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

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La$_{2-x}$Sr$_x$CuO$_4$

Hole-doped

$T_c$

$T^*$

$T_N$

AF

Hole doping / Sr content (x)
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).

Resistivity \( \sim \rho_0 + AT^n \)
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BaFe$_2$(As$_{1-x}$P$_x$)$_2$

Lower $T_c$ superconductivity in the heavy fermion compounds

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?
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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

Metal with “large” Fermi surface

Momenta with electronic states empty

Momenta with electronic states occupied
The electron spin polarization obeys

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

where $\vec{K}$ is the ordering wavevector.
Metal with “large” Fermi surface
Fermi surfaces translated by $\mathbf{K} = (\pi, \pi)$. 

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Electron and hole pockets in antiferromagnetic phase with $\langle \bar{\phi} \rangle \neq 0$
Fermi surface + antiferromagnetism

Metal with electron and hole pockets

\[ \langle \varphi \rangle \neq 0 \]

Metal with “large” Fermi surface

\[ \langle \varphi \rangle = 0 \]

Increasing interaction

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

Quantum oscillations

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

Fermi surface + antiferromagnetism

\[ \langle \tilde{\varphi} \rangle \neq 0 \]

Metal with electron and hole pockets

\[ \langle \tilde{\varphi} \rangle = 0 \]

Metal with “large” Fermi surface

Fluctuating Fermi pockets

Quantum Critical

Large Fermi surface

Underlying SDW ordering quantum critical point in metal at $x = x_m$
Fermi surface + antiferromagnetism

Fluctuating Fermi pockets

Quantum Critical

Large Fermi surface

Spin density wave (SDW)

Relaxation and equilibration times $\sim \hbar/k_BT$ are robust properties of strongly-coupled quantum criticality
Fluctuating Fermi pockets

Large Fermi surface

Strange Metal? 

Relaxation and equilibration times $\sim \hbar/k_B T$ are robust properties of strongly-coupled quantum criticality
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Boson-fermion theory for both phases

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

\[ \mathcal{L}_c = c_\alpha^\dagger \varepsilon (-i \nabla) c_\alpha \]

\[ \mathcal{L}_\varphi = \frac{1}{2} (\nabla \varphi_\alpha)^2 + \frac{r}{2} \varphi_\alpha^2 + \frac{u}{4} (\varphi_\alpha^2)^2 \]
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\[ \mathcal{L}_{c\varphi} = \lambda \varphi_\alpha e^{i K \cdot r} c_a^\dagger \sigma_{ab}^\alpha c_b. \]

“Yukawa” coupling between fermions and antiferromagnetic order:
\[ \lambda^2 \sim U, \text{ the Hubbard repulsion} \]
Hertz-Moriya-Millis theory

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

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

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

- This is dangerous, and will lead to non-local in the $\bar{\varphi}$ 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.

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

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• 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” graphics is required (at least): this theory is even more complicated than QCD.

Fermi surfaces translated by \( \mathbf{K} = (\pi, \pi) \).
“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 $v_{1,2}$) and boson order parameter $\tilde{\varphi}$, interacting with coupling $\lambda$.
Two loop results: Non-Fermi liquid spectrum at hot spots

\[ G_{\text{fermion}} \sim \frac{1}{\sqrt{i\omega - v \cdot k}} \]

Two loop results: Quasiparticle weight vanishes upon approaching hot spots

\[ G_{\text{fermion}} = \frac{Z(k_{||})}{\omega - v_F(k_{||})k_\perp}, \quad Z(k_{||}) \sim v_F(k_{||}) \sim k_{||} \]

Fluctuating Fermi pockets

Large Fermi surface

Strange Metal ?

Increasing SDW order $T^*$

Spin density wave (SDW)

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

Fluctuating, paired Fermi pockets

Strange Metal

Large Fermi surface

d-wave superconductor

Spin density wave (SDW)

Pairing “glue” from antiferromagnetic fluctuations


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Pairing “glue” from antiferromagnetic fluctuations

*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 \( (d_{x^2-y^2} \text{ and } d_{3z^2-r^2}) \) 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
Unconventional pairing at and near hot spots

\[ \langle c^\dagger_{k\alpha} c^\dagger_{-k\beta} \rangle = \varepsilon_{\alpha\beta} \Delta (\cos k_x - \cos k_y) \]
At stronger coupling, different effects compete:

- Pairing glue becomes stronger.
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- There is stronger fermion-boson scattering, and fermionic quasi-particles lose their integrity.
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- 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/striped order.
BCS theory

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

Electron-phonon coupling

Debye frequency
Enhancement of pairing susceptibility by interactions

Antiferromagnetic critical point

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

$\theta$ 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))

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.

**Summary:**

Field theory/RG provide strong evidence that there is unconventional ("pairing-amplitude-sign-changing") spin-singlet superconductivity at the antiferromagnetic 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 $1/(\text{ego})$ as an expansion parameter (R. Shankar)
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- Use $1/\langle \text{ego} \rangle$ as an expansion parameter (R. Shankar)
- Learn string theory
  (string duals cannot treat quantum phase transitions with Fermi surface reconstruction, yet...)

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For the future........

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

- Learn string theory
  (string duals cannot treat quantum phase transitions with Fermi surface reconstruction, yet...)

- Solve on a computer: sign problem........
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$\psi_1$ fermions occupied

$\psi_2$ fermions occupied
Theory has fermions $\psi_{1,2}$ (with Fermi velocities $v_{1,2}$) and boson order parameter $\bar{\phi}$, interacting with coupling $\lambda$.

