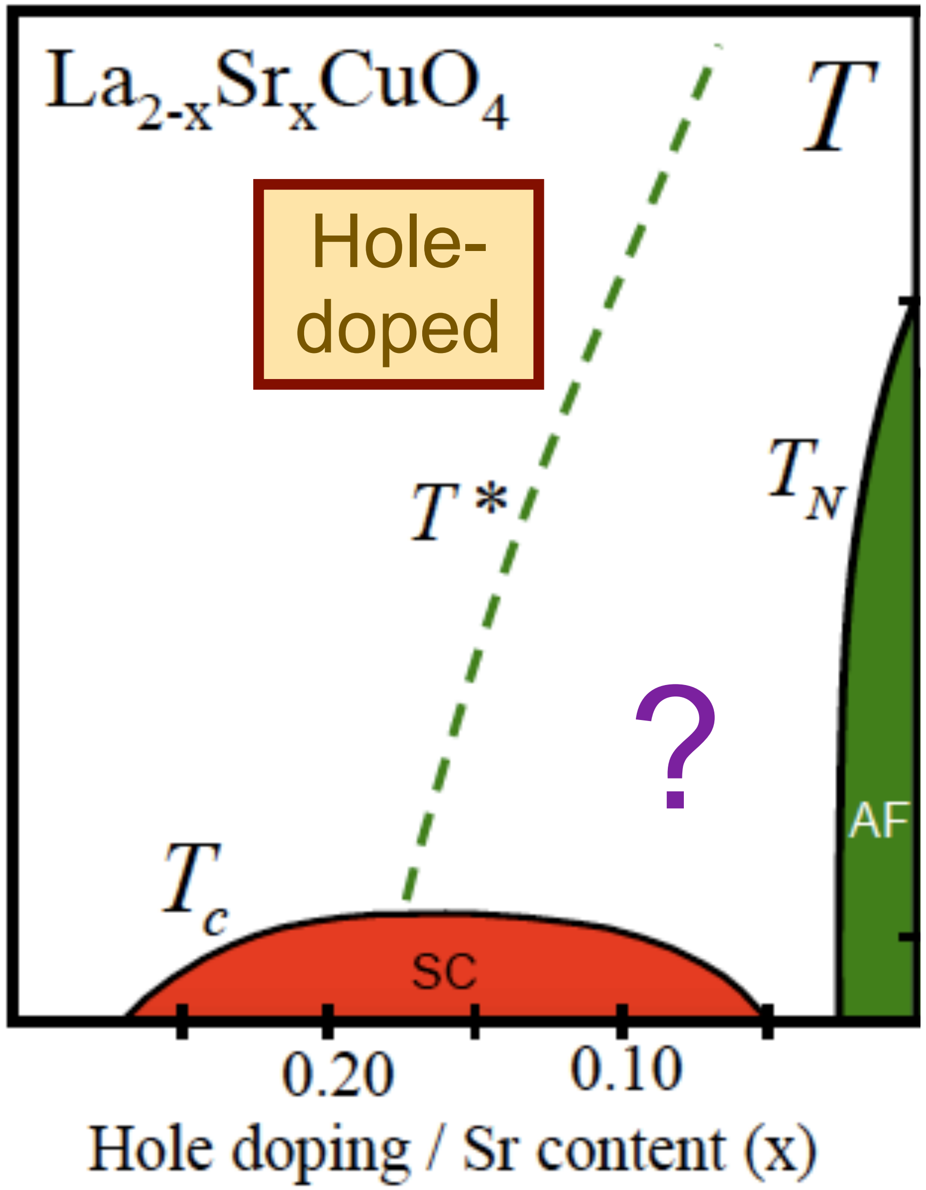


$La_{2-x}Sr_xCuO_4$
T
Hole-
doped
T^*
T_N
AF
T_c
SC
0.20
0.10
Hole doping / Sr content (x)


$La_{2-x}Sr_xCuO_4$
T
Hole-
doped
T^*
T_N
?
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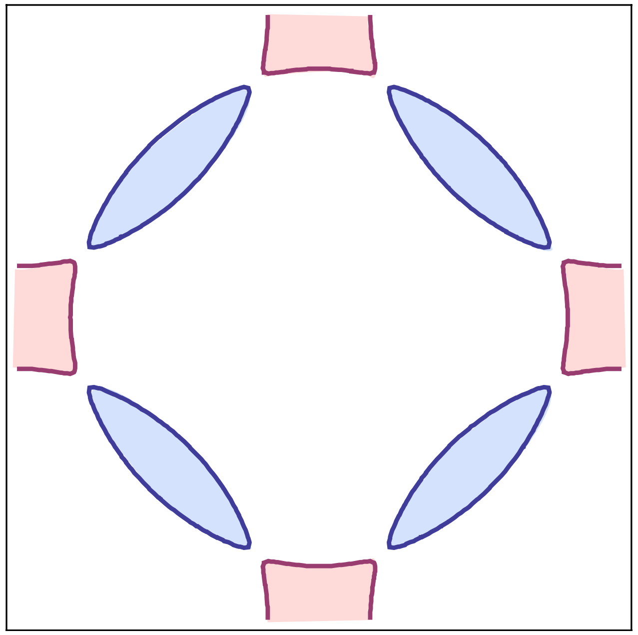
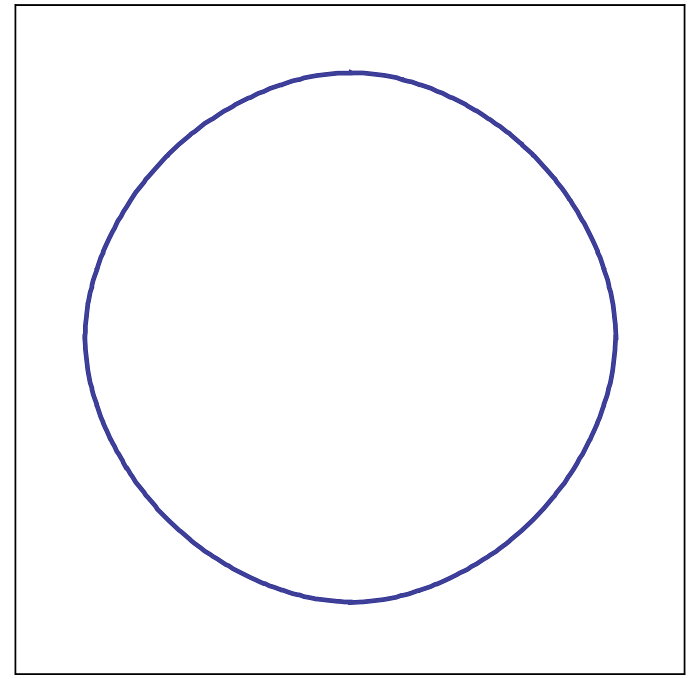
T_c
SC
0.20
0.10
Hole doping / Sr content (x)

