Quantum critical metals near the onset of antiferromagnetism: superconductivity and other instabilities

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The electron spin polarization obeys

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

where $K$ is the ordering wavevector.
Metal with electron and hole pockets

Increasing interaction

Metal with “large” Fermi surface

Lower $T_c$ superconductivity in the heavy fermion compounds

Hole-doped cuprates

G. Grissonnanche et al., preprint
Temperature (K)

Hole doping

YBCO

Charge order

Spin order

Spin order

Charge order

T_{\text{max}}

T_0

T_c

ρ_a (\mu \Omega \text{cm})

\Delta T_c / T_c (\%)

G. Grissonnanche et al., preprint

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Figure 4: Fermi surface reconstruction from order that is biaxial within each bilayer and staggered perpendicular to the bilayers. (A) A schematic of biaxial order yielding inequivalent sites (depicted by symbols of varying color and size) within the bilayers (considering an example where $\delta_1 \approx \delta_2 \approx 0.25$) resulting in a body-centered tetragonal superstructure. (B) Reconstruction of the Brillouin zone, with one instance of the pocket location indicated at the 'X' point in relation to the original Fermi surface (purple) and nodes in the superconducting wave function. (C) A three-dimensional rendition of the concentrically arranged Fermi surfaces resulting from bilayer splitting exhibiting a twofold screw warping.

Our finding of a twofold screw symmetry rules out an origin of the pockets from non-conductors [17, 18, 19] (see Fig. 1B)). Materials with a body-centered tetragonal structure (see Fig. 1C), by contrast, exhibit a unique twofold screw symmetry at the Brillouin zone corner 'X' (see Fig. 1D). Examples of layered materials with Fermi surface warpings exhibiting this symmetry include the ruthenates [7], the overdoped Tl-based cuprates [9] and pnictide superconductors of the '122' composition [8].

The symmetry of the Fermi surface warping is determined by fitting to the angular-dependence of the quantum oscillation frequencies and amplitudes in tilted magnetic fields [7, 9]. In the case...
Outline

1. Weak coupling theory of SDW ordering, and d-wave superconductivity

2. Universal critical theory of SDW ordering

3. Emergent pseudospin symmetry, and quadrupolar density wave

4. Quantum Monte Carlo without the sign problem
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1. Weak coupling theory of SDW ordering, and d-wave superconductivity

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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
Fermi surface + antiferromagnetism

Metal with electron and hole pockets

Increasing interaction

Metal with “large” Fermi surface


Theory of quantum criticality in the cuprates

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

Large Fermi surface

Strange Metal

Spin density wave (SDW)

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

Theory of quantum criticality in the cuprates
Theory of quantum criticality in the cuprates

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
Pairing by SDW fluctuation exchange

We now allow the SDW field \( \tilde{\varphi} \) to be dynamical, coupling to electrons as

\[
H_{\text{sdw}} = - \sum_{\mathbf{k}, \mathbf{q}, \alpha, \beta} \tilde{\varphi}_\mathbf{q} \cdot \mathbf{c}_\mathbf{k}\alpha \tilde{\sigma}_{\alpha\beta} \mathbf{c}_{\mathbf{k}+\mathbf{K}+\mathbf{q},\beta}.
\]

Exchange of a \( \tilde{\varphi} \) quantum leads to the effective interaction

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

where the pairing interaction is

\[
V_{\alpha\beta,\gamma\delta}(\mathbf{q}) = \tilde{\sigma}_{\alpha\beta} \cdot \tilde{\sigma}_{\gamma\delta} \frac{\chi_0}{\xi^{-2} + (\mathbf{q} - \mathbf{K})^2},
\]

with \( \chi_0 \xi^2 \) the SDW susceptibility and \( \xi \) the SDW correlation length.
In BCS theory, this interaction leads to the ‘gap equation’ for the pairing gap $\Delta_k \propto \langle c_{k\uparrow} c_{-k\downarrow} \rangle$.

$$\Delta_k = -\sum_p \left( \frac{3\chi_0}{\xi^{-2} + (p - k - K)^2} \right) \frac{\Delta_p}{2\sqrt{\varepsilon_p^2 + \Delta_p^2}}$$

