

Title: Entangling Superconductivity and antiferromagnetism: Quantum Monte Carlo without the sign Problem

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Abstract: It has long been known that a metal near an instability to antiferromagnetism also has a weak-coupling Cooper instability to spin-singlet d-wave-like superconductivity.

However, the theory of the antiferromagnetic quantum critical point flows to strong-coupling in two spatial dimensions, and so the fate of the superconductivity has also been unclear.

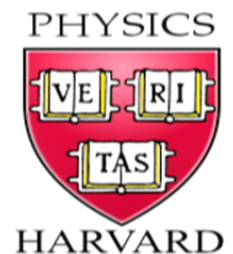
I will describe a method to realize the generic antiferromagnetic quantum critical in a metal in a sign-problem-free Monte Carlo simulation. Results showing Fermi surface reconstruction and unconventional spin-singlet superconductivity across the critical point are obtained.

Entangling antiferromagnetism and superconductivity: Quantum Monte Carlo without the sign problem

Perimeter Institute, July 11, 2012

Subir Sachdev

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Max Metlitski

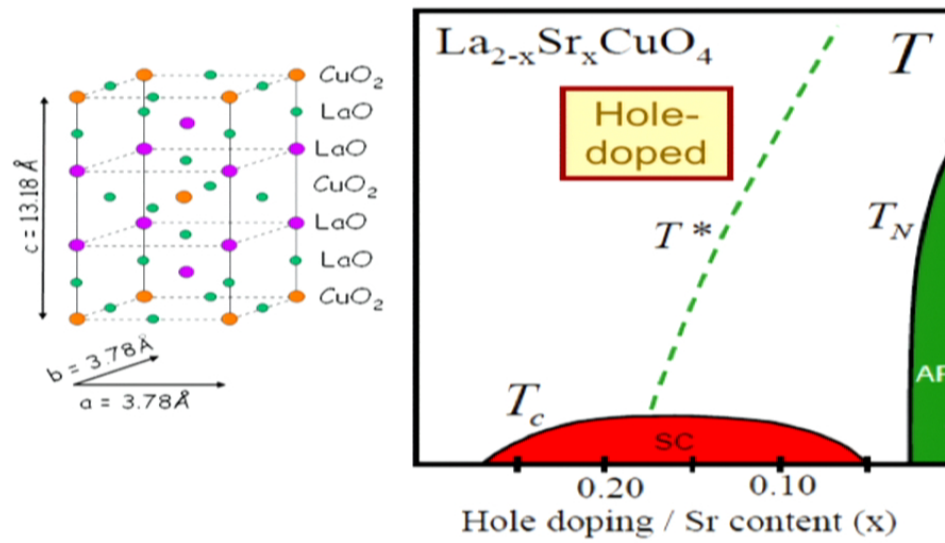


Erez Berg

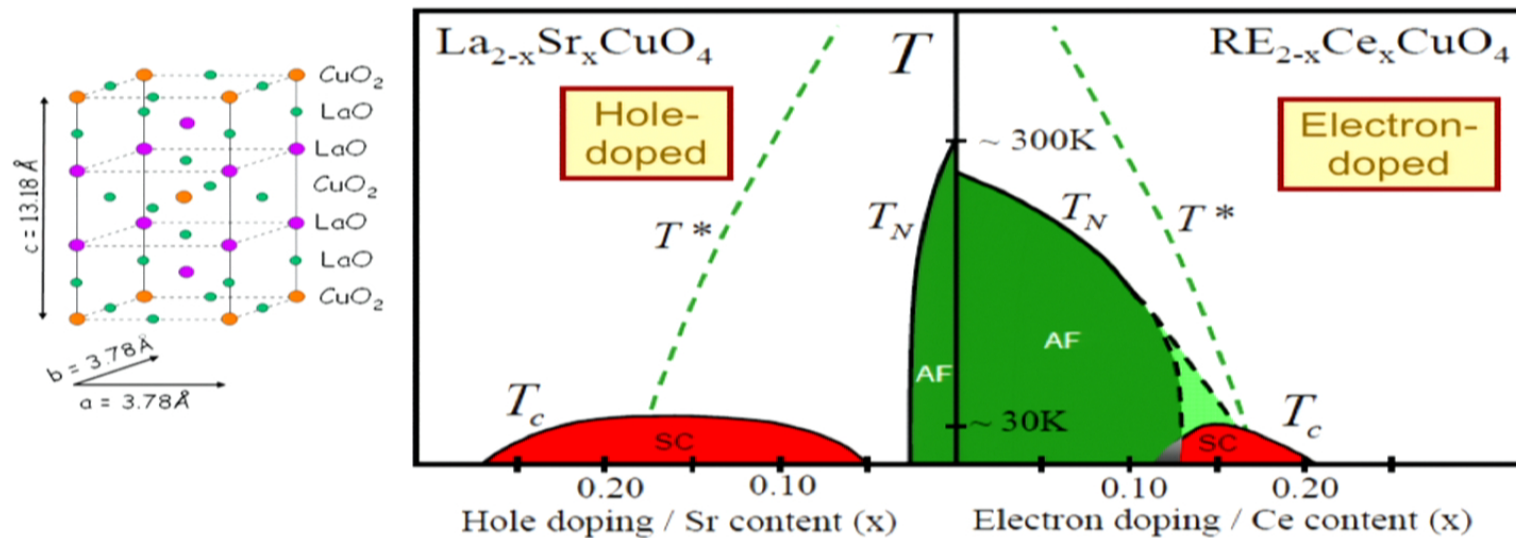


Matthias Punk





Electron-doped cuprate superconductors



Electron-doped cuprate superconductors

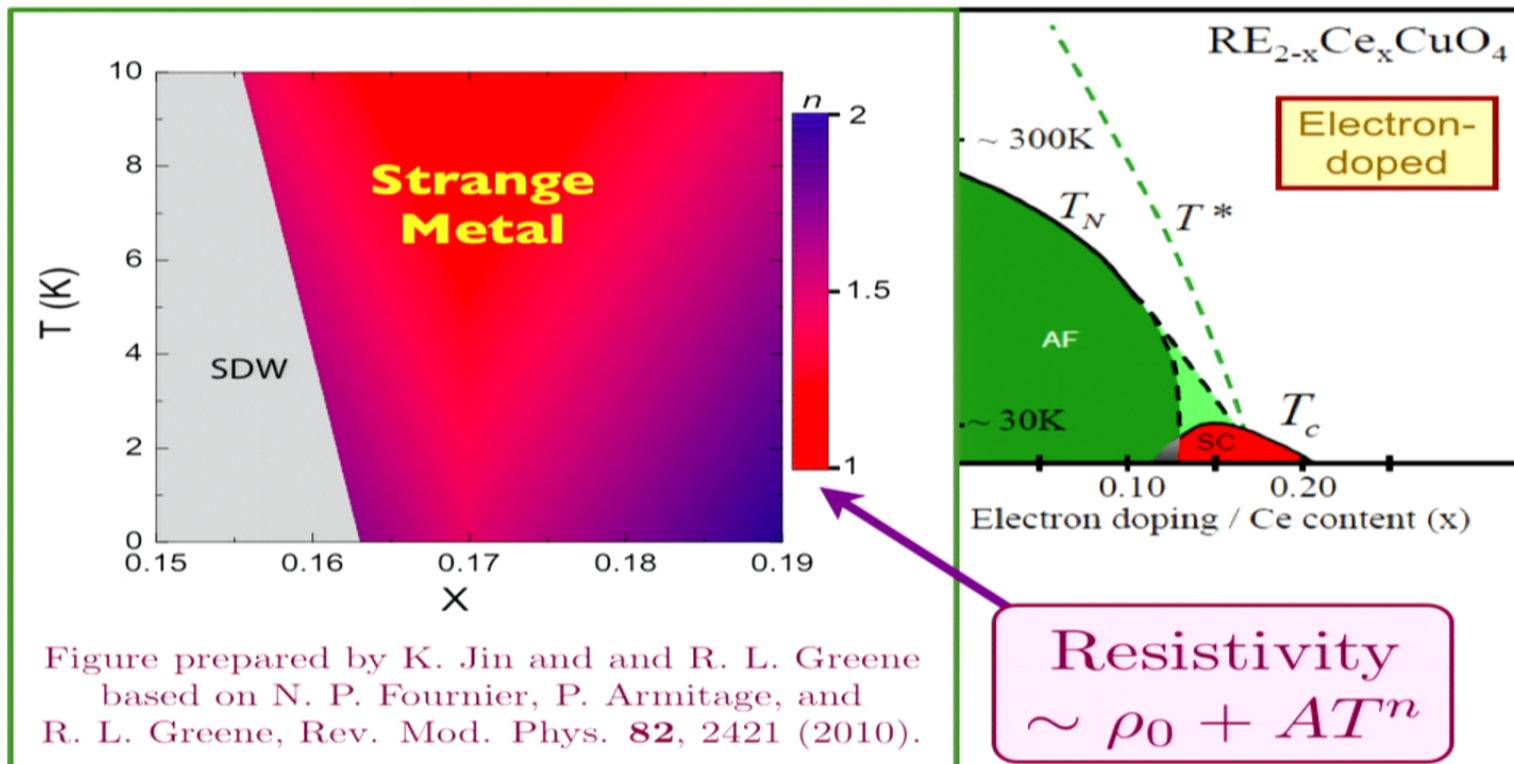
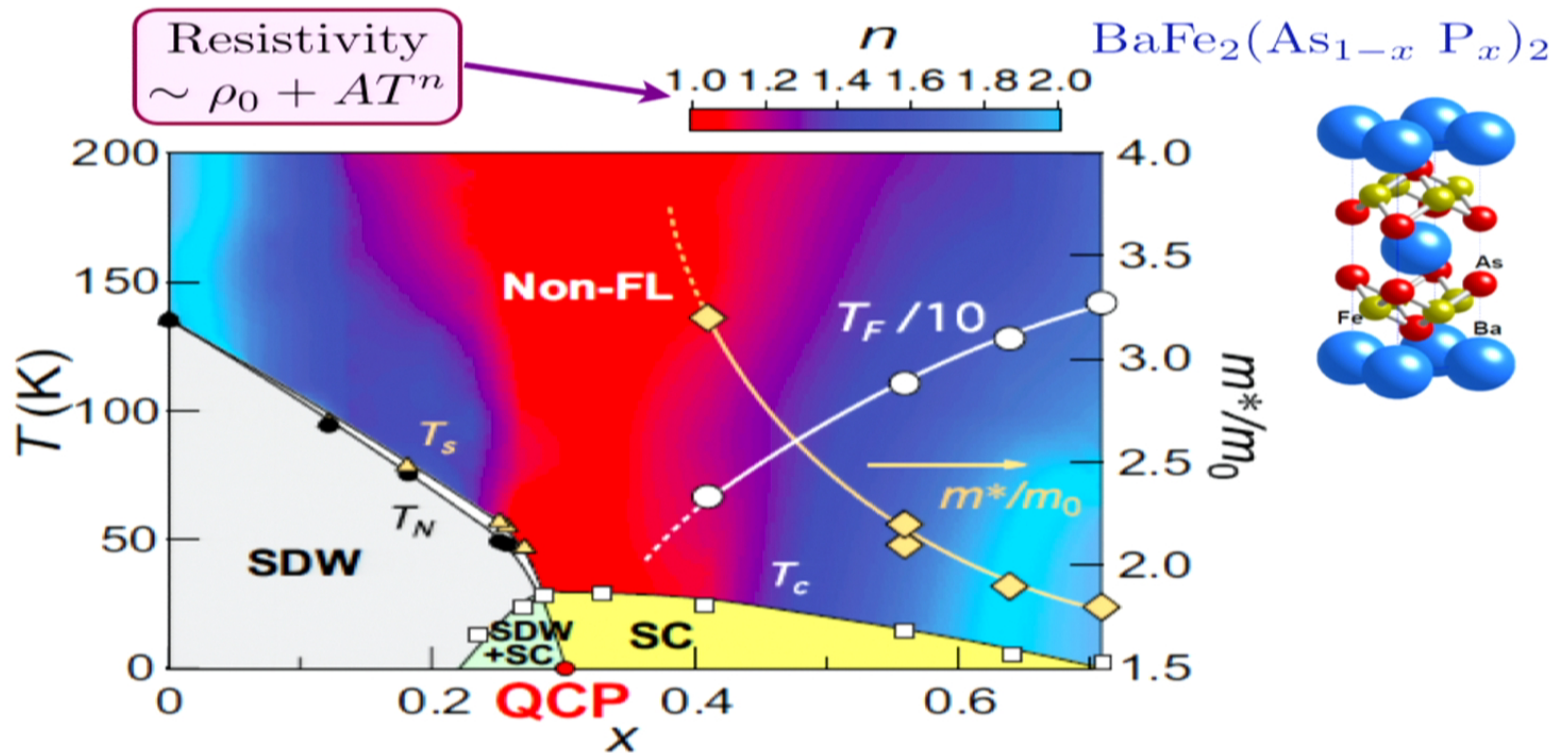
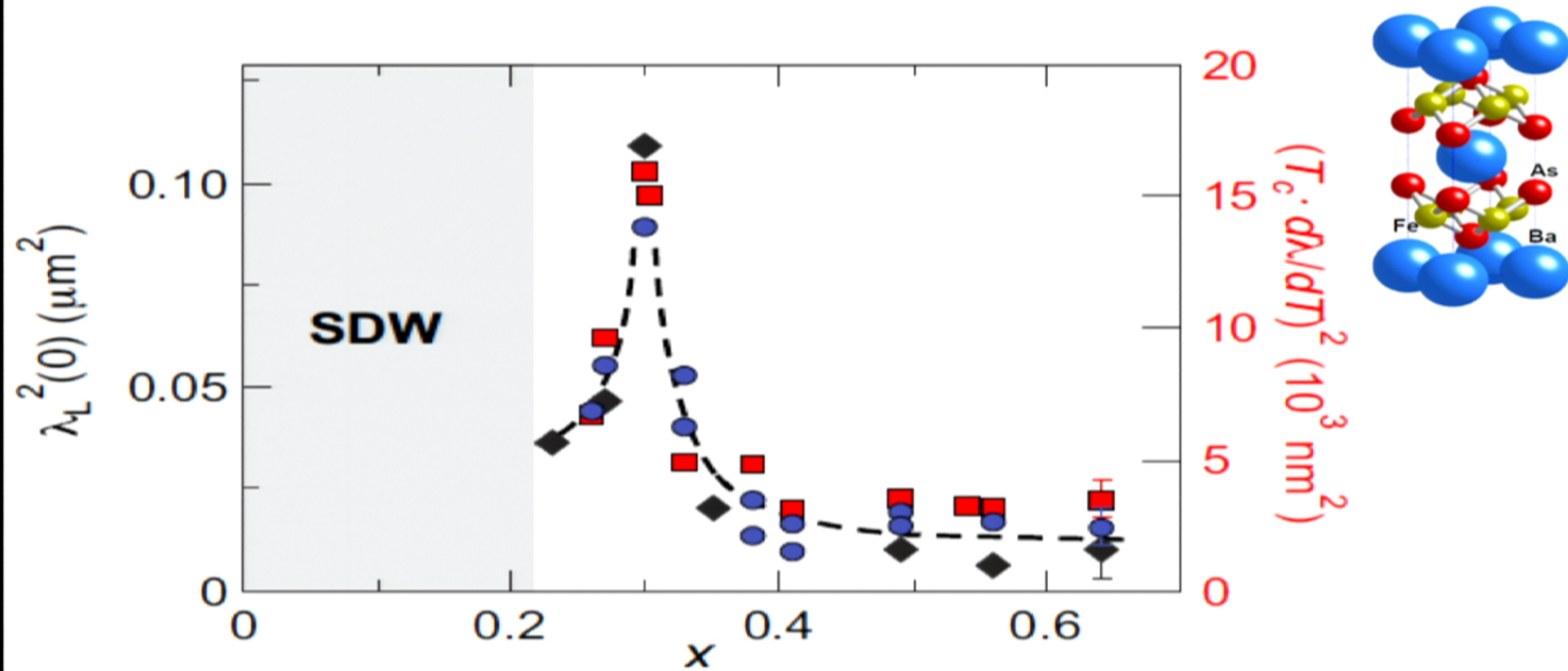