To faithfully realize low energy theory in quantum Monte Carlo, we need a UV completion in which Fermi lines don’t end and all weights are positive.
QMC for the onset of antiferromagnetism

Hot spots in a single band model
QMC for the onset of antiferromagnetism

Hot spots in a two band model

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742
QMC for the onset of antiferromagnetism

Hot spots in a two band model

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.

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742
QMC for the onset of antiferromagnetism

Electrons with dispersion $\varepsilon_k$
interacting with fluctuations of the antiferromagnetic order parameter $\bar{\phi}$.

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

$$S = \int d\tau \sum_k c_{k\alpha}^\dagger \left( \frac{\partial}{\partial \tau} - \varepsilon_k \right) c_{k\alpha}$$

$$+ \int d\tau d^2x \left[ \frac{1}{2} (\nabla_x \bar{\phi})^2 + \frac{r}{2} \bar{\phi}^2 + \ldots \right]$$

$$- \lambda \int d\tau \sum_i \bar{\phi}_i \cdot (-1)^{x_i} c_{i\alpha}^\dagger \tilde{\sigma}_{\alpha\beta} c_{i\beta}$$
Electrons with dispersions $\varepsilon_k^{(x)}$ and $\varepsilon_k^{(y)}$ interacting with fluctuations of the antiferromagnetic order parameter $\bar{\varphi}$.

$$Z = \int Dc_{\alpha}^{(x)} Dc_{\alpha}^{(y)} D\bar{\varphi} \exp (-S)$$

$$S = \int d\tau \sum_k c_{k\alpha}^{(x)} \left( \frac{\partial}{\partial \tau} - \varepsilon_k^{(x)} \right) c_{k\alpha}^{(x)}$$

$$+ \int d\tau \sum_k c_{k\alpha}^{(y)} \left( \frac{\partial}{\partial \tau} - \varepsilon_k^{(y)} \right) c_{k\alpha}^{(y)}$$

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

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

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Electrons with dispersions $\varepsilon^{(x)}_k$ and $\varepsilon^{(y)}_k$ interacting with fluctuations of the antiferromagnetic order parameter $\vec{\phi}$.

$$Z = \int \mathcal{D}c^{(x)}_\alpha \mathcal{D}c^{(y)}_\alpha \mathcal{D}\vec{\phi} \exp (-S)$$

$$S = \int d\tau \sum_k c^{(x)}_k \left( \frac{\partial}{\partial \tau} - \varepsilon^{(x)}_k \right) c^{(x)}_k$$

$$+ \int d\tau \sum_k c^{(y)}_k \left( \frac{\partial}{\partial \tau} - \varepsilon^{(y)}_k \right) c^{(y)}_k$$

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

$$- \lambda \int d\tau \sum_i \vec{\phi}_i \cdot (-1)^{x_i} c^{(x)}_{i\alpha} \sigma_{\alpha\beta} c^{(y)}_{i\beta} + \text{H.c.}$$

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No sign problem!
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Hot spots in a two band model

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742
QMC for the onset of antiferromagnetism

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

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742
QMC for the onset of antiferromagnetism

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

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742
QMC for the onset of antiferromagnetism

Now hot spots are at Fermi surface intersections

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742
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Expected Fermi surfaces in the AFM ordered phase

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

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QMC for the onset of antiferromagnetism

Electron occupation number $n_k$ 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, $\chi_\varphi$, 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
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.
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Hole-doped

$La_{2-x}Sr_xCuO_4$

$T^*$

$T_c$

$T_N$

SC

AF

Hole doping / Sr content (x)
Quantum phase transition with Fermi surface reconstruction

Metal with electron and hole pockets

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

Metal with “large” Fermi surface

$\langle \tilde{\varphi} \rangle = 0$
Separating onset of SDW order and Fermi surface reconstruction

\[ \langle \phi \rangle \neq 0 \]

Metal with electron and hole pockets

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Metal with “large” Fermi surface
Separating onset of SDW order and Fermi surface reconstruction

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

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

Magnetic order and the heavy Fermi liquid in the Kondo lattice

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

$\langle \varphi \rangle \neq 0$

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

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

Heavy Fermi liquid with “large” Fermi surface of hybridized $f$ and $c$-conduction electrons

$\langle \varphi \rangle \neq 0$

$\langle \varphi \rangle = 0$

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

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

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

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

Magnetic Metal: 
- $f$-electron moments and
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Fractionalized Fermi liquid (FL*) phase with no symmetry breaking and “small” Fermi surface

Heavy Fermi liquid with “large” Fermi surface of hybridized $f$ and $c$-conduction electrons

Experimental perspective on same phase diagrams of Kondo lattice

Fractionalized Fermi liquid (FL*)

YbAgGe
YbRh$_2$(Si$_{0.95}$ Ge$_{0.05}$)$_2$
Yb(Rh$_{0.94}$ Ir$_{0.06}$)$_2$Si$_2$
YbRh$_2$Si$_2$
Yb(Rh$_{0.93}$ Co$_{0.07}$)$_2$Si$_2$
CeCu$_2$Si$_2$

AFM Metal

large Fermi surface heavy Fermi liquid

Kondo screened paramagnet

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

$\langle \phi \rangle = 0$

Metal with “large” Fermi surface

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

Reconstructed Fermi Surface of Underdoped Bi$_2$Sr$_2$CaCu$_2$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. Kidd$^3$
Characteristics of FL* phase

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• 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.

Questions

1. Can quantum fluctuations near the onset of antiferromagnetism induce higher temperature superconductivity?

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

3. What is the physics of the strange metal?
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

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