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

\[ \langle c_{k\alpha}^\dagger c_{-k\beta}^\dagger \rangle = \varepsilon_{\alpha\beta} \Delta (\cos k_x - \cos k_y) \]
Fluctuating Fermi pockets

Large Fermi surface

Underlying SDW ordering quantum critical point in metal at $x = x_m$
Theory of quantum criticality in the cuprates

Fluctuating, paired Fermi pockets

Strange Metal

Large Fermi surface

d-wave superconductor

SDW quantum critical point is unstable to $d$-wave superconductivity. This instability is stronger than that in the BCS theory.
Theory of quantum criticality in the cuprates

Competition between SDW order and superconductivity moves the actual quantum critical point to $x = x_s < x_m$. 

Theory of quantum criticality in the cuprates


**Fluctuating, paired Fermi pockets**

**Large Fermi surface**

**Strange Metal**

**d-wave superconductor**

**Spin density wave (SDW)**

Competition between SDW order and superconductivity moves the actual quantum critical point to $x = x_s < x_m$. 

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Theory of quantum criticality in the cuprates

Fluctuating, paired Fermi pockets

Strange Metal

Large Fermi surface

d-wave superconductor


Spin density wave (SDW)

Competition between SDW order and superconductivity moves the actual quantum critical point to $x = x_s < x_m$. 

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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.
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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1. Weak coupling theory of SDW ordering, and d-wave superconductivity

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4. Quantum Monte Carlo without the sign problem
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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 $\langle \bar{\Phi} \rangle \neq 0$
“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 $\varphi$, interacting with coupling $\lambda$. 

Diagram showing fermions $\psi_1$ and $\psi_2$ with Fermi velocities $v_1$ and $v_2$. 

$\psi_1$ fermions occupied

$\psi_2$ fermions occupied
\[ \mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \]

\[
\begin{align*}
\psi_1 \text{ fermions} & \quad \text{occupied} \\
\psi_2 \text{ fermions} & \quad \text{occupied}
\end{align*}
\]

$$\mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_{\tau} - i \mathbf{v}_1 \cdot \mathbf{\nabla}_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_{\tau} - i \mathbf{v}_2 \cdot \mathbf{\nabla}_r) \psi_{2\alpha}$$

\[ \mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \]

Order parameter: \[ \mathcal{L}_\varphi = \frac{1}{2} (\nabla_r \varphi)^2 + \frac{\zeta}{2} (\partial_\tau \varphi)^2 + \frac{s}{2} \varphi^2 + \frac{u}{4} \varphi^4 \]

\[ \mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \]

Order parameter:
\[ \mathcal{L}_\varphi = \frac{1}{2} (\nabla_r \bar{\varphi})^2 + \frac{\zeta}{2} (\partial_\tau \bar{\varphi})^2 + \frac{s}{2} \bar{\varphi}^2 + \frac{u}{4} \bar{\varphi}^4 \]

“Yukawa” coupling:
\[ \mathcal{L}_c = -\lambda \bar{\varphi} \cdot \left( \psi_{1\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{1\beta} \right) \]

\[ \mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \]

**Fermion dispersions:** \( \varepsilon_{k1} = \mathbf{v}_1 \cdot \mathbf{k} \) and \( \varepsilon_{k2} = \mathbf{v}_2 \cdot \mathbf{k} \)

**Metal with “large” Fermi surface**

\[ \langle \phi \rangle = 0 \]
\[
\mathcal{L}_f = \psi_1^\dagger (\zeta \partial_\tau - iv_1 \cdot \nabla_r) \psi_1 + \psi_2^\dagger (\zeta \partial_\tau - iv_2 \cdot \nabla_r) \psi_2
\]
\[
-\lambda \bar{\varphi} \cdot \left( \psi_1^\dagger \sigma_{\alpha\beta} \psi_2\beta + \psi_2^\dagger \sigma_{\alpha\beta} \psi_1\beta \right)
\]

Fermion dispersions:

\[
E_{k\pm} = \frac{\varepsilon_{k1} + \varepsilon_{k2}}{2} \pm \sqrt{\left( \frac{\varepsilon_{k1} - \varepsilon_{k2}}{2} \right)^2 + \lambda^2 |\bar{\varphi}|^2}
\]

Metal with hole and electron pockets \( \langle \varphi \rangle \neq 0 \)
Hertz action.