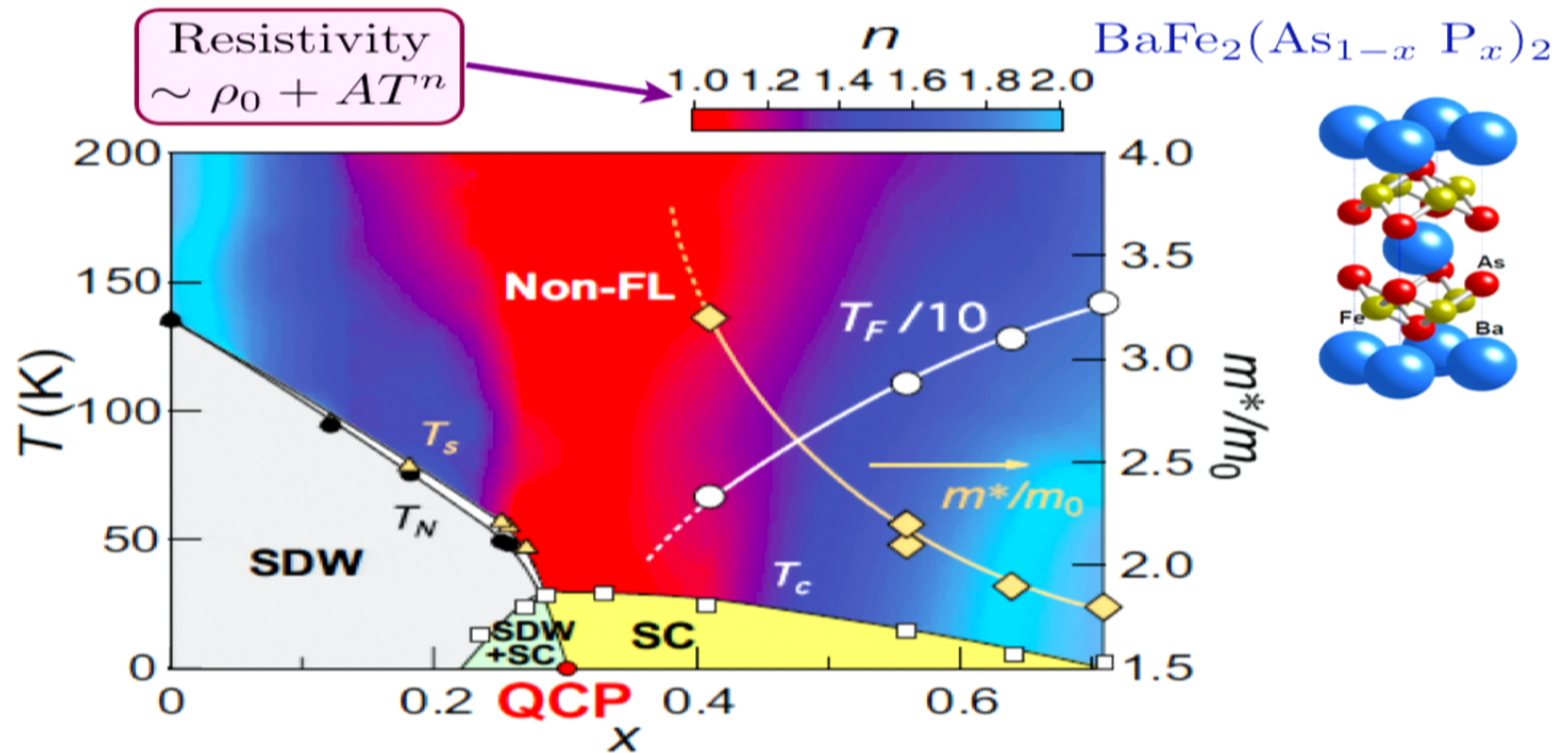
Figure prepared by K. Jin and R. L. Greene based on N. P. Fournier, P. Armitage, and R. L. Greene, Rev. Mod. Phys. **82**, 2421 (2010).



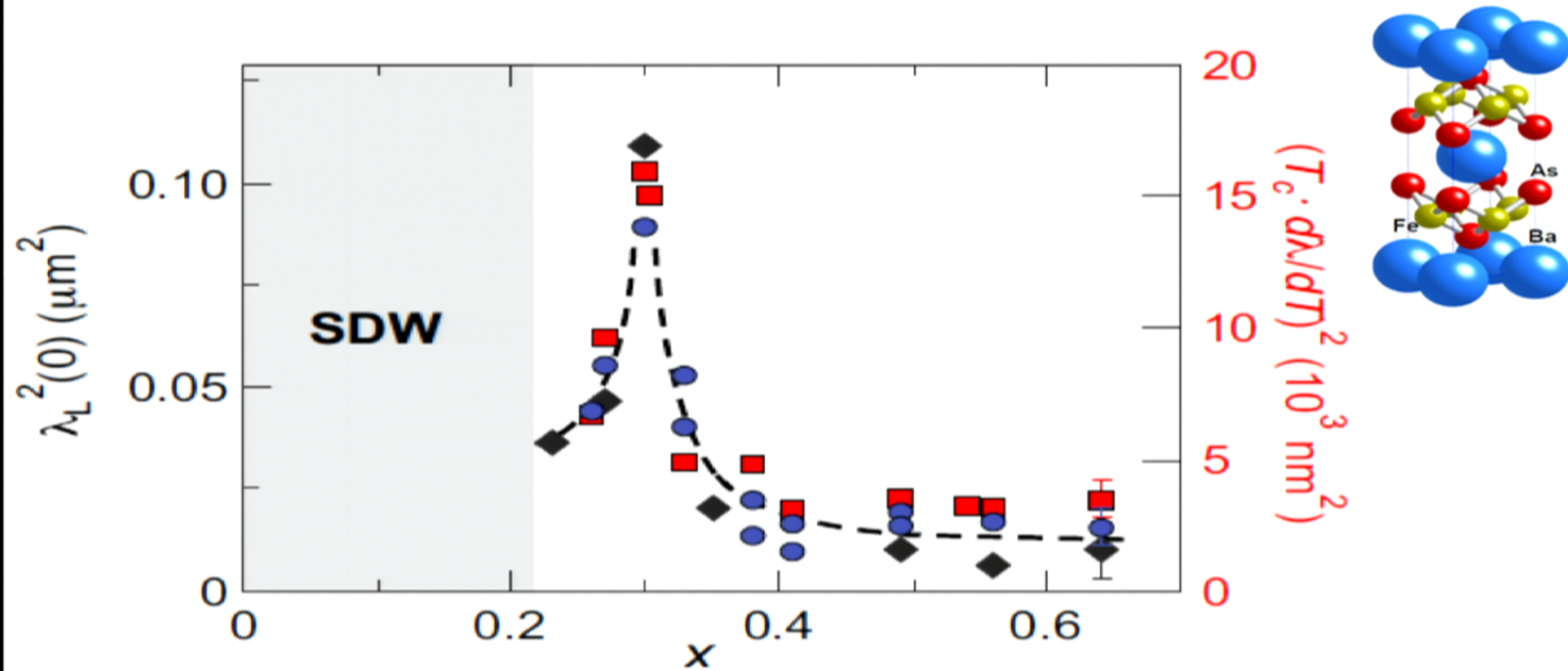
K. Hashimoto, K. Cho, T. Shibauchi, S. Kasahara, Y. Mizukami, R. Katsumata, Y. Tsuruhara, T. Terashima, H. Ikeda, M. A. Tanatar, H. Kitano, N. Salovich, R. W. Giannetta, P. Walmsley, A. Carrington, R. Prozorov, and Y. Matsuda, *Science* **336**, 1554 (2012).



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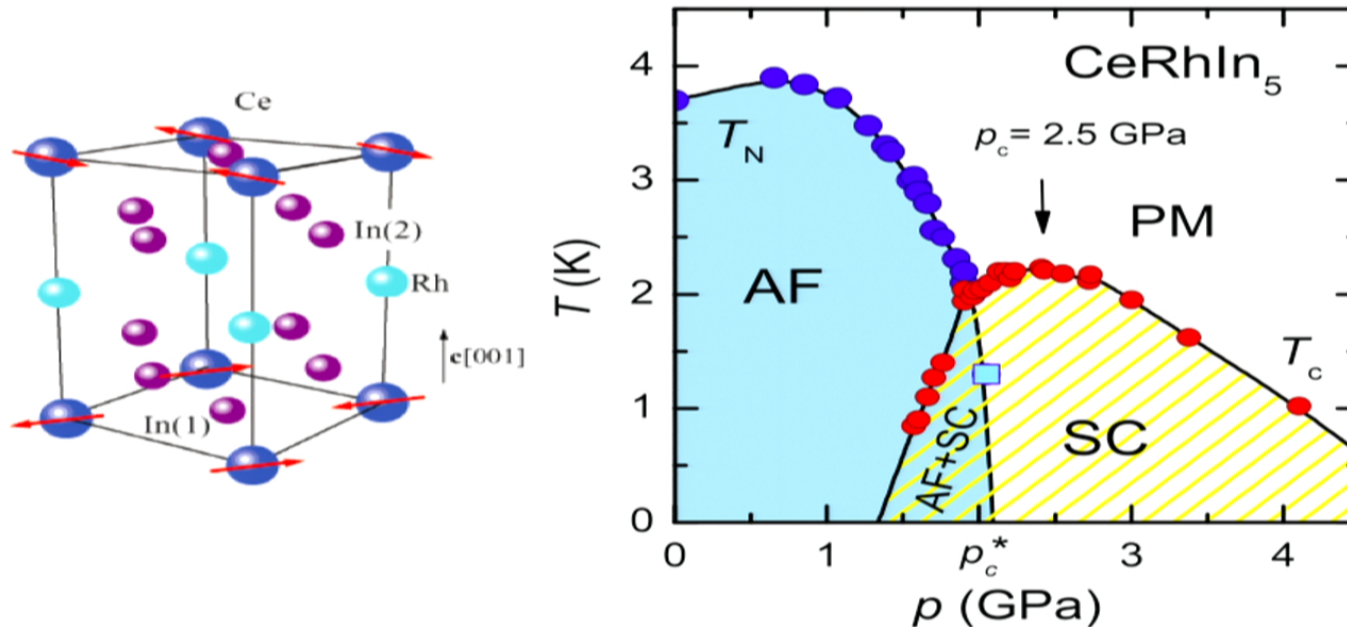


