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

Perimeter Institute, July 11, 2012

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Electron-doped cuprate superconductors



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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).

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



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Lower T_c superconductivity in the heavy fermion compounds



G. Knebel, D. Aoki, and J. Flouquet, arXiv:0911.5223. Tuson Park, F. Ronning, H. Q. Yuan, M. B. Salamon, R. Movshovich, J. L. Sarrao, and J. D. Thompson, *Nature* **440**, 65 (2006)

<u>Outline</u>

I.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

$$S = \int d^2 r d\tau \left[\mathcal{L}_c + \mathcal{L}_{\varphi} + \mathcal{L}_{c\varphi} \right]$$
$$\mathcal{L}_c = c_a^{\dagger} \varepsilon (-i \mathbf{\nabla}) c_a$$

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

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

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



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.

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}

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

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

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



Metal with "large" Fermi surface

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





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



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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Photoemission in Nd_{2-x}Ce_xCuO₄



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

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Quantum oscillations

$$Nd_{2-x}Ce_{x}CuO_{4}$$

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



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)

Pairing by SDW fluctuation exchange

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

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

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

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

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



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



Unconventional pairing at <u>and near</u> hot spots

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

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

Metal with electron and hole pockets Metal with "large" Fermi surface

S

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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Pairing "glue" from antiferromagnetic fluctuations

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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Low energy theory for critical point near hot spots



Low energy theory for critical point near hot spots

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



- In d = 2, we must work in local theores 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.

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)

 k_x

Two loop results: Quasiparticle weight vanishes upon approaching hot spots



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

Pairing by SDW fluctuation exchange



Pairing by SDW fluctuation exchange



(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

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



- Universal log² 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.

Solution For 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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 k_y

 k_x

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 !



Hot spots in a single band model



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



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



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

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}c_{\alpha}\mathcal{D}\vec{\varphi}\exp\left(-\mathcal{S}\right) \\ \mathcal{S} &= \int d\tau \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^{\dagger} \left(\frac{\partial}{\partial\tau} - \varepsilon_{\mathbf{k}}\right) c_{\mathbf{k}\alpha} \\ &+ \int d\tau d^{2}x \left[\frac{1}{2} \left(\boldsymbol{\nabla}_{x}\vec{\varphi}\right)^{2} + \frac{r}{2}\vec{\varphi}^{2} + \ldots\right] \\ &- \lambda \int d\tau \sum_{i} \vec{\varphi}_{i} \cdot (-1)^{\mathbf{x}_{i}} c_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta} \end{aligned}$$

1206.0742

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

$$\begin{split} \mathcal{Z} &= \int \mathcal{D} c_{\alpha}^{(x)} \mathcal{D} c_{\alpha}^{(y)} \mathcal{D} \vec{\varphi} \exp\left(-\mathcal{S}\right) & \stackrel{\text{E.Berg,}}{\underset{\text{M. Meditski, and}}{\text{S. Sachdev,}}} \\ \mathcal{S} &= \int d\tau \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^{(x)\dagger} \left(\frac{\partial}{\partial \tau} - \varepsilon_{\mathbf{k}}^{(x)}\right) c_{\mathbf{k}\alpha}^{(x)} & \text{arXiv:1206.0742} \\ &+ \int d\tau \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^{(y)\dagger} \left(\frac{\partial}{\partial \tau} - \varepsilon_{\mathbf{k}}^{(y)}\right) c_{\mathbf{k}\alpha}^{(y)} \\ &+ \int d\tau d^{2}x \left[\frac{1}{2} \left(\mathbf{\nabla}_{x} \vec{\varphi}\right)^{2} + \frac{r}{2} \vec{\varphi}^{2} + \ldots\right] \\ &- \lambda \int d\tau \sum_{i} \vec{\varphi}_{i} \cdot (-1)^{\mathbf{x}_{i}} c_{i\alpha}^{(x)\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta}^{(y)} + \text{H.c.} \end{split}$$

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





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







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

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



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



....

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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Quantum phase transition with Fermi surface reconstruction





Metal with electron and hole pockets



 $\left<\vec{\varphi}\right>=0$

Metal with "large" Fermi surface

<u>Separating onset of SDW order</u> and Fermi surface reconstruction



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

Metal with electron and hole pockets



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

Metal with "large" Fermi surface

<u>Separating onset of SDW order</u> and Fermi surface reconstruction



 $\left<\vec{\varphi}\right>\neq 0$

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

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

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<u>Separating onset of SDW order</u> and Fermi surface reconstruction



 $\left<\vec{\varphi}\right>\neq 0$

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

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

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



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

Metal with "large" Fermi surface

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



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

M. Punk and S. Sachdev, Phys. Rev. B 85, 195123 (2012)



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. 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)

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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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