Quantum phase transition with Fermi surface reconstruction



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

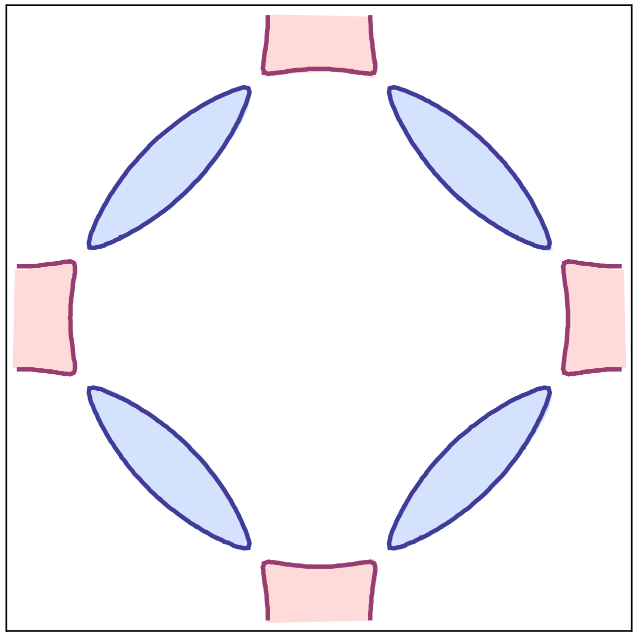
Metal with electron and hole pockets



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

Metal with "large" Fermi surface

Separating onset of SDW order and Fermi surface reconstruction



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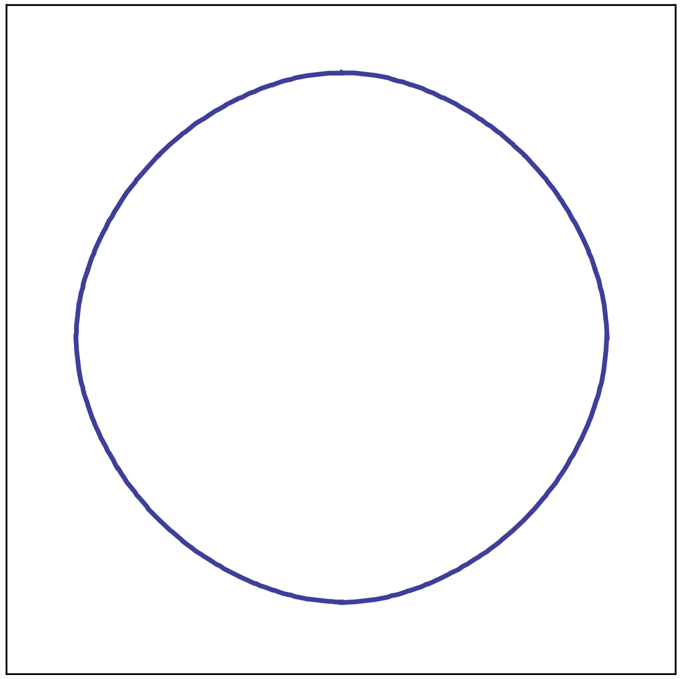

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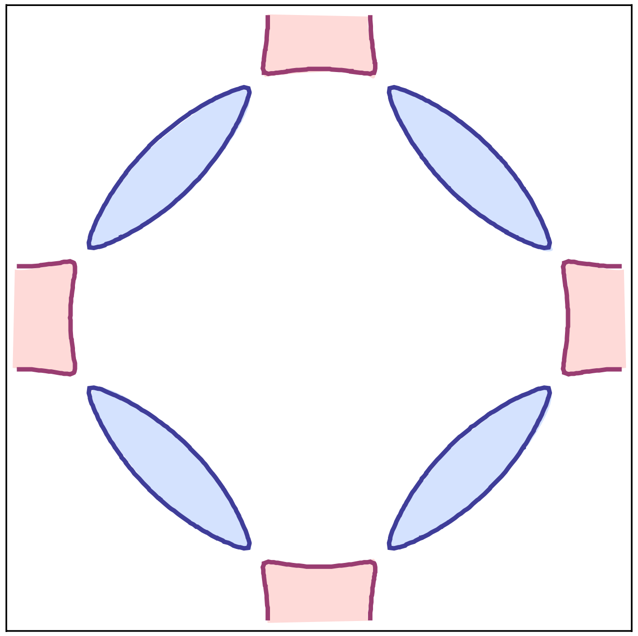
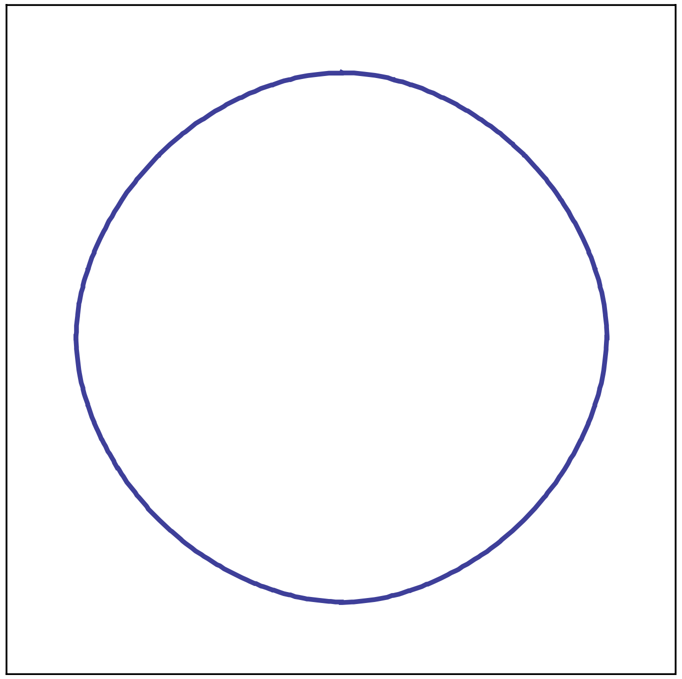


Electron and/or hole Fermi pockets form in "local" SDW order, but quantum fluctuations destroy long-range SDW order