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Lower T_c superconductivity in the heavy fermion compounds



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 for 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

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 $\alpha = \uparrow, \downarrow$

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

$$\begin{aligned} c_{i\alpha}^\dagger c_{j\beta} + c_{j\beta} c_{i\alpha}^\dagger &= \delta_{ij} \delta_{\alpha\beta} \\ c_{i\alpha} c_{j\beta} + c_{j\beta} c_{i\alpha} &= 0 \end{aligned}$$

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:

$\lambda^2 \sim U$, the Hubbard repulsion

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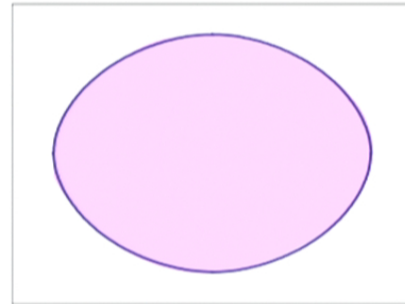
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Fermi surface+antiferromagnetism

Metal with “large”
Fermi surface

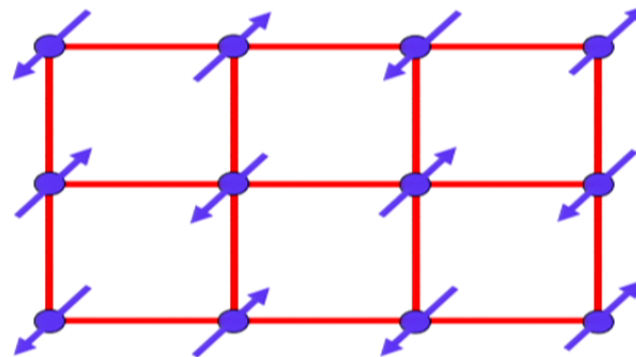


+

The electron spin polarization obeys

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

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



Fermi surface+antiferromagnetism

Mean field theory

In the presence of spin density wave order, $\vec{\varphi}$ at wavevector $\mathbf{K} = (\pi, \pi)$, we have an additional term which mixes electron states with momentum separated by $\mathbf{K}$

$$H_{\text{sdw}} = \lambda \vec{\varphi} \cdot \sum_{\mathbf{k}, \alpha, \beta} c_{\mathbf{k}, \alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{\mathbf{k}+\mathbf{K}, \beta}$$

where $\vec{\sigma}$ are the Pauli matrices. The electron dispersions obtained by diagonalizing $H_0 + H_{\text{sdw}}$ for $\vec{\varphi} \propto (0, 0, 1)$ are

$$E_{\mathbf{k}\pm} = \frac{\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}+\mathbf{K}}}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{K}}}{2}\right)^2 + \lambda^2 \varphi^2}$$

Fermi surface+antiferromagnetism

Mean field theory

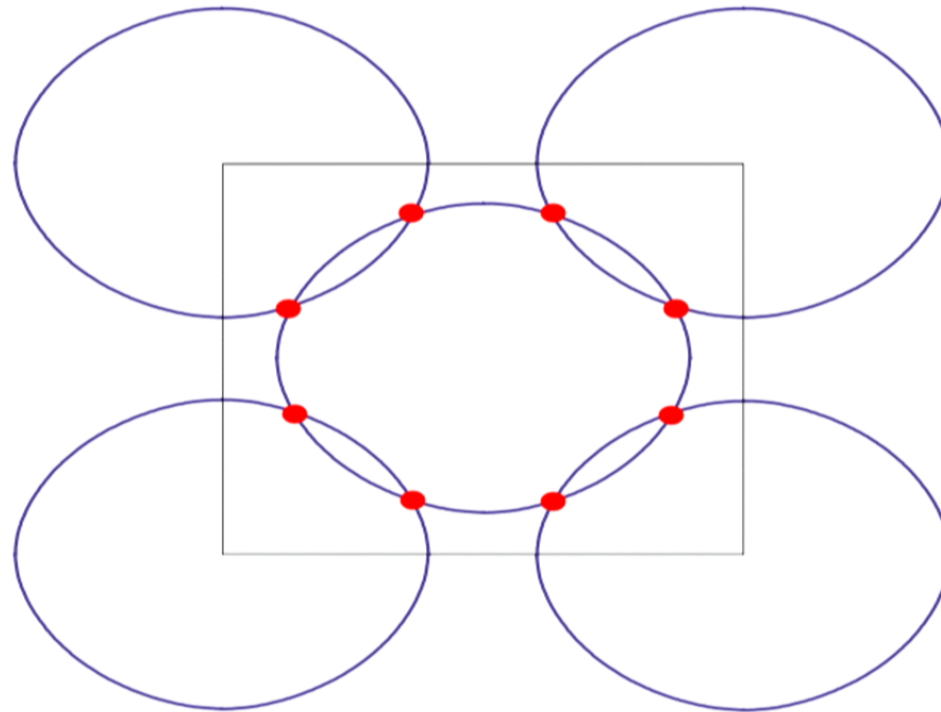
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Fermi surface+antiferromagnetism



“Hot” spots

Fermi surface+antiferromagnetism

Mean field theory

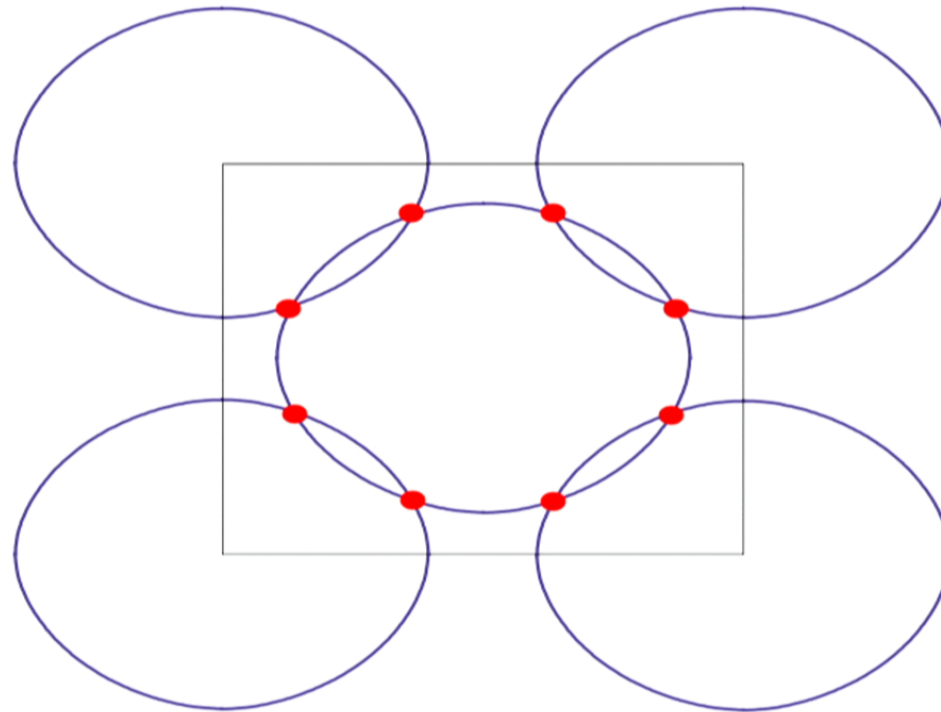
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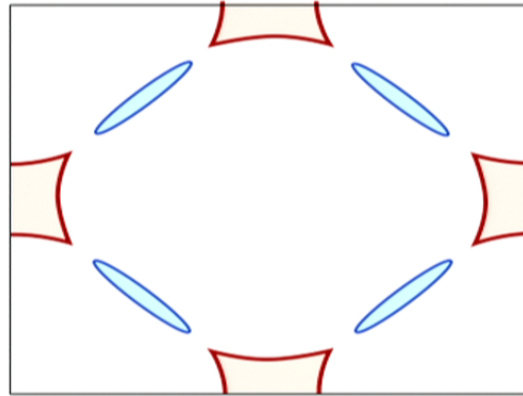
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Fermi surface+antiferromagnetism



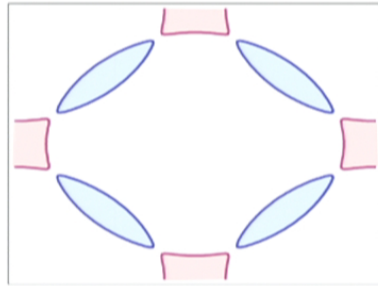
“Hot” spots

Fermi surface+antiferromagnetism



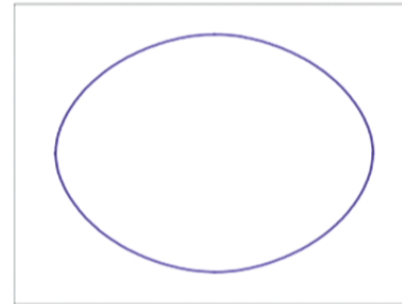
Electron and hole pockets in
antiferromagnetic phase with $\langle \vec{\varphi} \rangle \neq 0$

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).

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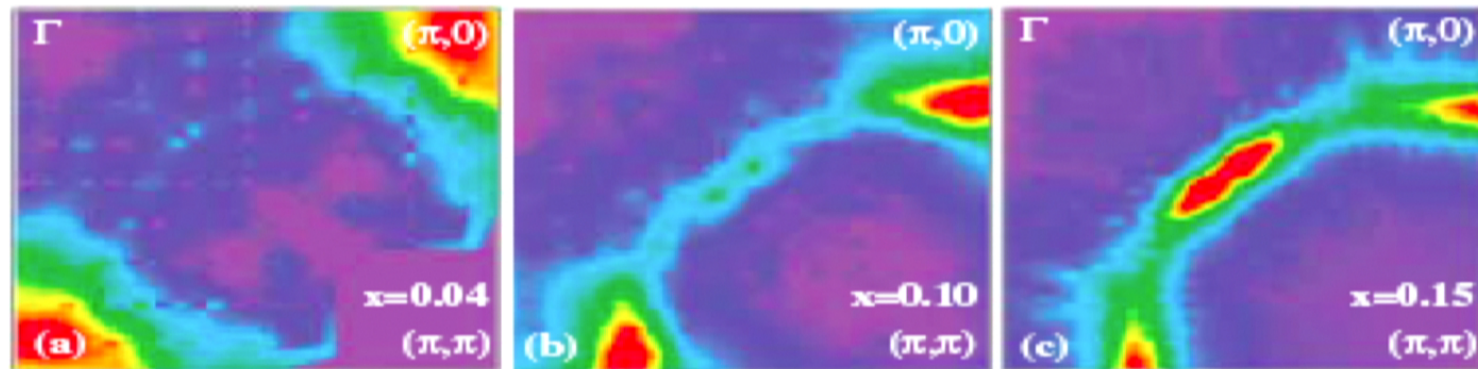
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antiferromagnetic order:

$\lambda^2 \sim U$, the Hubbard repulsion

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

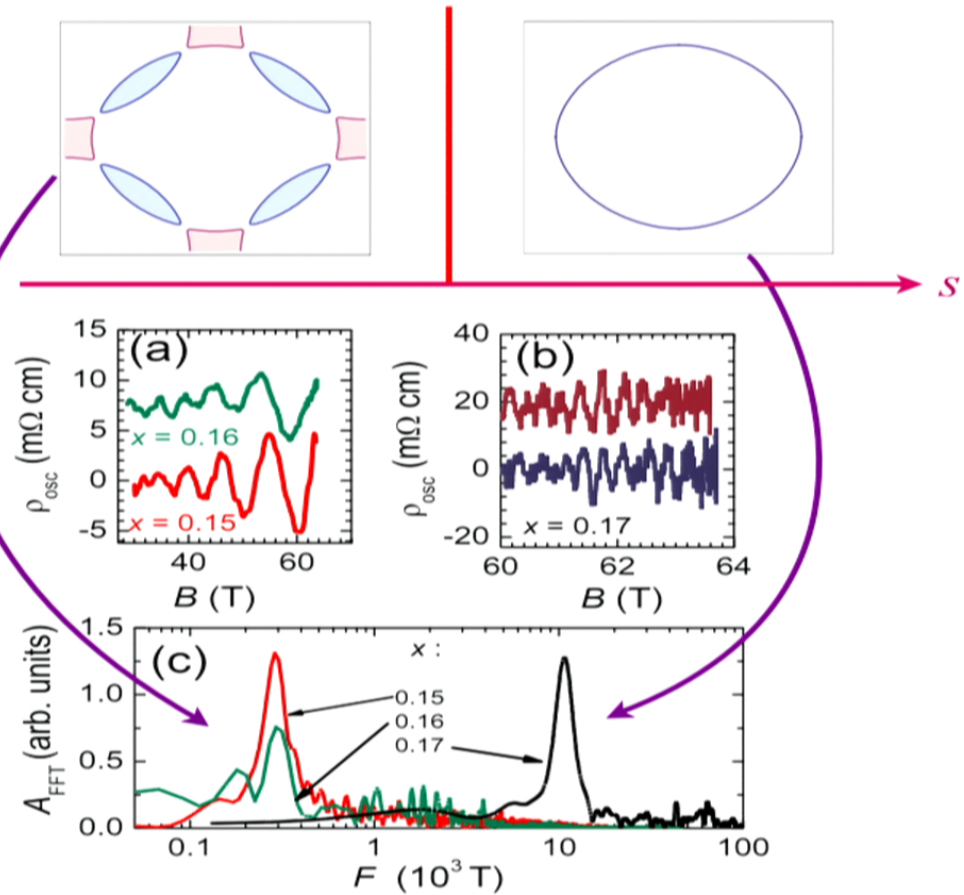


N. P.Armitage *et al.*, Phys. Rev. Lett. **88**, 257001 (2002).

Quantum oscillations



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



***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)

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

Pairing by SDW fluctuation exchange

We now allow the SDW field $\vec{\varphi}$ to be dynamical, coupling to electrons as

$$H_{\text{sdw}} = - \sum_{\mathbf{k}, \mathbf{q}, \alpha, \beta} \vec{\varphi}_{\mathbf{q}} \cdot c_{\mathbf{k}, \alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{\mathbf{k}+\mathbf{K}+\mathbf{q}, \beta}.$$

Exchange of a $\vec{\varphi}$ quantum leads to the effective interaction

$$H_{ee} = -\frac{1}{2} \sum_{\mathbf{q}} \sum_{\mathbf{p}, \gamma, \delta} \sum_{\mathbf{k}, \alpha, \beta} V_{\alpha\beta, \gamma\delta}(\mathbf{q}) c_{\mathbf{k}, \alpha}^{\dagger} c_{\mathbf{k}+\mathbf{q}, \beta} c_{\mathbf{p}, \gamma}^{\dagger} c_{\mathbf{p}-\mathbf{q}, \delta},$$

where the pairing interaction is

$$V_{\alpha\beta, \gamma\delta}(\mathbf{q}) = \vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta} \frac{\lambda^2}{\xi^{-2} + (\mathbf{q} - \mathbf{K})^2},$$

with $\lambda^2 \xi^2$ the SDW susceptibility and ξ the SDW correlation length.