Upon integrating the fermions out, the leading term in the $\bar{\phi}$ effective action is $-\Pi(q, \omega_n)|\bar{\phi}(q, \omega_n)|^2$, where $\Pi(q, \omega_n)$ is the fermion polarizability. This is given by a simple fermion loop diagram

\[
\Pi(q, \omega_n) = \int \frac{d^d k}{(2\pi)^d} \int \frac{d\epsilon_n}{2\pi} \frac{1}{[-i\zeta(\epsilon_n + \omega_n) + \mathbf{v}_1 \cdot (\mathbf{k} + \mathbf{q})][-i\zeta\epsilon_n + \mathbf{v}_2 \cdot \mathbf{k}]} \tag{1}
\]

We define oblique co-ordinates $p_1 = \mathbf{v}_1 \cdot \mathbf{k}$ and $p_2 = \mathbf{v}_2 \cdot \mathbf{k}$. It is then clear that the integrand in (1) is independent of the $(d - 2)$ transverse momenta, whose integral yields an overall factor $\Lambda^{d-2}$ (in $d = 2$ this factor is precisely 1). Also, by shifting the integral
over $k_1$ we note that the integral is independent of $q$. So we have

$$
\Pi(q, \omega_n) = \frac{\Lambda^{d-2}}{|\mathbf{v}_1 \times \mathbf{v}_2|} \int \frac{dp_1 dp_2 d\epsilon_n}{8\pi^3} \frac{1}{[-i\zeta(\epsilon_n + \omega_n) + p_1][-i\zeta\epsilon_n + p_2]}.
$$

(2)

Next, we evaluate the frequency integral to obtain

$$
\Pi(q, \omega_n) = \frac{\Lambda^{d-2}}{\zeta|\mathbf{v}_1 \times \mathbf{v}_2|} \int \frac{dp_1 dp_2}{4\pi^2} \frac{[\text{sgn}(p_2) - \text{sgn}(p_1)]}{-i\zeta\omega_n + p_1 - p_2}
$$

$$
= -\frac{|\omega_n|\Lambda^{d-2}}{4\pi|\mathbf{v}_1 \times \mathbf{v}_2|}.
$$

(3)

In the last step, we have dropped a frequency-independent, cutoff-dependent constant which can absorbed into a redefinition of $r$. Notice also that the factor of $\zeta$ has cancelled.

Inserting this fermion polarizability in the effective action for $\bar{\varphi}$, we obtain the Hertz action for the SDW transition:

$$
S_H = \int \frac{d^d k}{(2\pi)^d} T \sum_{\omega_n} \frac{1}{2} \left[ k^2 + \gamma|\omega_n| + s \right] |\bar{\varphi}(k, \omega_n)|^2
$$

$$
+ \frac{u}{4} \int d^d x d\tau \left( \bar{\varphi}^2(x, \tau) \right)^2.
$$

(4)
**Exercise:** Perform a tree-level RG rescaling on $S_H$. Now we rescale co-ordinates as $x' = xe^{-\ell}$ and $\tau' = \tau e^{-z\ell}$. Here $z$ is the dynamic critical exponent. Show that the gradient and non-local terms become invariant for $z = 2$ (previous theories considered here had $z = 1$). Then show that the transformation of the quartic term is $u' = ue^{(2-d)\ell}$. This led Hertz to conclude that the SDW quantum critical point was described by a Gaussian theory for the SDW order parameter in $d \geq 2$. 
Fate of the fermions.