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

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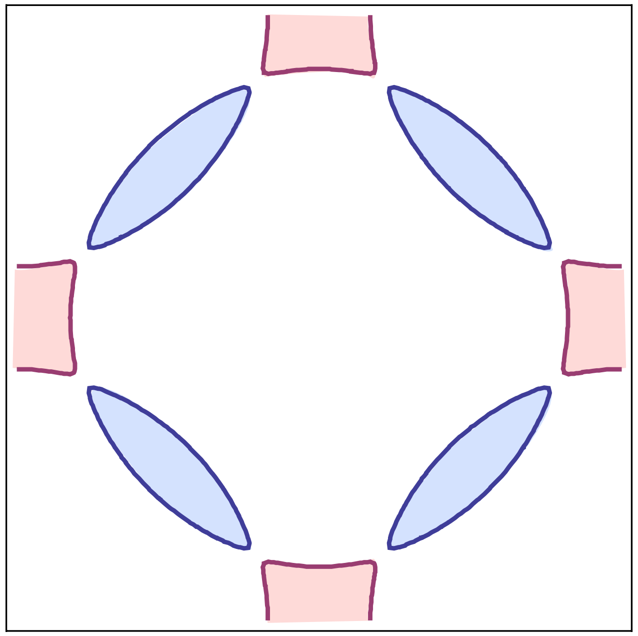

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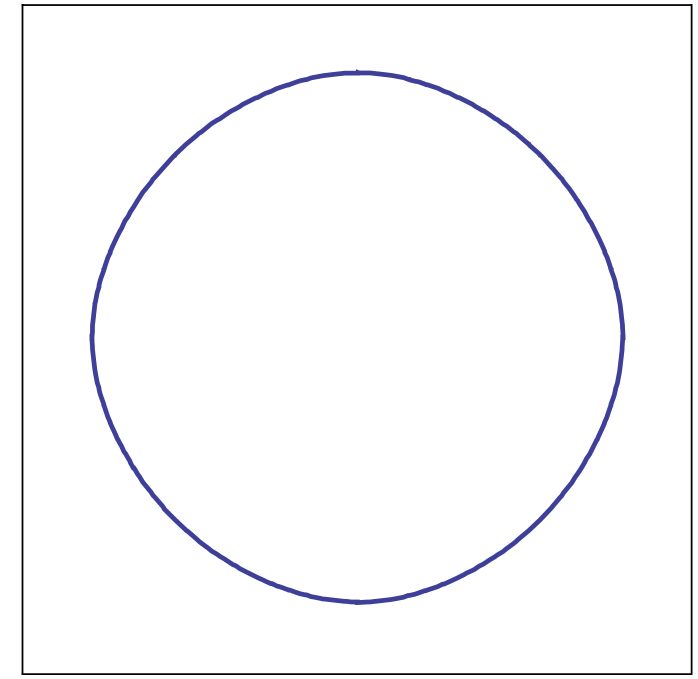

$\langle \vec{\varphi} \rangle \neq 0$

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

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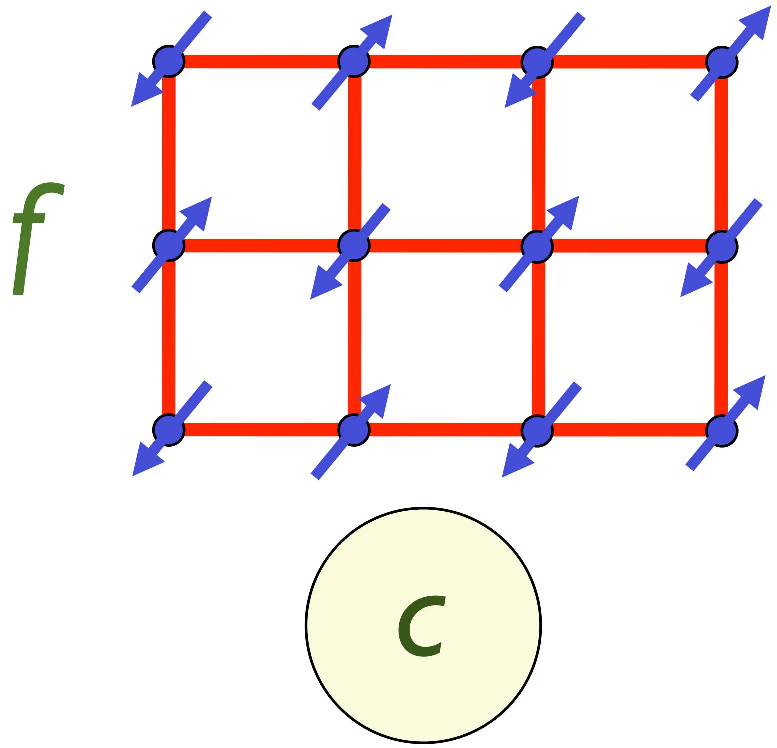
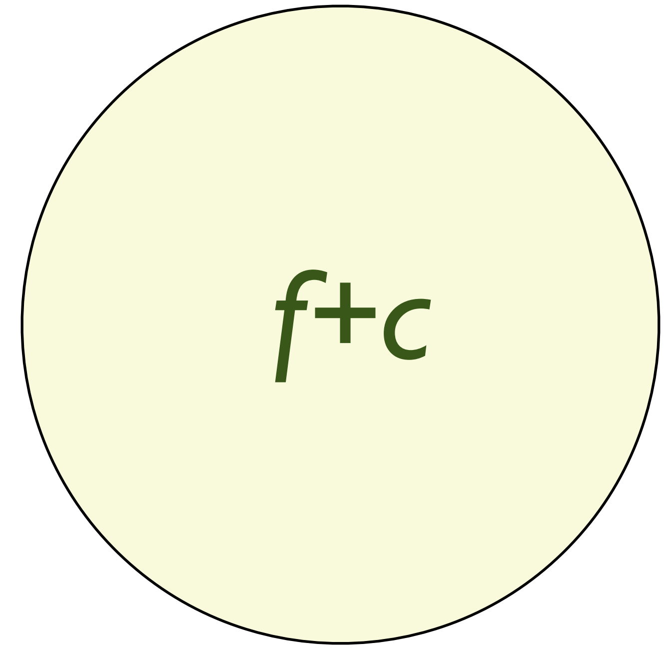
T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