Pairing by SDW fluctuation exchange

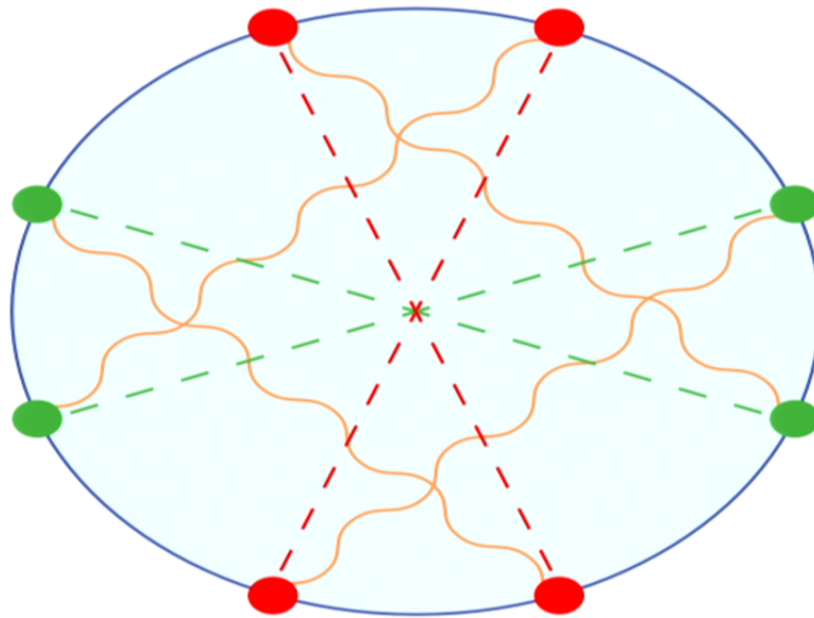
BCS Gap equation

In BCS theory, this interaction leads to the 'gap equation' for the pairing gap $\Delta_{\mathbf{k}} \propto \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$.

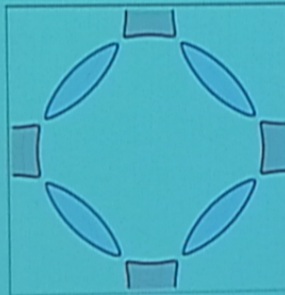
$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{p}} \left(\frac{3\lambda^2}{\xi^{-2} + (\mathbf{p} - \mathbf{k} - \mathbf{K})^2} \right) \frac{\Delta_{\mathbf{p}}}{2\sqrt{\varepsilon_{\mathbf{p}}^2 + \Delta_{\mathbf{p}}^2}}$$

Non-zero solutions of this equation require that $\Delta_{\mathbf{k}}$ and $\Delta_{\mathbf{p}}$ have opposite signs when $\mathbf{p} - \mathbf{k} \approx \mathbf{K}$.

Pairing “glue” from antiferromagnetic fluctuations

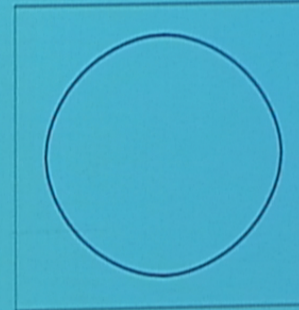


Fermi surface+antiferromagnetism



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

Metal with electron
and hole pockets

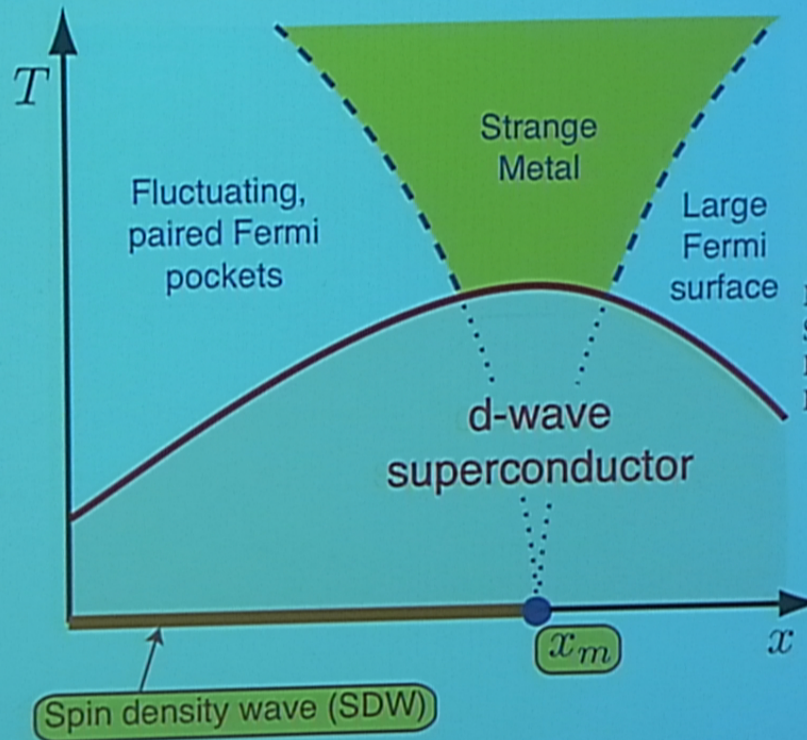


$$\langle \vec{\varphi} \rangle = 0$$

Metal with "large"
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S. Sachdev, A. V. Chubukov, and A. Sokol, *Phys. Rev. B* **51**, 14874 (1995).
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Fermi surface+antiferromagnetism



Large
Fermi
surface

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

d-wave
superconductor

Spin density wave (SDW)

Pairing "glue" from antiferromagnetic fluctuations

At stronger coupling,
different effects compete:

- Pairing glue becomes stronger.



At stronger coupling,
different effects compete:

- Pairing glue becomes stronger.
- There is stronger fermion-boson scattering, and fermionic quasi-particles lose their integrity.



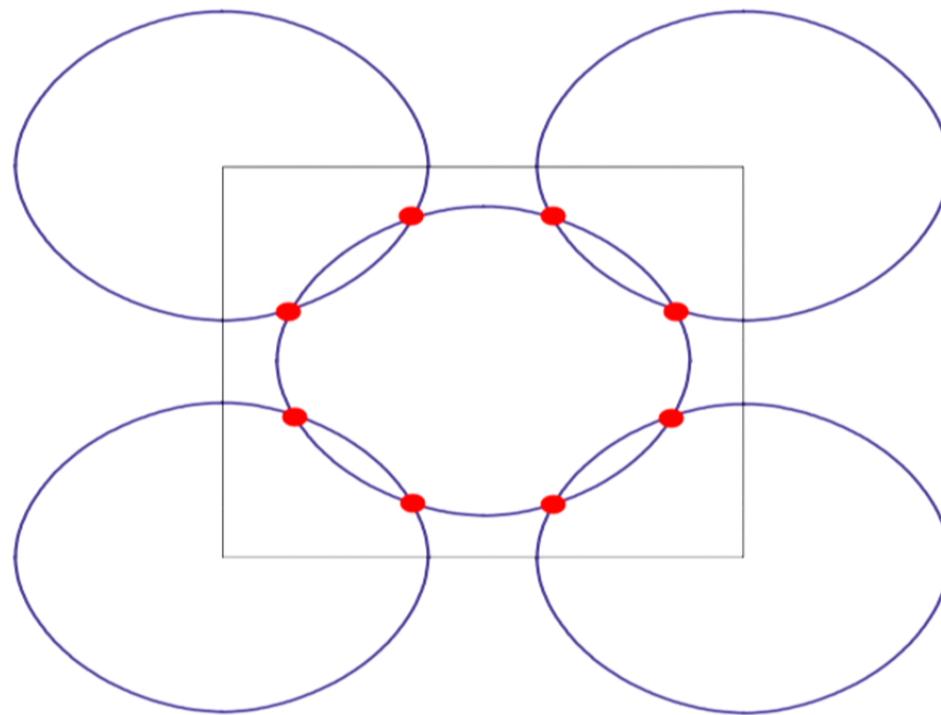
At stronger coupling,
different effects compete:

- Pairing glue becomes stronger.
- There is stronger fermion-boson scattering, and fermionic quasi-particles lose their integrity.
- Other instabilities can appear *e.g.* to charge density waves/stripe order.



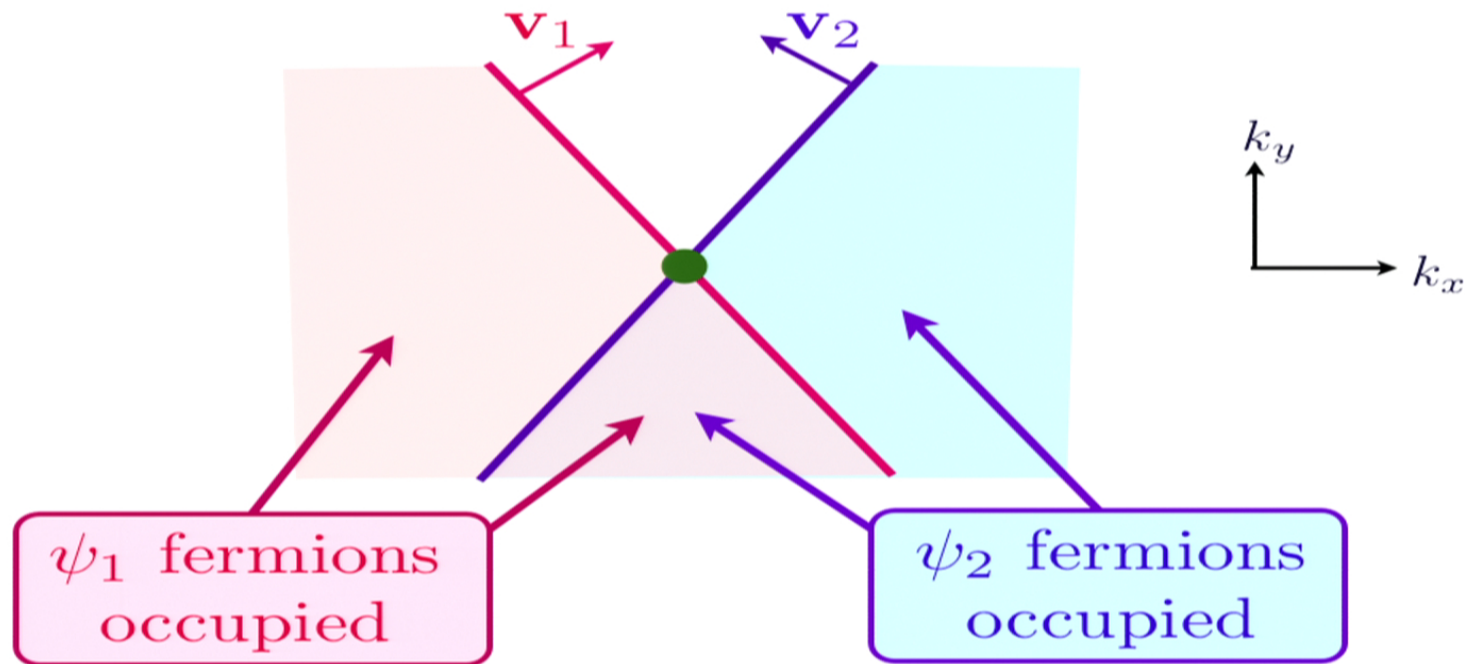
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“Hot” spots