Let us, for now, assume the validity of the Hertz Gaussian action, and compute the leading correction to the electronic Green’s function. This is given by the following Feynman graph for the electron self energy, $\Sigma$. At zero momentum for the $\psi_1$ fermion we have

$$
\Sigma_1(0, \omega_n) = \lambda^2 \int \frac{d^d q}{(2\pi)^d} \int \frac{d\epsilon_n}{2\pi} \frac{1}{[q^2 + \gamma|\epsilon_n|][-i\zeta(\epsilon_n + \omega_n) + \mathbf{v}_2 \cdot \mathbf{q}]}.
$$

We first perform the integral over the $\mathbf{q}$ direction parallel to $\mathbf{v}_2$, while ignoring the subdominant dependence on this momentum in the boson propagator. The dependence on $\zeta$ immediately
disappears, and we have

$$
\Sigma_1(0, \omega_n) = i \frac{\lambda^2}{|v_2|} \int \frac{d^{d-1}q}{(2\pi)^{d-1}} \int \frac{d\epsilon_n \operatorname{sgn}(\epsilon_n + \omega_n)}{2\pi} \frac{|q|^2 + \gamma |\epsilon_n|}{|q|^2 + |\epsilon_n|}
$$

$$
= i \frac{\lambda^2}{\pi |v_2| \gamma} \operatorname{sgn}(\omega_n) \int \frac{d^{d-1}q}{(2\pi)^{d-1}} \ln \left( \frac{|q|^2 + \gamma |\omega_n|}{|q|^2} \right). \quad (6)
$$

Evaluation of the $q$ integral shows that

$$
\Sigma_1(0, \omega_n) \sim |\omega_n|^{(d-1)/2} \quad (7)
$$

The most important case is $d = 2$, where we have

$$
\Sigma_1(0, \omega_n) = i \frac{\lambda^2}{\pi |v_2| \sqrt{\gamma}} \operatorname{sgn}(\omega_n) \sqrt{|\omega_n|}, \quad d = 2. \quad (8)
$$
Strong coupling physics in $d = 2$

The theory so far has the boson propagator

$$\sim \frac{1}{q^2 + \gamma|\omega|}$$

which scales with dynamic exponent $z_b = 2$, and now a fermion propagator

$$\sim \frac{1}{-i\zeta \omega + c_1|\omega|^{(d-1)/2} + v \cdot q}.$$  

First note that for $d < 3$, the bare $-i\zeta \omega$ term is less important than the contribution from the self energy at low frequencies. This indicates that $\zeta$ is *irrelevant* in the critical theory, and we can set $\zeta \to 0$. Fortunately, all the loop diagrams evaluated so far are independent of $\zeta$.

Setting $\zeta = 0$, we see that the fermion propagator scales with dynamic exponent $z_f = 2/(d-1)$. For $d > 2$, $z_f < z_b$, and so at small momenta the boson fluctuations have lower energy than the fermion fluctuations. Thus it seems reasonable to assume that the
fermion fluctuations are not as singular, and we can focus on an effective theory of the SDW order parameter $\vec{\phi}$ alone. In other words, the Hertz assumptions appear valid for $d > 2$.

However, in $d = 2$, we have $z_f = z_b = 2$. Thus fermionic and bosonic fluctuations are equally important, and it is not appropriate to integrate the fermions out at an initial stage. We have to return to the original theory of coupled bosons and fermions. This turns out to be strongly coupled, and exhibits complex critical behavior. For more details, see

Perform RG on both fermions and $\bar{\phi}$, using a local field theory.

\[ \mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \]

Order parameter:

\[ \mathcal{L}_\phi = \frac{1}{2} (\nabla_r \bar{\phi})^2 + \frac{\tilde{\zeta}}{2} (\partial_\tau \bar{\phi})^2 + \frac{s}{2} \bar{\phi}^2 + \frac{u}{4} \bar{\phi}^4 \]

“Yukawa” coupling:

\[ \mathcal{L}_c = -\lambda \bar{\phi} \cdot \left( \psi_{1\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{1\beta} \right) \]
\[ \mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \]

Order parameter: \[ \mathcal{L}_\varphi = \frac{1}{2} (\nabla_r \bar{\varphi})^2 + \frac{\zeta}{2} (\partial_\tau \bar{\varphi})^2 + \frac{s}{2} \bar{\varphi}^2 + \frac{u}{4} \bar{\varphi}^4 \]

