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

Perimeter Institute, July 11, 2012

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Electron-doped cuprate superconductors

- **Hole-doped**
  - $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$
  - $c = 13.18 \text{Å}$
  - $\mathbf{b} = 3.78 \text{Å}$
  - $\mathbf{a} = 3.78 \text{Å}$

- **Electron-doped**
  - $\text{RE}_{2-x}\text{Ce}_x\text{CuO}_4$
  - $T^*$
  - $T_N$
  - $\sim 300 \text{K}$
  - $T_c$
  - $\sim 30 \text{K}$

- Diagram showing the relationship between hole doping, electron doping, and superconductivity ($T_c$) for different materials.
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 \( \sim \rho_0 + A T^n \)
BaFe$_2$(As$_{1-x}$ P$_x$)$_2$

Resistivity $\sim \rho_0 + A T^n$

Lower $T_c$ superconductivity in the heavy fermion compounds

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
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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 \( \alpha = \uparrow, \downarrow \)

\[ n_{i\alpha} = c_{i\alpha}^\dagger c_{i\alpha} \]

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

\[ c_{i\alpha} c_{j\beta} + c_{j\beta} c_{i\alpha} = 0 \]
The Hubbard Model

Decouple $U$ term by a Hubbard-Stratanovich transformation

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

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

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

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

“Yukawa” coupling between fermions and antiferromagnetic order:

$\lambda^2 \sim U$, the Hubbard repulsion
The electron spin polarization obeys

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

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

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

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

$$E_{\mathbf{k}\pm} = \frac{\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k+K}}}{2} \pm \sqrt{\left(\frac{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k+K}}}{2}\right)^2 + \lambda^2 \varphi^2}$$
Metal with “large” Fermi surface
Fermi surfaces translated by $\mathbf{K} = (\pi, \pi)$. 
Fermi surface + antiferromagnetism

“Hot” spots
Electron and hole pockets in antiferromagnetic phase with $\langle \bar{\varphi} \rangle \neq 0$
Fermi surface + antiferromagnetism

Metal with electron and hole pockets

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

Metal with "large" Fermi surface

\[ \langle \phi \rangle = 0 \]

Increasing interaction

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

Quantum oscillations

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

T. Helm, M. V. Kartsovnik, M. Bartkowiak, N. Bittner, M. Lambacher, A. Erb, J. Wosnitza, and R. Gross,

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

D. J. Scalapino, E. Loh, Jr.,* and J. E. Hirsch†

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(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)
Pairing by SDW fluctuation exchange

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

$$H_{\text{sdw}} = - \sum_{\mathbf{k}, \mathbf{q}, \alpha, \beta} \varphi_{\mathbf{q}} \cdot c_{\mathbf{k} + \mathbf{q}, \alpha}^\dagger \sigma_{\alpha \beta} c_{\mathbf{k} + \mathbf{q} + \mathbf{K}, \beta}.$$ 

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

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

where the pairing interaction is

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

with $\lambda^2 \xi^2$ the SDW susceptibility and $\xi$ 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 $\Delta_k \propto \langle c_{k\uparrow}c_{-k\downarrow} \rangle$.

$$\Delta_k = -\sum_p \left( \frac{3\lambda^2}{\xi^{-2} + (p - k - K)^2} \right) \frac{\Delta_p}{2\sqrt{\varepsilon_p^2 + \Delta_p^2}}$$

Non-zero solutions of this equation require that $\Delta_k$ and $\Delta_p$ have opposite signs when $p - k \approx K$. 
Pairing “glue” from antiferromagnetic fluctuations
Unconventional pairing at and near hot spots
Fermi surface + antiferromagnetism

Metal with electron and hole pockets
\[ \langle \varphi \rangle \neq 0 \]

Metal with “large” Fermi surface
\[ \langle \varphi \rangle = 0 \]

Fluctuating Fermi pockets

Quantum Critical

Large Fermi surface

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

Large Fermi surface

Quantum Critical

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
Fermi surface + antiferromagnetism

Fluctuating Fermi pockets

Strange Metal ?