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



$$(\nabla\phi)^2 + \lambda\phi^2 + u\phi^4$$

$$+ \psi_1^\dagger (\partial_\tau - \vec{\nabla}_1 \cdot \vec{\nabla}) \psi_1$$

$$\psi_2^\dagger (\partial_\tau - \vec{\nabla}_2 \cdot \vec{\nabla}) \psi_2$$

$$+ \lambda \vec{\phi} (\psi_1^\dagger \vec{\sigma} \psi_2 + \text{h.c.})$$

$$(\nabla\phi)^2 + \lambda\phi^2 + u\phi^4$$

$$+ \psi_1^\dagger (\partial_t - \vec{\nabla}_1 \cdot \vec{\nabla}) \psi_1$$

$$+ \psi_2^\dagger (\partial_t - \vec{\nabla}_2 \cdot \vec{\nabla}) \psi_2$$

$$+ \lambda \phi (\psi_1^\dagger \vec{\psi}_2 + \text{h.c.})$$

$$= \epsilon_k = \vec{v} \cdot \vec{k} \neq |\vec{k}|$$

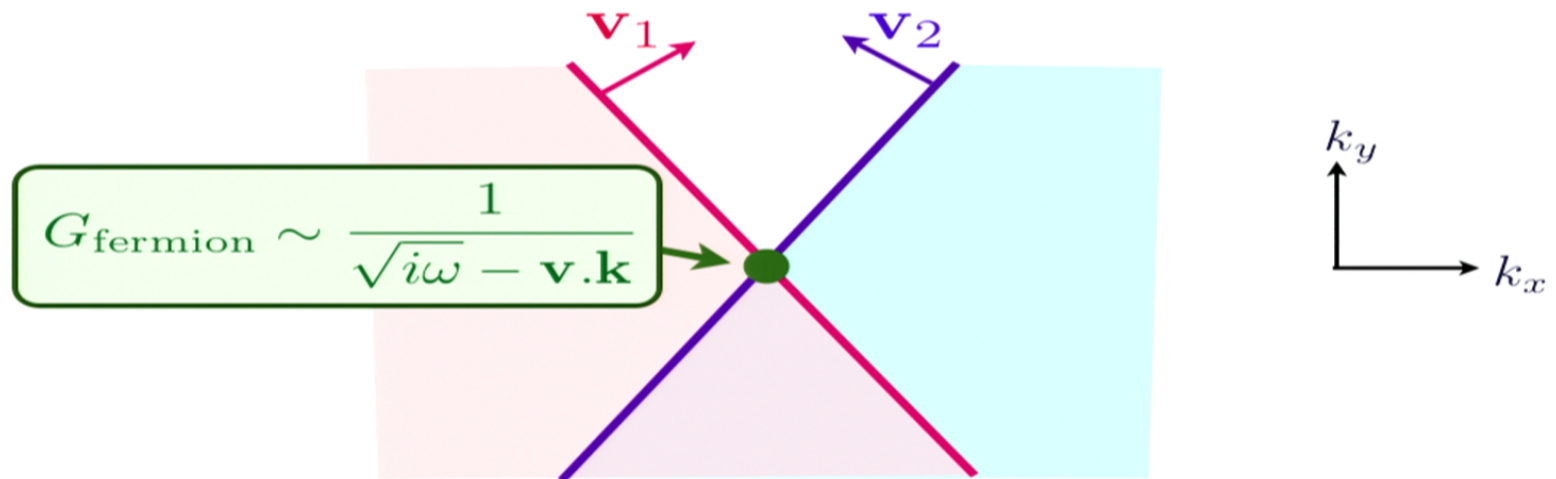
- In $d = 2$, we *must* work in local theories which keep both the order parameter and the Fermi surface quasiparticles “alive”.
- The theories can be organized in a $1/N$ expansion, where N is the number of fermion “flavors”.
- At subleading order, resummation of all “planar” graphs is required (at 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)

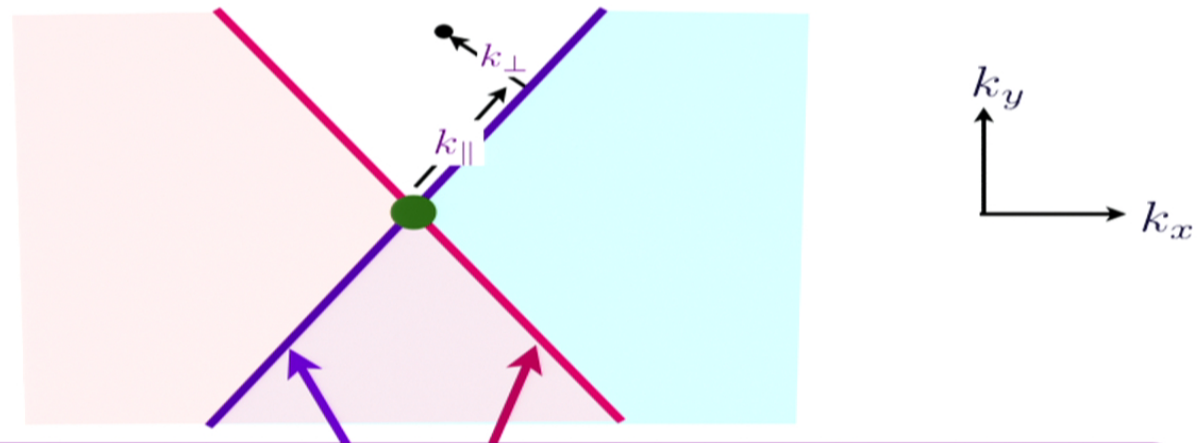
M.A. Metlitski and S. Sachdev, *Phys. Rev. B* **85**, 075128 (2010)

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* **85**, 075127 (2010)

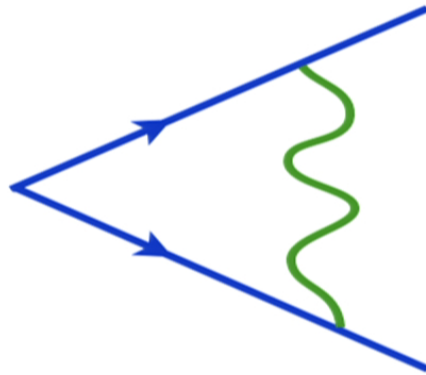
Pairing by SDW fluctuation exchange

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

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

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)

Pairing by SDW fluctuation exchange

Antiferromagnetic critical point

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Fermi
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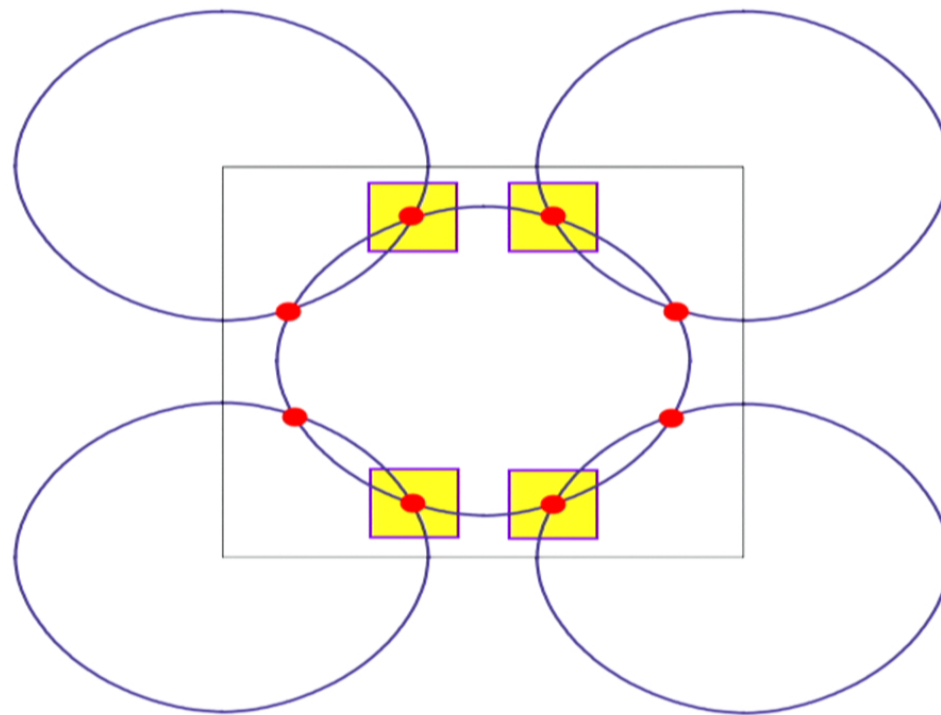


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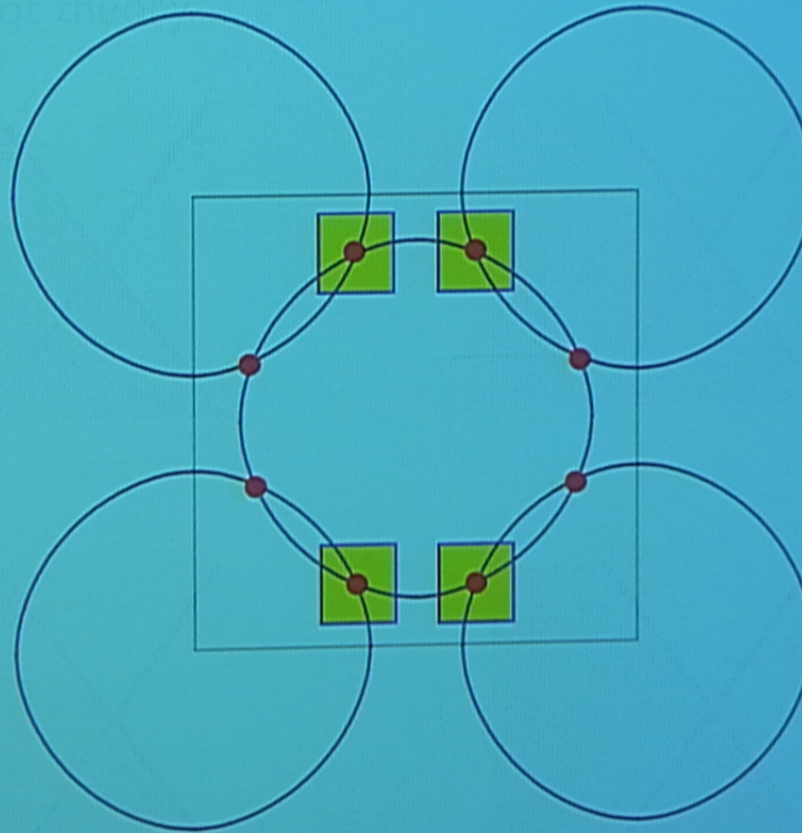
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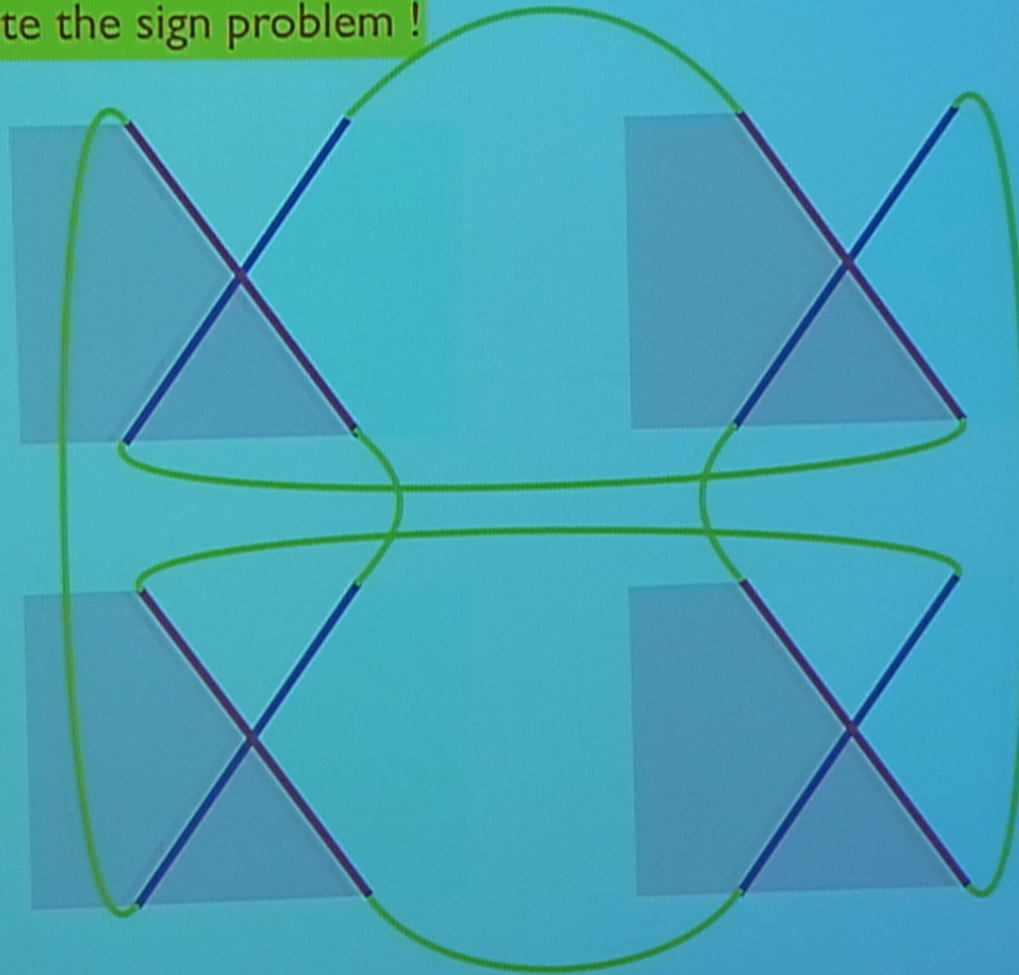
Low energy theory for critical point near hot spots