"Yukawa" coupling: \[ \mathcal{L}_c = -\lambda \bar{\varphi} \cdot \left( \psi_{1\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{1\beta} \right) \]

Under the rescaling \( x' = xe^{-\ell}, \tau' = \tau e^{-z\ell} \), the spatial gradients are fixed if the fields transform as

\[ \bar{\varphi}' = e^{(d+z-2)\ell/2} \bar{\varphi} ; \quad \psi' = e^{(d+z-1)\ell/2} \psi. \]

Then the Yukawa coupling transforms as

\[ \lambda' = e^{(4-d-z)\ell/2} \lambda \]

For \( d = 2 \), with \( z = 2 \) the bare time-derivative terms \( \zeta, \bar{\zeta} \) are irrelevant, but the Yukawa coupling is invariant. Thus we have to work at fixed \( \lambda = 1 \), and cannot expand in powers of \( \lambda \): critical theory is strongly coupled.
Critical point theory is strongly coupled in $d = 2$
Results are independent of coupling $\lambda$

$G_{\text{fermion}} \sim \frac{1}{i \sqrt{\omega - v.k}}$

Critical point theory is strongly coupled in $d = 2$
Results are independent of coupling $\lambda$

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

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Emergent $[\text{SU}(2)]^4$ pseudospin symmetry

\[ \mathcal{L}_f = \psi_{1\alpha}^{\dagger} (\zeta \partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^{\dagger} (\zeta \partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \]

Order parameter: \[ \mathcal{L}_\varphi = \frac{1}{2} (\nabla_r \bar{\varphi})^2 + \frac{\zeta}{2} (\partial_\tau \bar{\varphi})^2 + s \varphi^2 + u \varphi^4 \]

"Yukawa" coupling: \[ \mathcal{L}_c = -\lambda \bar{\varphi} \cdot \left( \psi_{1\alpha}^{\dagger} \tilde{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^{\dagger} \tilde{\sigma}_{\alpha\beta} \psi_{1\beta} \right) \]
Emergent $[\text{SU}(2)]^4$ pseudospin symmetry

\[ \mathcal{L}_f = \psi_{1\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\zeta \partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \]

Order parameter: \[ \mathcal{L}_\varphi = \frac{1}{2} (\nabla_r \bar{\varphi})^2 + \frac{\zeta}{2} (\partial_\tau \bar{\varphi})^2 + \frac{s}{2} \bar{\varphi}^2 + \frac{u}{4} \bar{\varphi}^4 \]

“Yukawa” coupling: \[ \mathcal{L}_c = -\lambda \bar{\varphi} \cdot \left( \psi_{1\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \bar{\sigma}_{\alpha\beta} \psi_{1\beta} \right) \]

Introduce the spinors

\[ \Psi_{1\alpha} = \left( \begin{array}{c} \psi_{1\alpha} \\ \epsilon_{\alpha\beta} \psi_{1\beta}^\dagger \end{array} \right), \quad \Psi_{2\alpha} = \left( \begin{array}{c} \psi_{2\alpha} \\ \epsilon_{\alpha\beta} \psi_{2\beta}^\dagger \end{array} \right) \]

Then the Lagrangian is invariant under the SU(2) transformation $U$ with \[ \Psi_1 \rightarrow U \Psi_1, \quad \Psi_2 \rightarrow U \Psi_2 \]

Note that $U$ can be chosen independently at the 4 pairs of hotspots.