Magnetic order and the heavy Fermi liquid in the Kondo lattice



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

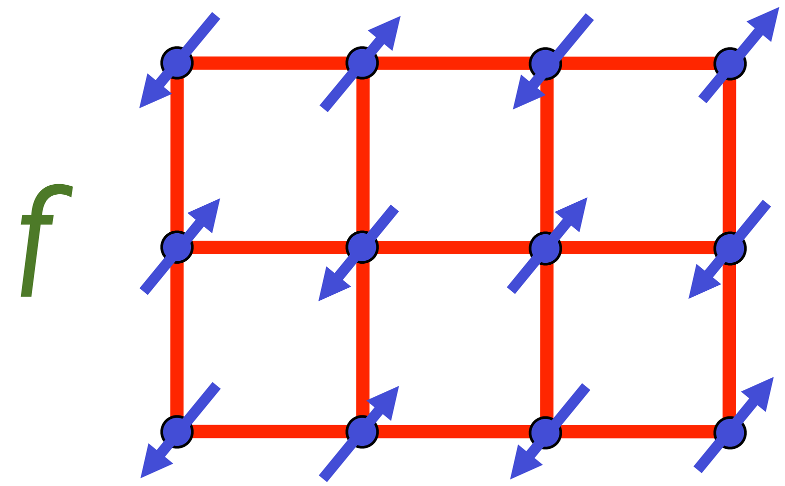
Magnetic Metal:
f-electron moments
and
c-conduction electron
Fermi surface

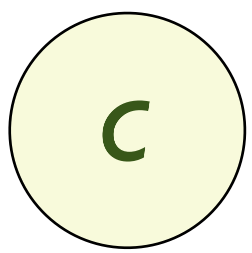


$$\langle \vec{\varphi} \rangle = 0$$

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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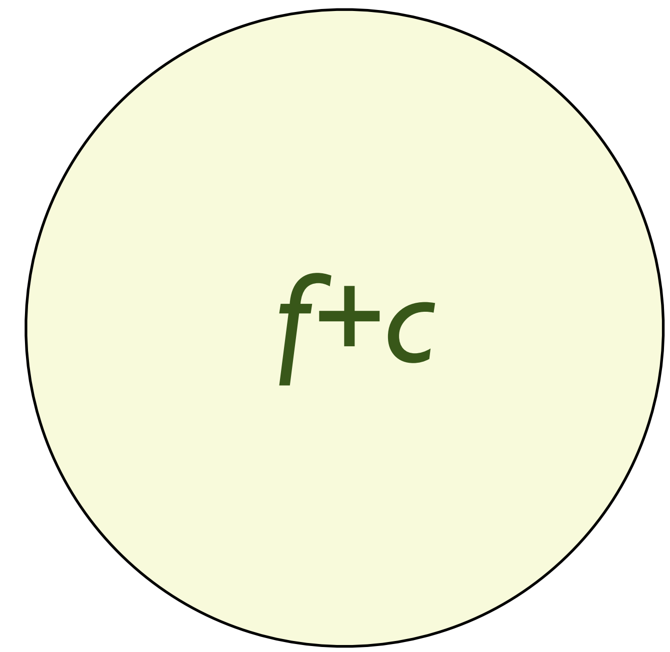

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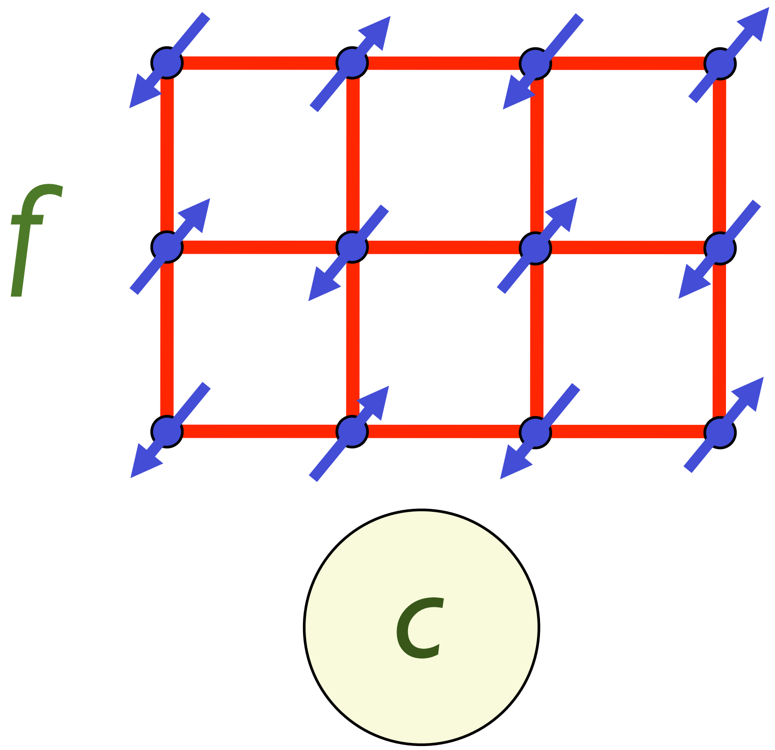