We have 4 copies
of the hot spot in the
unit cell

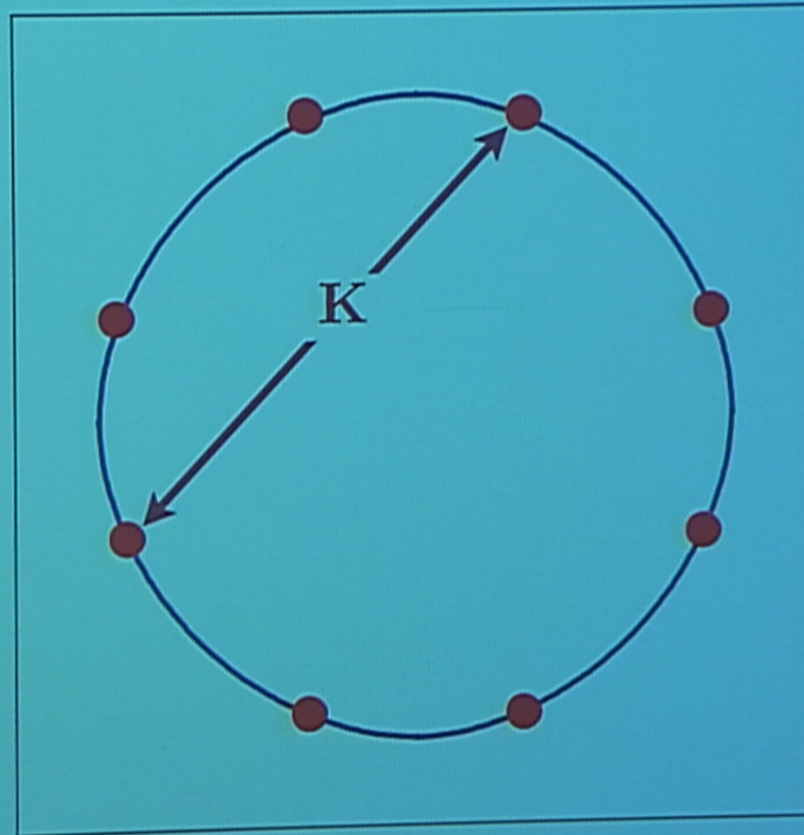


Low energy theory for critical point near hot spots

Reconnect Fermi lines and
eliminate the sign problem !

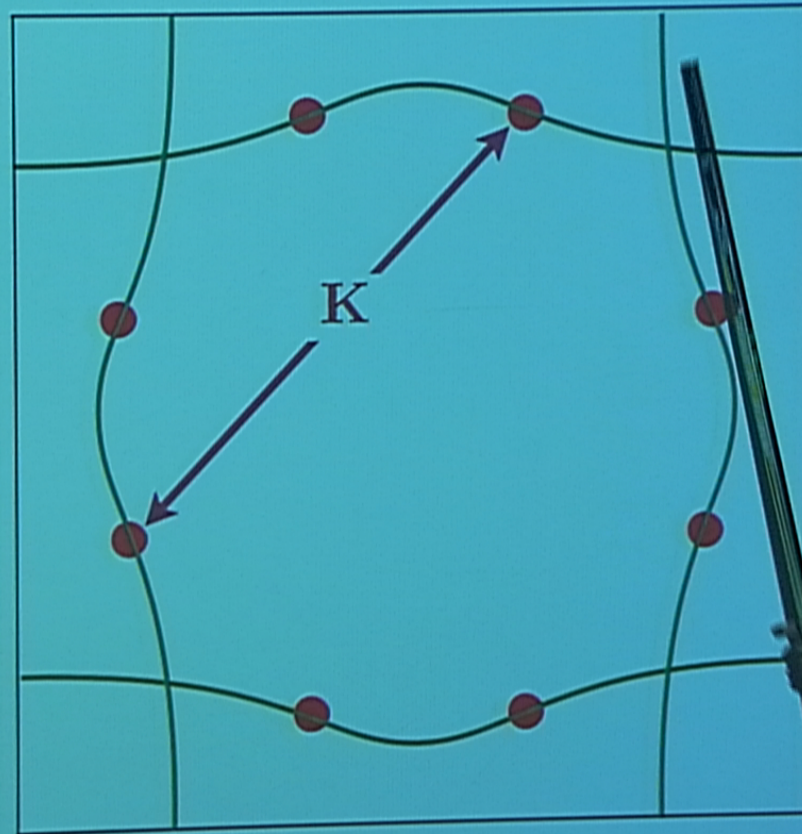


QMC for the onset of antiferromagnetism



Hot spots in a single band model

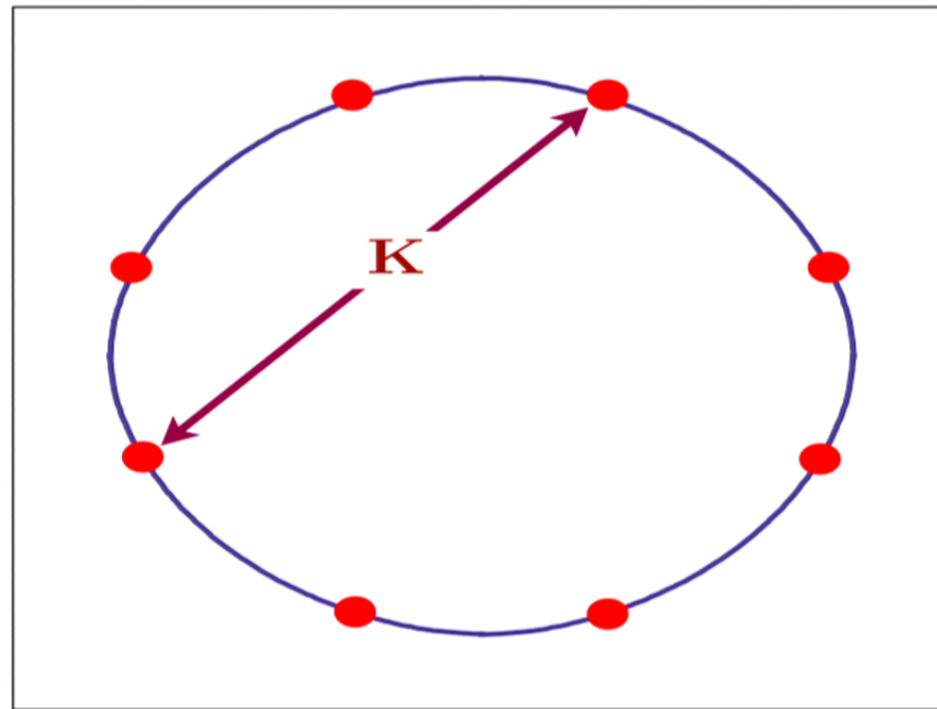
QMC for the onset of antiferromagnetism



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

Hot spots in a two band model

QMC for the onset of antiferromagnetism



Hot spots in a single band model

QMC for the onset of antiferromagnetism

Electrons with dispersion $\varepsilon_{\mathbf{k}}$
interacting with fluctuations of the
antiferromagnetic order parameter $\vec{\varphi}$.

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

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

$$+ \int d\tau d^2x \left[\frac{1}{2} (\nabla_x \vec{\varphi})^2 + \frac{r}{2} \vec{\varphi}^2 + \dots \right]$$
$$- \lambda \int d\tau \sum_i \vec{\varphi}_i \cdot (-1)^{\mathbf{x}_i} c_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta}$$

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 $\vec{\varphi}$.

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

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

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

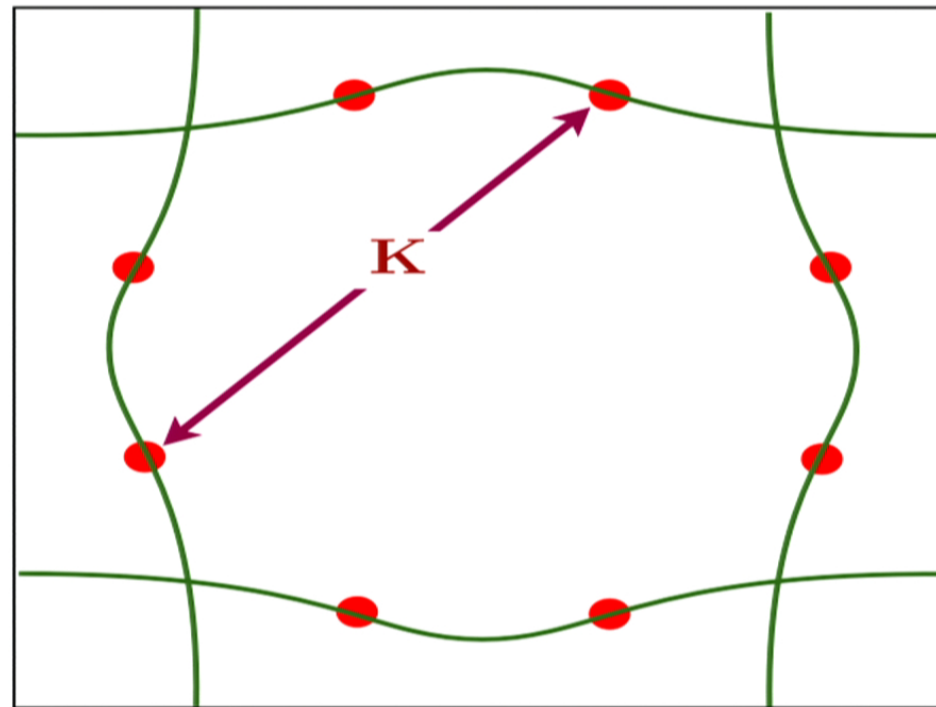
$$+ \int d\tau d^2x \left[\frac{1}{2} (\nabla_x \vec{\varphi})^2 + \frac{r}{2} \vec{\varphi}^2 + \dots \right]$$

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

No sign problem !