Large Fermi surface

Spin density wave (SDW)

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

Pairing “glue” from antiferromagnetic fluctuations

At stronger coupling, different effects compete:

- Pairing glue becomes stronger.
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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.
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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 $\bar{\varphi}$, interacting with coupling $\lambda$. 

\begin{align*}
\psi_1 \text{ fermions} & \text{ occupied} \\
\psi_2 \text{ fermions} & \text{ occupied}
\end{align*}
• In $d = 2$, we must work in local theories which keeps 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” graphics is required (at least): this theory is even more complicated than QCD.

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

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

Weak-coupling theory

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

Pairing by SDW fluctuation exchange

Fermi energy

Density of states at Fermi energy
Pairing by SDW fluctuation exchange

Antiferromagnetic critical point

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

\( \theta \) 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))

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.

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........
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\begin{itemize}
  \item $\psi_1$ fermions occupied
  \item $\psi_2$ fermions occupied
\end{itemize}
Theory has fermions $\psi_{1,2}$ (with Fermi velocities $v_{1,2}$) and boson order parameter $\bar{\varphi}$, 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.
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
Hot spots in a two band model

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

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

Hot spots in a two band model
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 $\vec{\varphi}$.

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

$$
S = \int d\tau \sum_k c^\dagger_k \alpha \left( \frac{\partial}{\partial \tau} - \varepsilon_k \right) c_k \alpha
$$

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

$$
- \lambda \int d\tau \sum_i \vec{\varphi}_i \cdot (-1)^{x_i} c^\dagger_{i\alpha} \vec{\sigma}_{\alpha\beta} c_{i\beta}
$$
QMC for the onset of antiferromagnetism

Electrons with dispersions $\varepsilon_{k}(x)$ and $\varepsilon_{k}(y)$ interacting with fluctuations of the antiferromagnetic order parameter $\bar{\varphi}$.

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

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

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

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

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

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742
Electrons with dispersions $\varepsilon^{(x)}_k$ and $\varepsilon^{(y)}_k$
interacting with fluctuations of the antiferromagnetic order parameter $\vec{\varphi}$.

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

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

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

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

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

No sign problem!
Hot spots in a two band model

QMC for the onset of antiferromagnetism

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

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

Wednesday, July 11, 12
QMC for the onset of antiferromagnetism

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

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
QMC for the onset of antiferromagnetism

Expected Fermi surfaces in the AFM ordered phase

E. Berg, M. Metlitski, and S. Sachdev, arXiv:1206.0742
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, $\chi_\phi$, 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
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

$La_{2-x}Sr_xCuO_4$

Hole doping / Sr content (x)

$T_c$

$T^*$

$T_N$

AF
Hole-doped

\( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \)

Hole doping / Sr content (x)

\( T_c \)

\( T^* \)

\( T_N \)

AF

Wednesday, July 11, 12
Quantum phase transition with Fermi surface reconstruction

Metal with electron and hole pockets

$\langle \varphi \rangle \neq 0$

Metal with "large" Fermi surface

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

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

Metal with electron and hole pockets

\[ \langle \phi \rangle = 0 \]

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

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

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

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

Metal with electron and hole pockets

Metal with “large” Fermi surface

Separating onset of SDW order and Fermi surface reconstruction

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

Metal with electron and hole pockets

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

Metal with “large” Fermi surface

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

Reconstructed Fermi Surface of Underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ Cuprate Superconductors

Characteristics of FL* phase

- Fermi surface volume does not count all electrons.

- Such a phase \textit{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**

- 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

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?

What is the physics of the strange metal?
Can quantum fluctuations near the onset of antiferromagnetism induce higher temperature superconductivity?

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The QCP shift from the metal to the superconductor is large. New physics (charge order, fractionalization...) is likely present in the intermediate regime

What is the physics of the strange metal?
Questions and Answers

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What is the physics of the strange metal?

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