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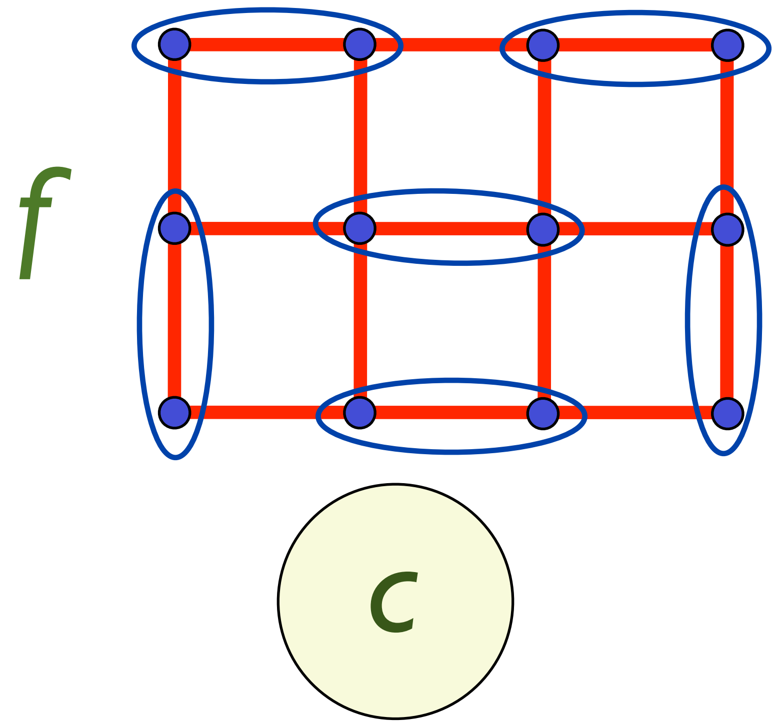
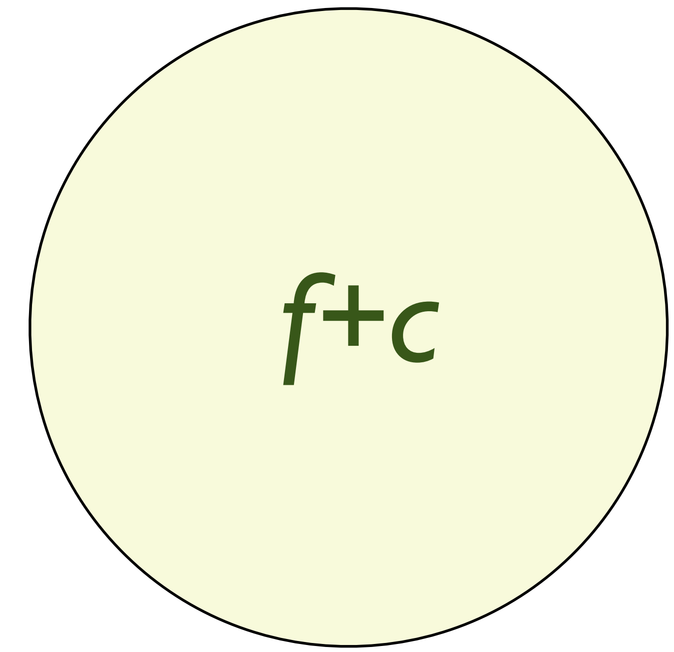


$$\langle \vec{\varphi} \rangle = 0$$

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



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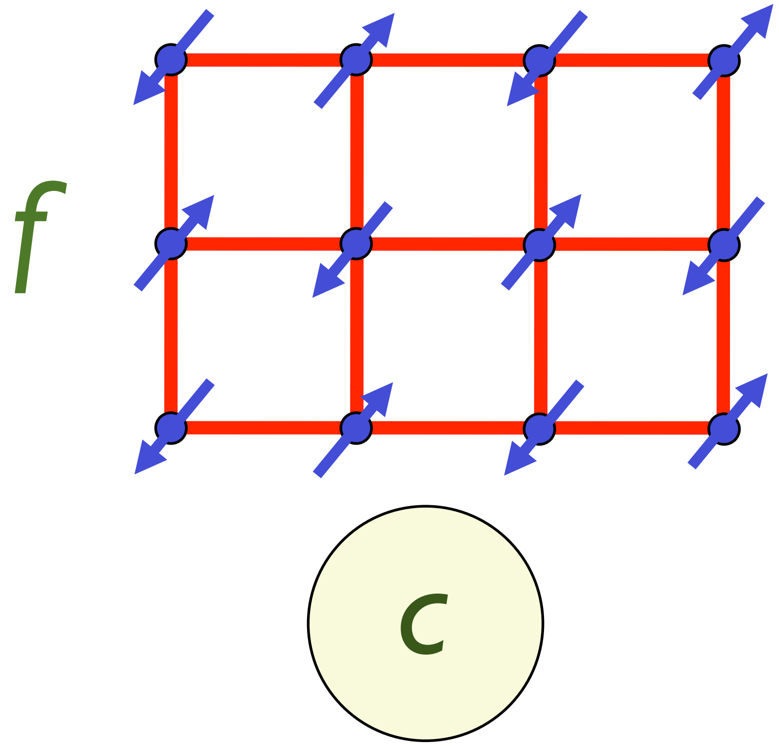

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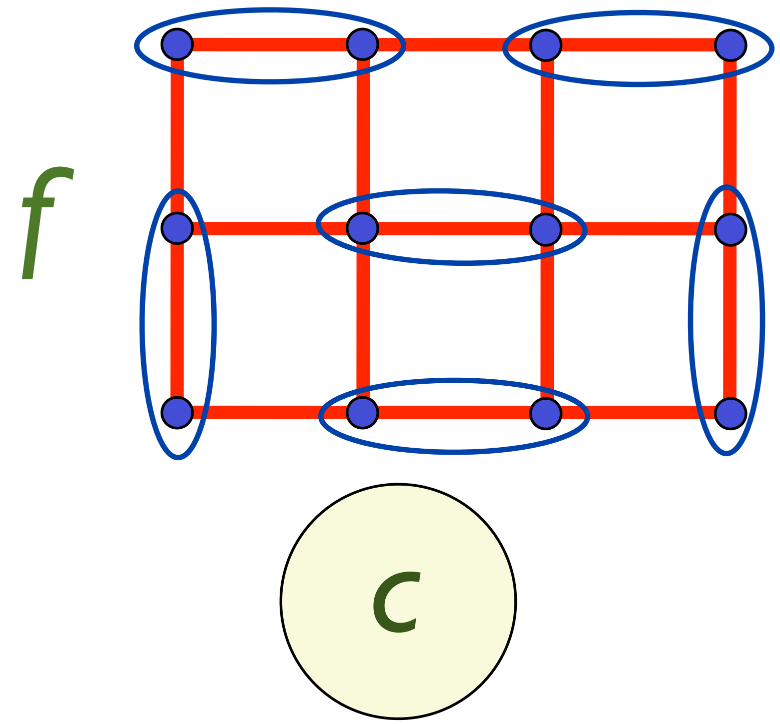

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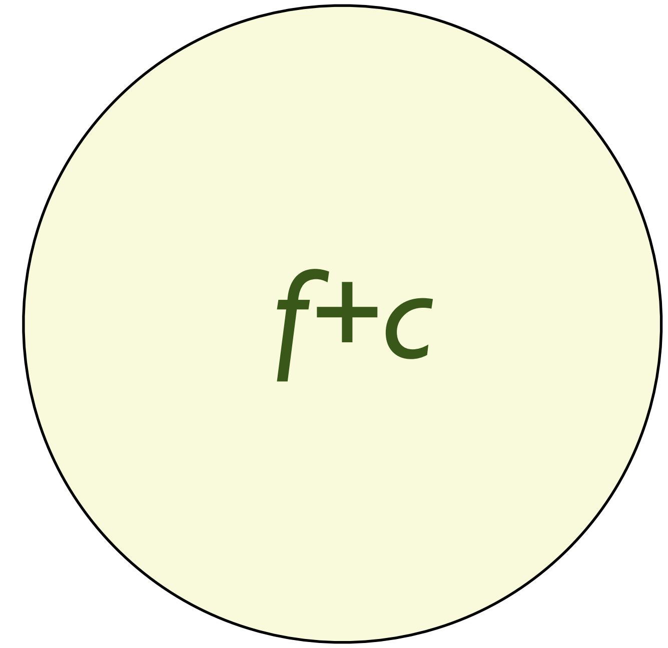
Fractionalized Fermi liquid (FL*) phase with no symmetry breaking and "small" Fermi surface