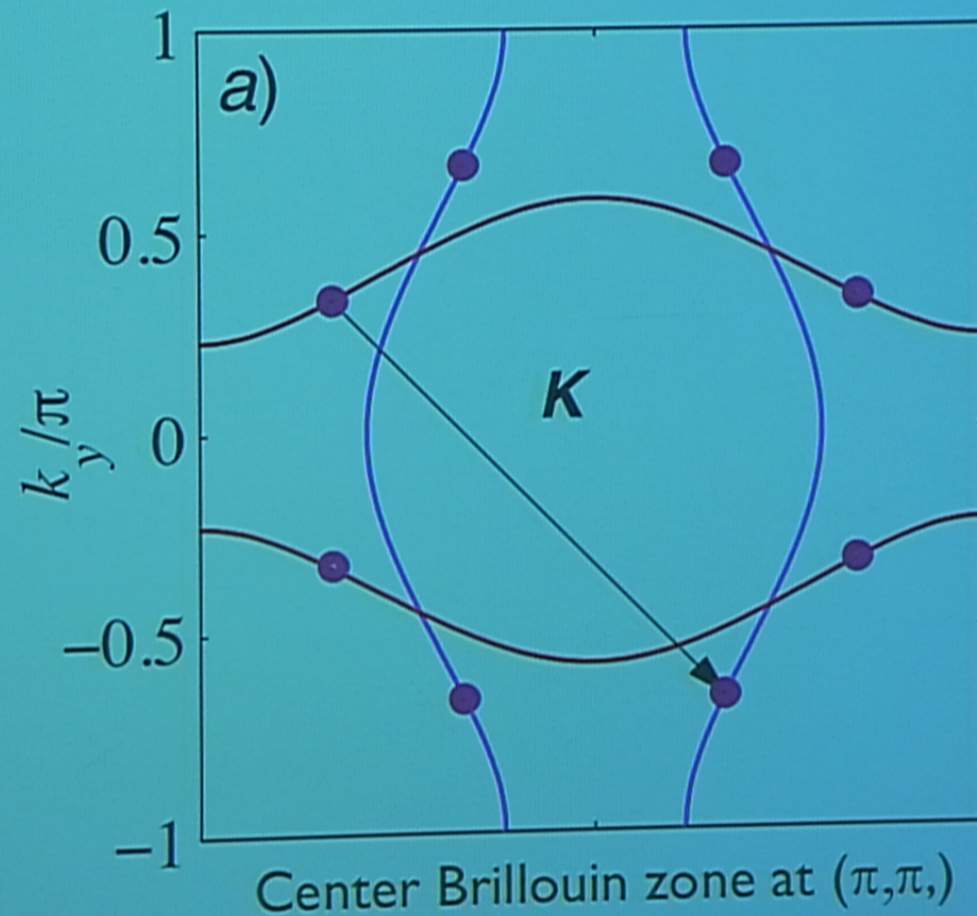
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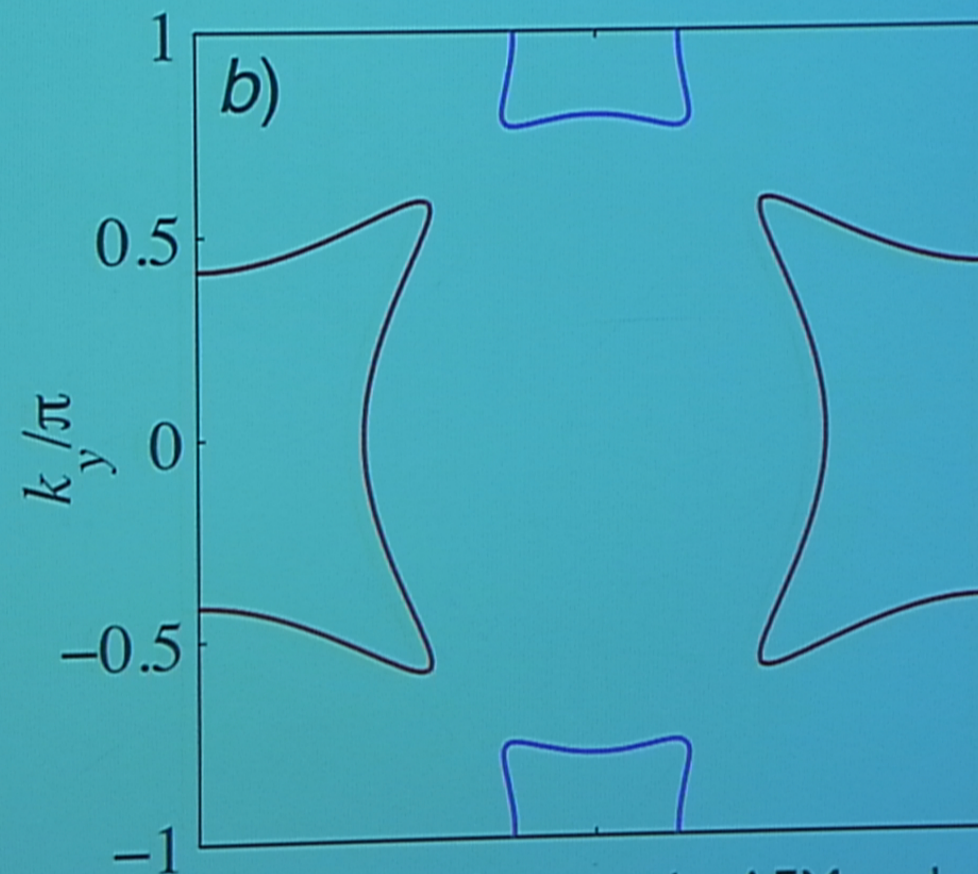
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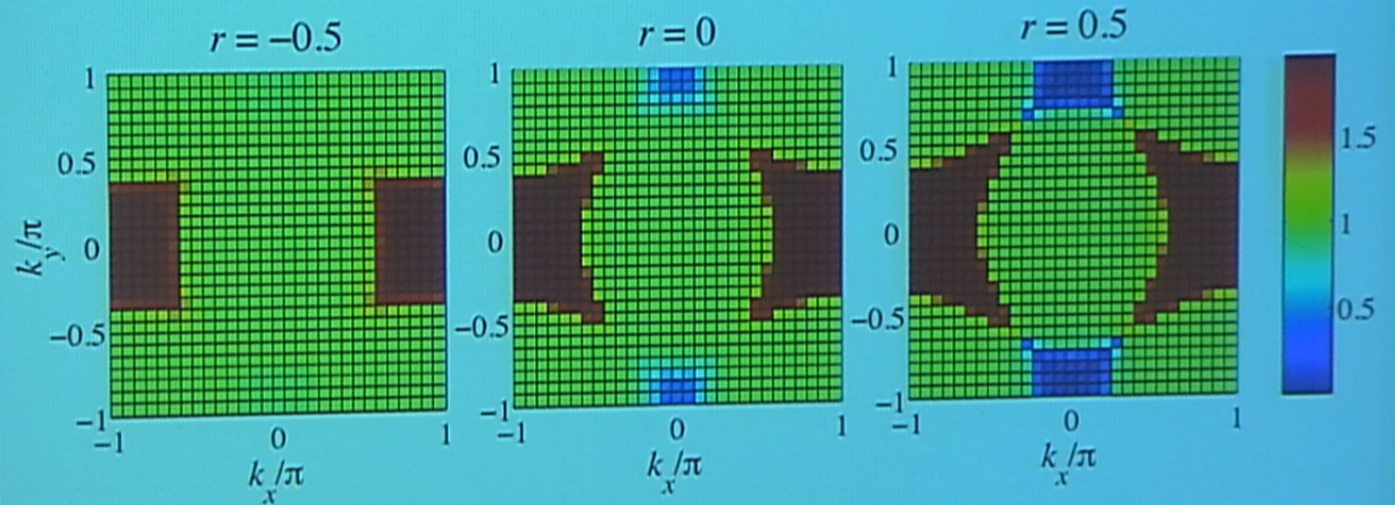
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E. Berg,
M. Metlitski, and
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Expected Fermi surfaces in the AFM ordered phase

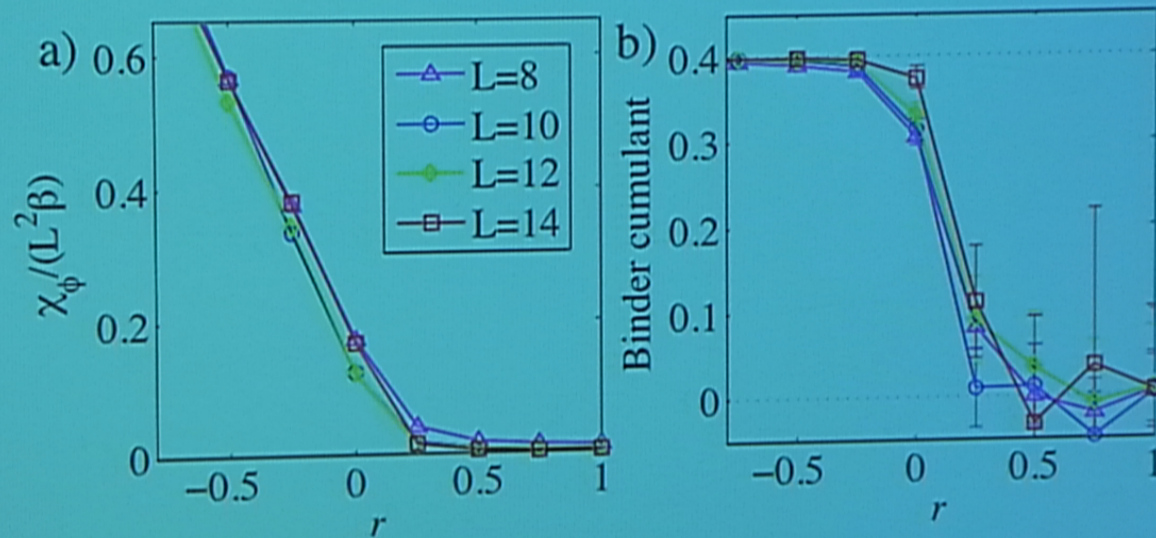
QMC for the onset of antiferromagnetism



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

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

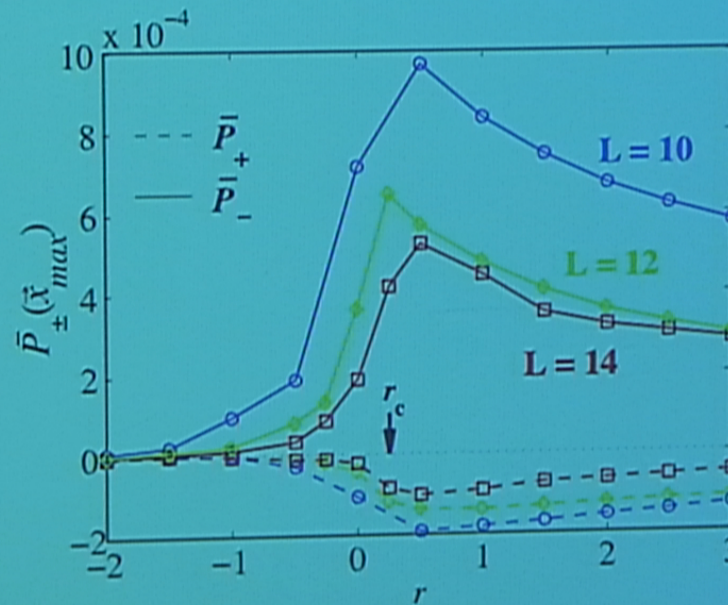
QMC for the onset of antiferromagnetism



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

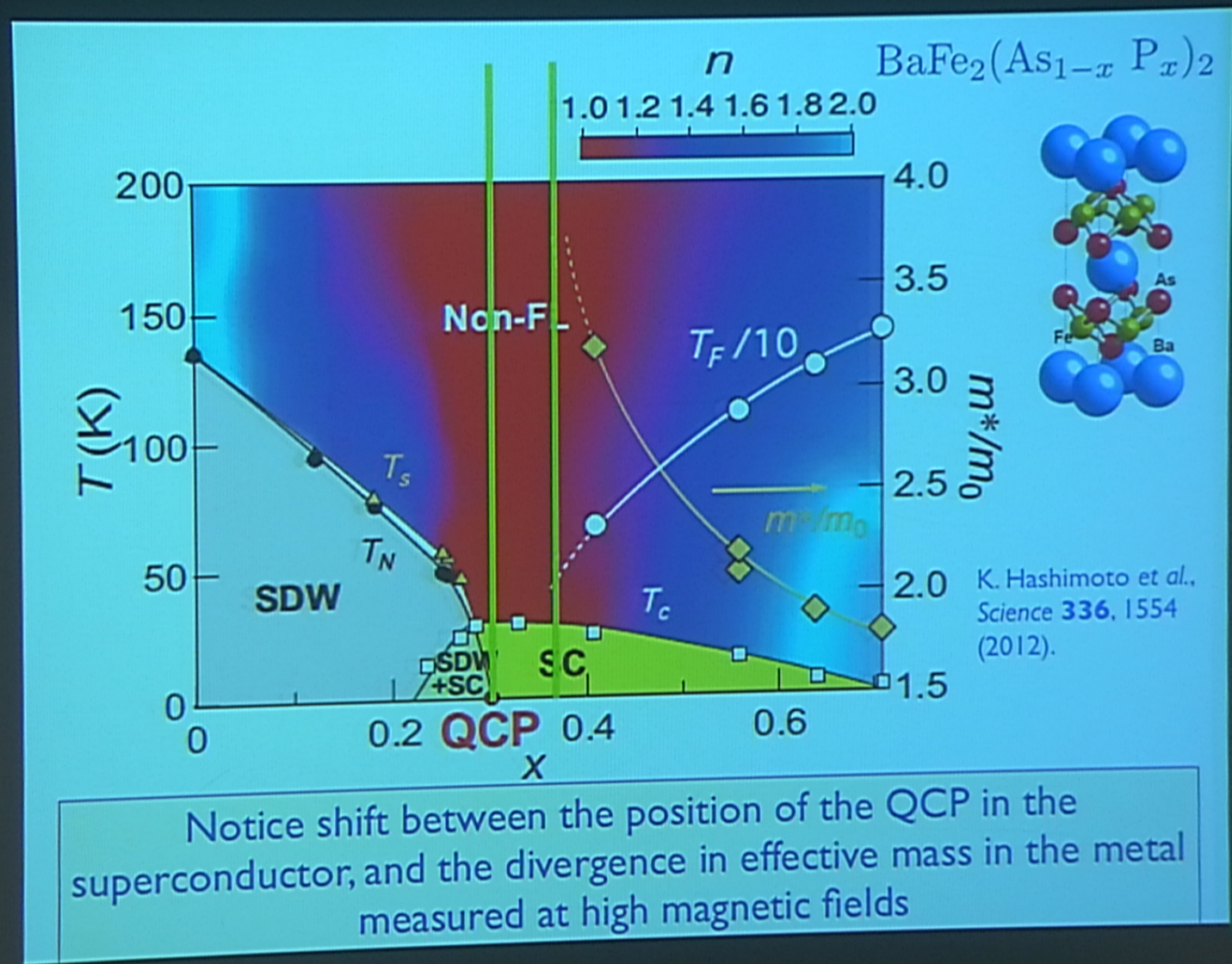
E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742