This symmetry relies on the linearization of the fermion dispersion about the hot spots.
Unconventional pairing at and near hot spots

\[
\left\langle c_{k\alpha}^\dagger c_{-k\beta}^\dagger \right\rangle = \varepsilon_{\alpha\beta} \Delta (\cos k_x - \cos k_y)
\]
Unconventional particle-hole pairing at and near hot spots

\[ \left\langle c_{k-Q/2,\alpha}^\dagger c_{k+Q/2,\alpha} \right\rangle = \Phi(\cos k_x - \cos k_y) \]

Q is ‘2k_F’ wavevector

After pseudospin rotation


Unconventional particle-hole pairing at and near hot spots

After pseudospin rotation

\[ \left\langle c_{k-Q/2,\alpha}^{\dagger} c_{k+Q/2,\alpha} \right\rangle = \Phi(\cos k_x - \cos k_y) \]

\( Q \) is ‘2\( k_F \)’ wavevector

\( \Phi \) corresponds to a 2\( k_F \) bond-nematic or a quadrupole density wave


Quadrupole density wave
Quadrupole density wave
Quadrupole density wave
Quadrupole density wave

\[ \langle c_{\mathbf{k}+\mathbf{Q}/2,\alpha}^{\dagger} c_{\mathbf{k}-\mathbf{Q}/2,\alpha} \rangle = \Phi(\cos k_x - \cos k_y) \]
Quadrupole density wave

No modulations on sites, $\langle c^\dagger_{\mathbf{r}\alpha} c_{\mathbf{s}\alpha} \rangle$ is modulated only for $\mathbf{r} \neq \mathbf{s}$.

$$\left\langle c^\dagger_{\mathbf{k}-\mathbf{Q}/2,\alpha} c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \right\rangle = \Phi(\cos k_x - \cos k_y)$$

“Bond density” measures amplitude for electrons to be in spin-singlet valence bond.
Quadrupole density wave

No modulations on sites, $\langle c^\dagger_{r\alpha} c_{s\alpha} \rangle$ is modulated only for $r \neq s$.

$$\left\langle c^\dagger_{k-Q/2,\alpha} c_{k+Q/2,\alpha} \right\rangle = \Phi(\cos k_x - \cos k_y)$$
No modulations on sites, $\langle c^\dagger_{r\alpha} c_{s\alpha} \rangle$ is modulated only for $r \neq s$.

$$\left\langle c^\dagger_{k-Q/2,\alpha} c_{k+Q/2,\alpha} \right\rangle = \Phi(\cos k_x - \cos k_y)$$
No modulations on sites, $\langle c_{\mathbf{r}\alpha}^\dagger c_{\mathbf{s}\alpha} \rangle$ is modulated only for $\mathbf{r} \neq \mathbf{s}$.

$$\langle c_{\mathbf{k}-\mathbf{Q}/2,\alpha}^\dagger c_{\mathbf{k}+\mathbf{Q}/2,\alpha} \rangle = \Phi(\cos k_x - \cos k_y)$$
Strength of instability at quantum criticality

BCS theory

\[ 1 + \lambda_{e-ph} \log \left( \frac{\omega D}{\omega} \right) \]
Strength of instability at quantum criticality

BCS theory

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

Electron-phonon coupling

Debye frequency

Implies

\[ T_c \sim \omega_D \exp \left( -\frac{1}{\lambda} \right) \]
Strength of instability at quantum criticality

Spin density wave quantum critical point

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


Y. Wang and A. Chubukov, arXiv:1210.2408
Spin density wave quantum critical point

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

\[ \alpha = \tan \theta, \text{ where } 2\theta \text{ is the angle between Fermi lines.} \]

Independent of interaction strength $U$ in 2 dimensions.


Y. Wang and A. Chubukov, arXiv:1210.2408
\[ G_{\text{fermion}} = \frac{Z(k_{\parallel})}{i\omega - v_F(k_{\parallel})k_{\perp}}, \quad Z(k_{\parallel}) \sim v_F(k_{\parallel}) \sim k_{\parallel} \]

\[ \int dk_{\parallel} \frac{1}{k_{\parallel}^2} \left( \frac{Z^2(k_{\parallel})}{v_F(k_{\parallel})} \right) \log \frac{k_{\parallel}^2}{\omega} \]
\[ G_{\text{fermion}} = \frac{Z(k_{||})}{i\omega - v_F(k_{||})k_{\perp}}, \quad Z(k_{||}) \sim v_F(k_{||}) \sim k_{||} \]

\[ \int dk_{||} \frac{1}{k_{||}^2} \left( \frac{Z^2(k_{||})}{v_F(k_{||})} \right) \log \frac{k_{||}^2}{\omega} \]