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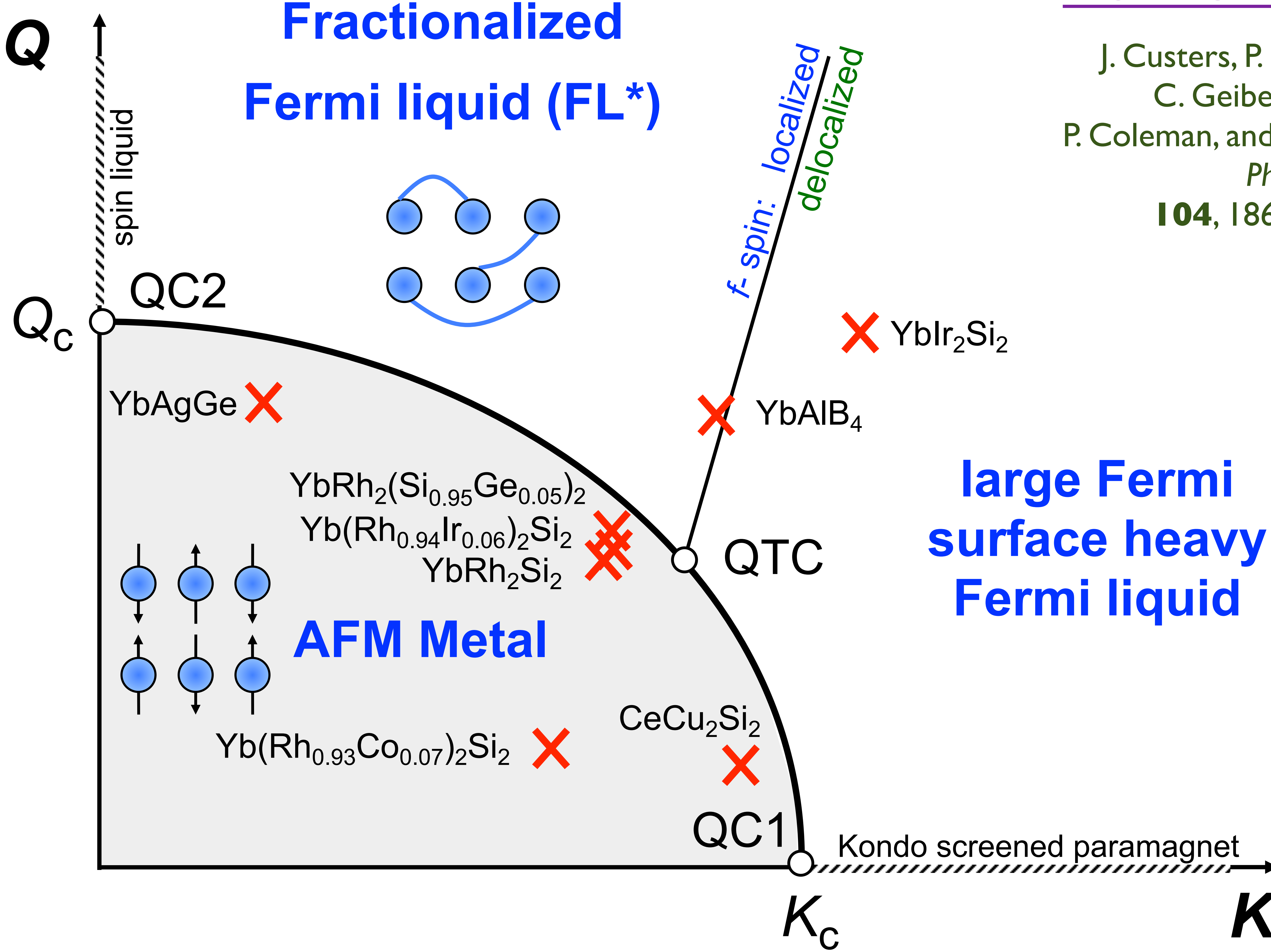
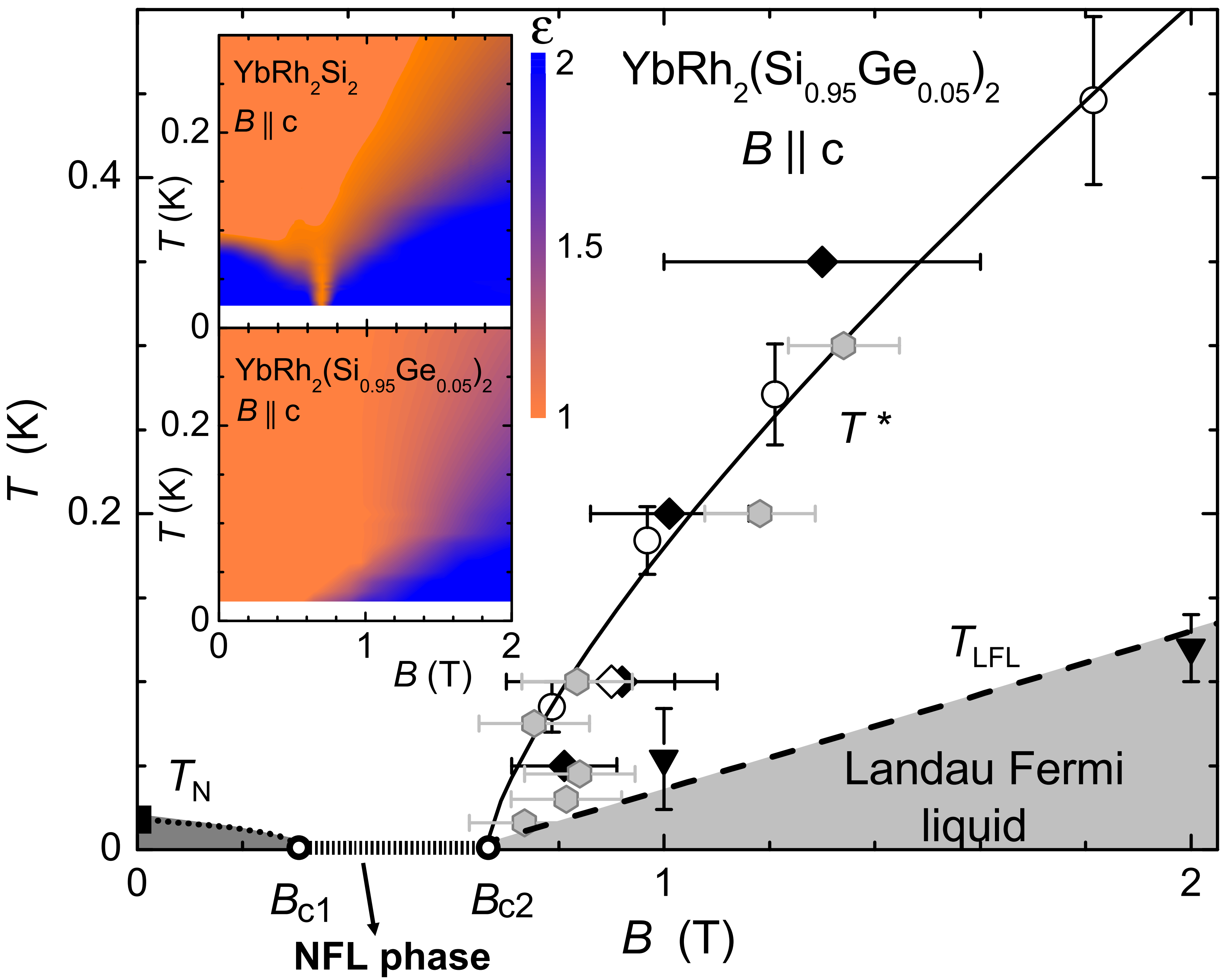
T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