QMC for the onset of antiferromagnetism

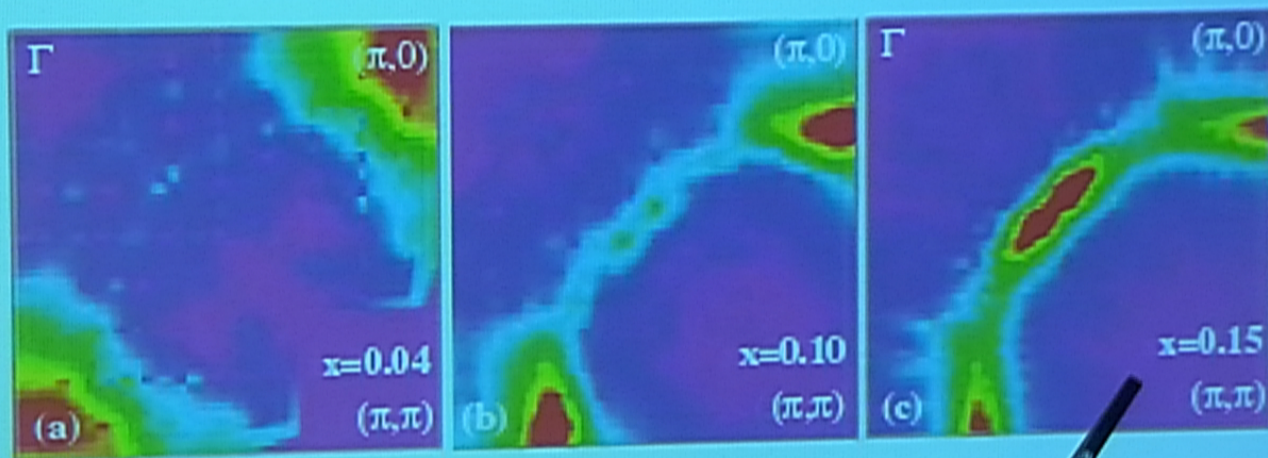


s/d pairing amplitudes P_+/P_-
as a function of the tuning parameter r

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

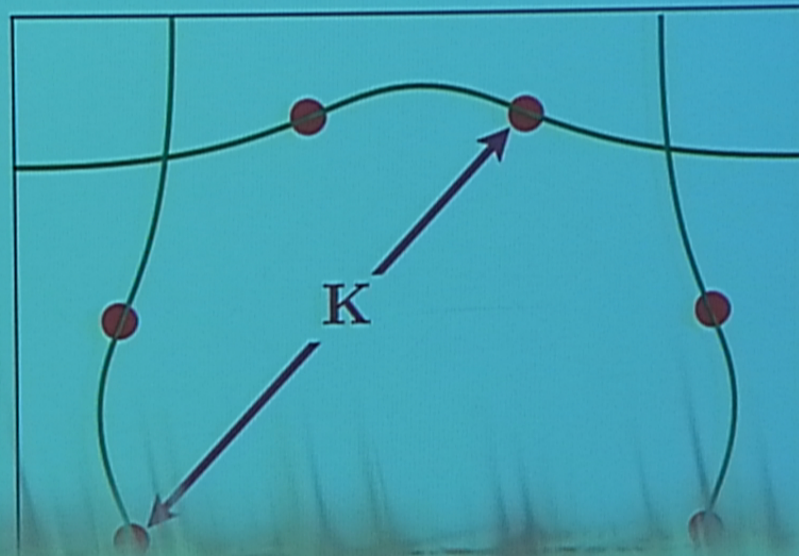


Photoemission in $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$



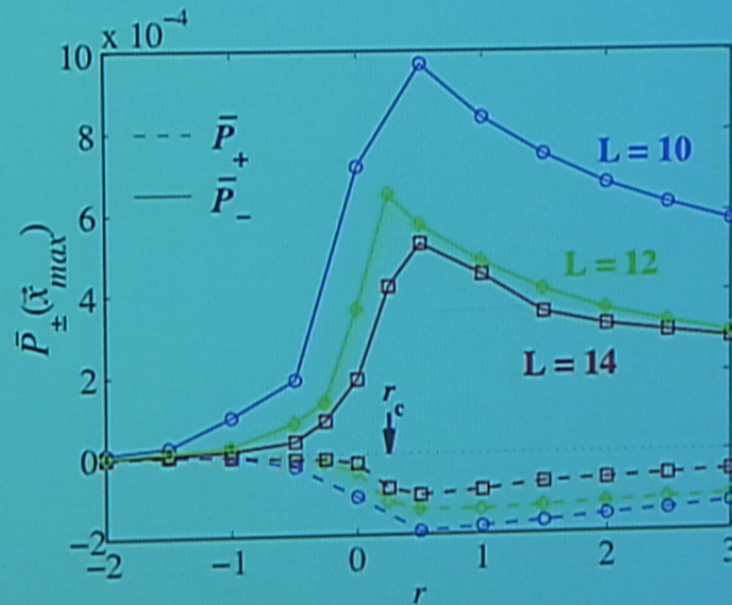
N. P. Armitage et al., Phys. Rev. Lett. **89**, 257001 (2002).

QMC for the onset of antiferromagnetism



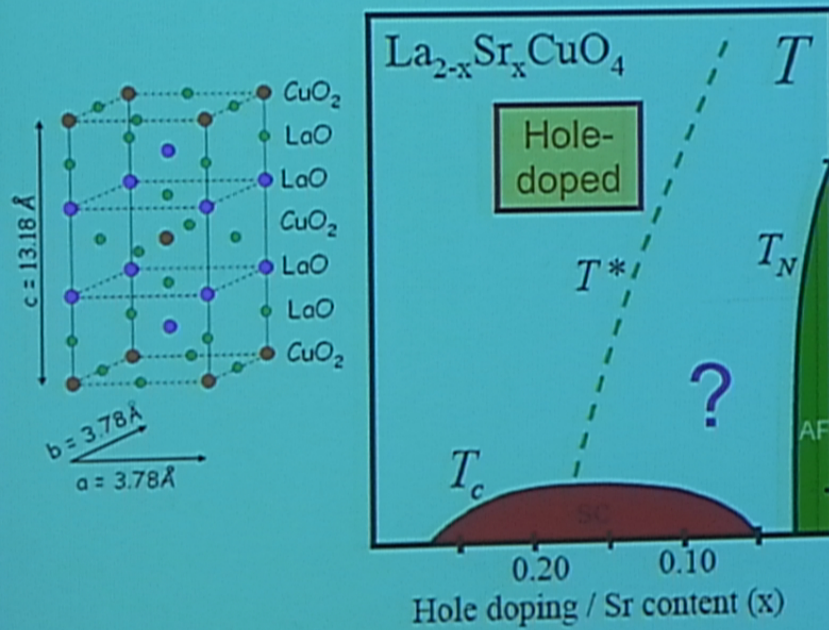
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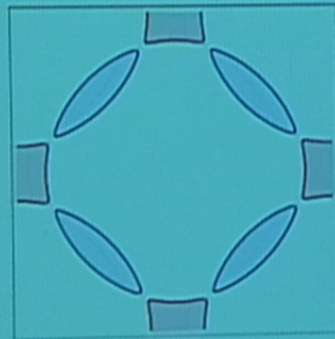


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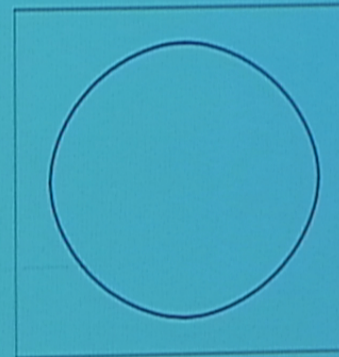


Quantum phase transition with Fermi surface reconstruction



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

Metal with electron
and hole pockets

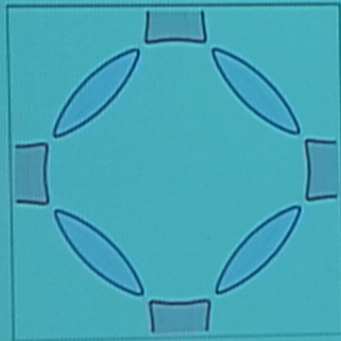


$$\langle \vec{\varphi} \rangle = 0$$

Metal with “large”
Fermi surface

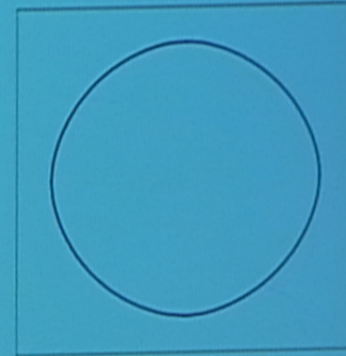


Separating onset of SDW order and Fermi surface reconstruction



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

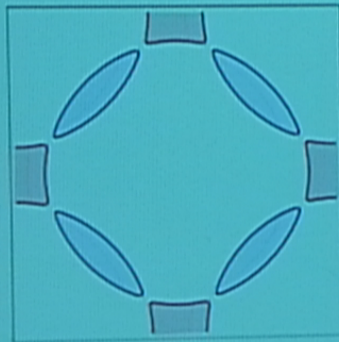
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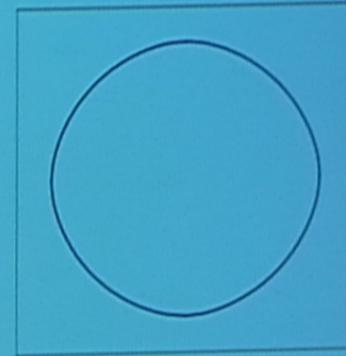


$$\langle \vec{\varphi} \rangle \neq 0$$

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

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

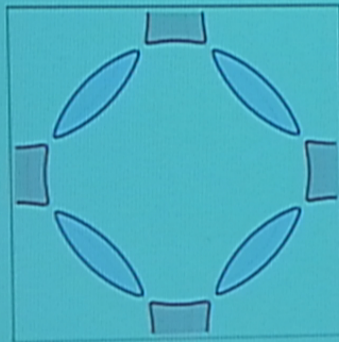


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Metal with “large”
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T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)

Separating onset of SDW order and Fermi surface reconstruction



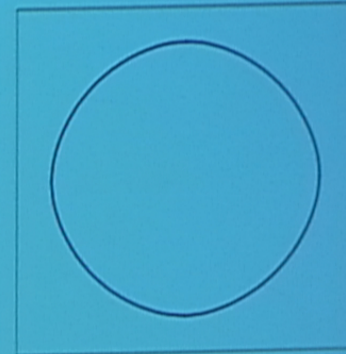
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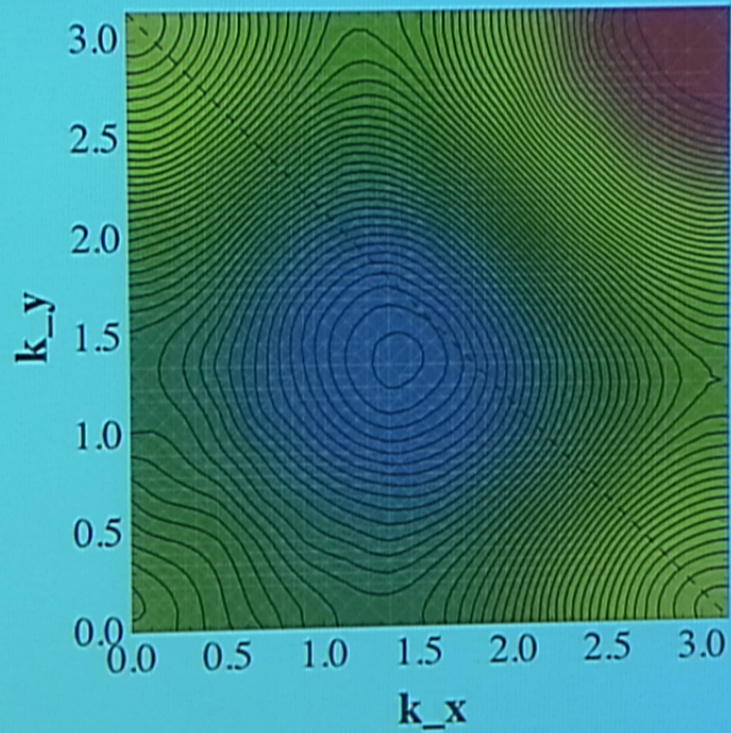
Fractionalized Fermi
liquid (FL*) phase
with no symmetry
breaking and “small”
Fermi surface



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

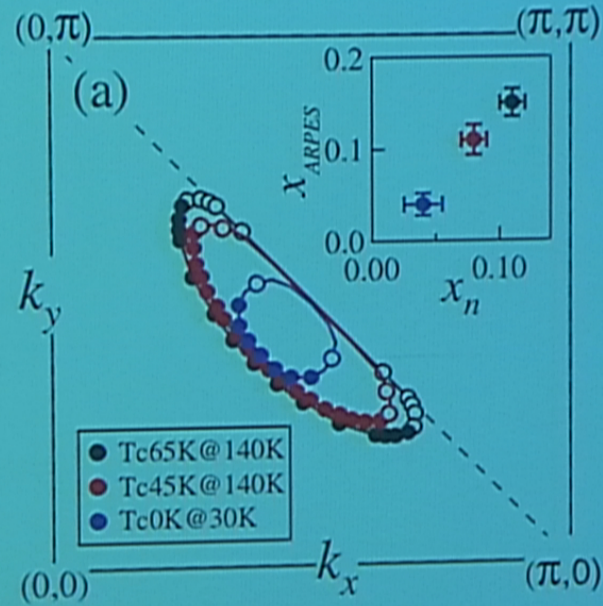
Metal with “large”
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← T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* **90**, 216403 (2003)



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 $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ 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. Kidd³

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)

$$(\nabla\phi)^2 + \lambda\phi^2 + u\phi^4$$

$$+ \psi_1^\dagger (\partial_\tau - \vec{\nabla}_1 \cdot \vec{\nabla}) \psi_1 = \epsilon_k = \vec{v} \cdot \vec{k}$$

$$\neq |\vec{k}|$$

$$\psi_2^\dagger (\partial_\tau - \vec{\nabla}_2 \cdot \vec{\nabla}) \psi_2$$

$$+ \lambda \phi (\psi_1^\dagger \vec{\psi}_2 + \text{h.c.})$$

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

Questions and Answers

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

Yes; convincing evidence from field theory and sign-problem free quantum Monte Carlo

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

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