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)





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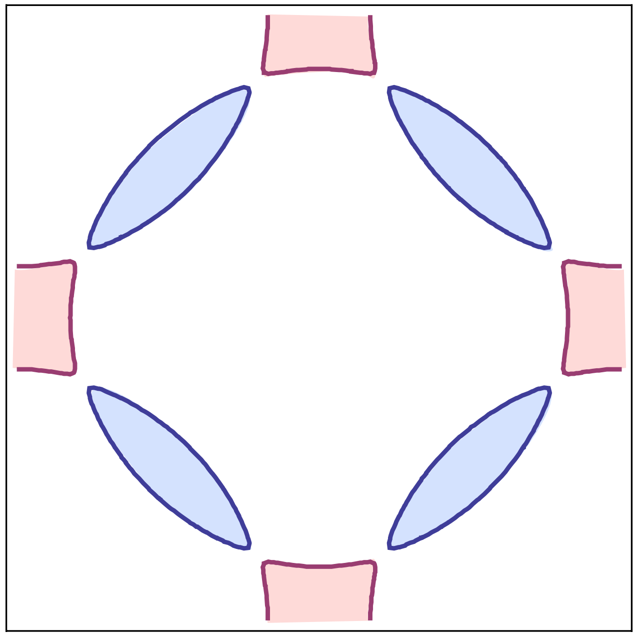

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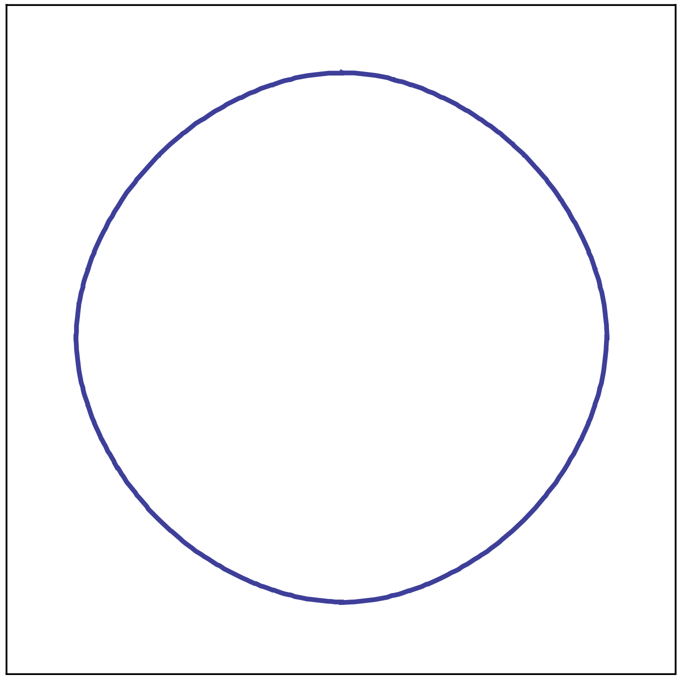

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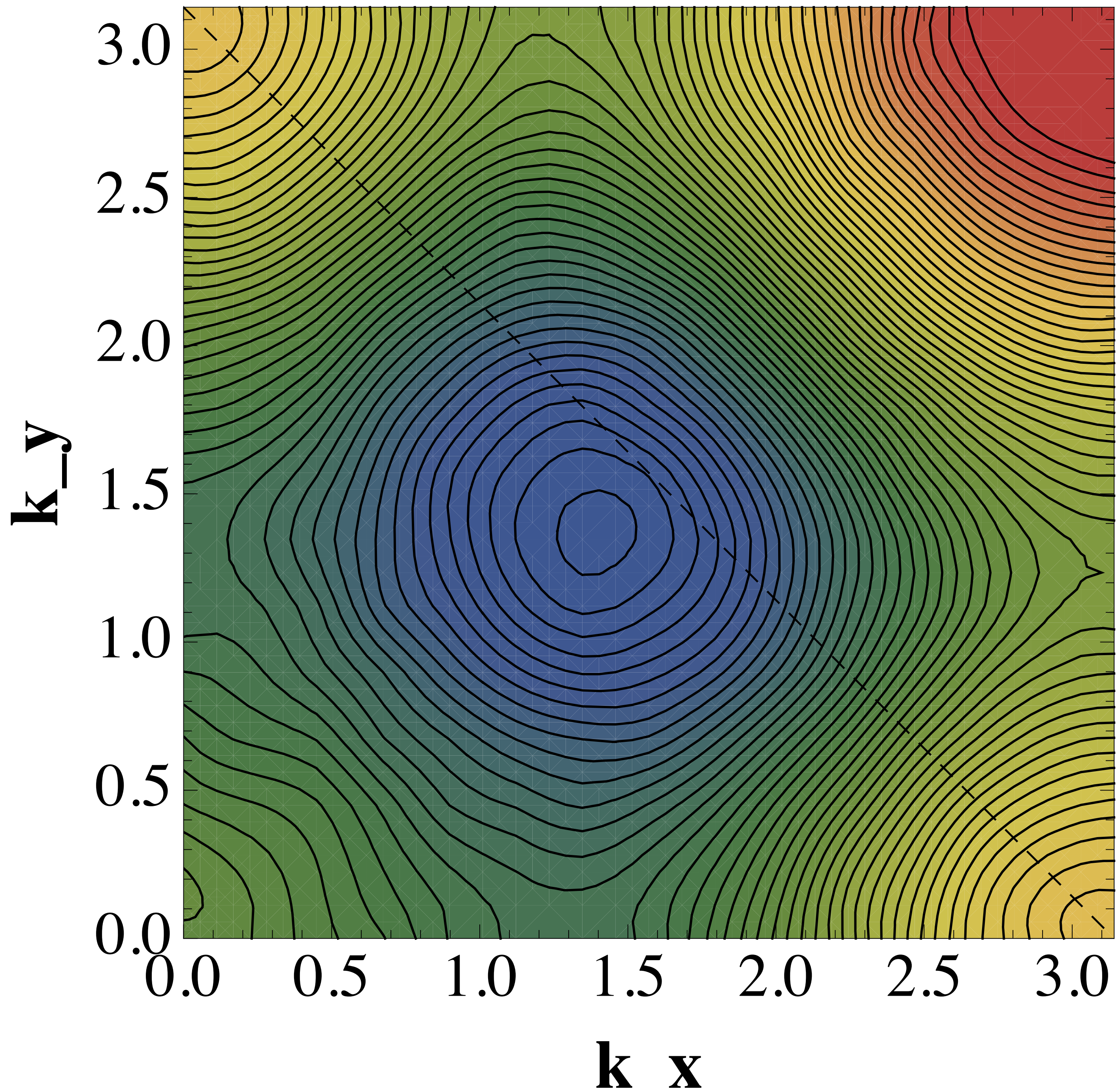
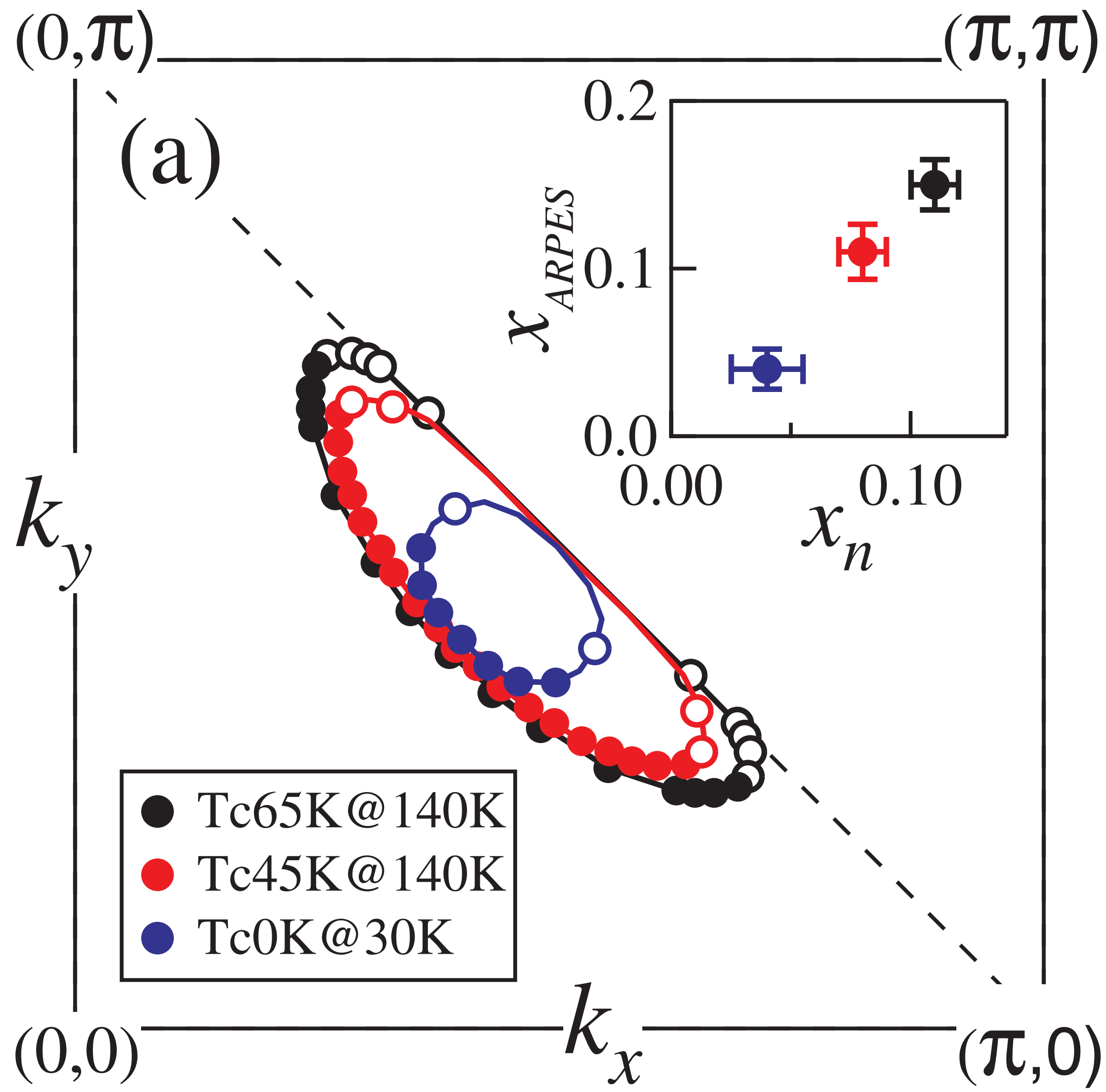
Metal with "large" Fermi surface

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]

Tuesday, June 19, 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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- 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)

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- 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)

Questions

- *Can quantum fluctuations near the onset of antiferromagnetism induce higher temperature superconductivity ?*

- *How should such a theory be extended to apply to the hole-doped cuprates ?*

- *What is the physics of the strange metal ?*

Questions and Answers

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  Strongly-coupled quantum criticality of Fermi surface change in a metal