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

\[ \int dk_{||} \frac{1}{k_{||}^2} \left( \frac{Z^2(k_{||})}{v_F(k_{||})} \right) \log \frac{k_{||}^2}{\omega} \]

**Spin fluctuation propagator**

**Cooper logarithm**
Enhancement of pairing susceptibility by interactions

Spin density wave quantum critical point

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

- \(\log^2\) 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.
Enhancement of $\Phi$ susceptibility by interactions

Spin density wave quantum critical point

$$1 + \frac{\alpha}{3\pi(1 + \alpha^2)} \log^2 \left( \frac{E_F}{\omega} \right)$$

- Emergent pseudospin symmetry of low energy theory also induces $\log^2$ in a single “$d$-wave” particle-hole channel. Fermi-surface curvature reduces prefactor by $1/3$.
- $\Phi$ corresponds to a $2k_F$ bond-nematic or a quadrupole density wave

Outline

1. Weak coupling theory of SDW ordering, and d-wave superconductivity

2. Universal critical theory of SDW ordering

3. Emergent pseudospin symmetry, and quadrupolar density wave

4. Quantum Monte Carlo without the sign problem
Outline

1. Weak coupling theory of SDW ordering, and d-wave superconductivity

2. Universal critical theory of SDW ordering

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4. Quantum Monte Carlo without the sign problem
Low energy theory for critical point near hot spots
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

QMC for the onset of antiferromagnetism

Faithful realization of the *generic* universal low energy theory for the onset of antiferromagnetism.


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

Hot spots in a two band model

Sign problem is absent as $K$ connects hotspots in distinct bands.
QMC for the onset of antiferromagnetism

Sign problem is absent as long as $K$ connects hotspots in distinct bands.

Particle-hole or point-group symmetries or commensurate densities not required!

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QMC for the onset of antiferromagnetism

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

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

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

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

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

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

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

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

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

$$- \lambda \int d\tau \sum_{i} \vec{\varphi}_{i} \cdot (-1)^{x_{i}} c_{i\alpha}^{(x)\dagger} \vec{\sigma}_{\alpha\beta} c_{i\beta}^{(y)} + H.c.$$
QMC for the onset of antiferromagnetism

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

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

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

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

$$- \lambda \int d\tau \sum_i \bar{\varphi}_i \cdot (-1)^{x_i} c^{(x)\dagger}_{i\alpha} \sigma_{\alpha\beta} c^{(y)\dagger}_{i\beta} + H.c.$$
**QMC for the onset of antiferromagnetism**

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

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

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

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

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

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

**E. Berg, M. Metlitski, and S. Sachdev, Science 338, 1606 (2012).**

Applies without changes to the microscopic band structure in the iron-based superconductors.
QMC for the onset of antiferromagnetism

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

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

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

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

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

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

Can integrate out $\vec{\varphi}$ to obtain an extended Hubbard model. The interactions in this model only couple electrons in separate bands.

QMC for the onset of antiferromagnetism

Hot spots in a two band model

QMC for the onset of antiferromagnetism

QMC for the onset of antiferromagnetism

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

QMC for the onset of antiferromagnetism


Now hot spots are at Fermi surface intersections

Friday, January 11, 13
QMC for the onset of antiferromagnetism

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

Expected Fermi surfaces in the AFM ordered phase
QMC for the onset of antiferromagnetism

Electron occupation number $n_k$ as a function of the tuning parameter $r$

QMC for the onset of antiferromagnetism

\[ \chi_\varphi/(L^2 \beta) \]

AF susceptibility, \( \chi_\varphi \), and Binder cumulant as a function of the tuning parameter \( r \)

QMC for the onset of antiferromagnetism

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

Conclusions

Solved sign-problem for generic universal theory for the onset of antiferromagnetism in two-dimensional metals.
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Obtained (first ?) convincing evidence for the presence of unconventional superconductivity at strong coupling and near SDW quantum criticality.
Conclusions

Solved sign-problem for generic universal theory for the onset of antiferromagnetism in two-dimensional metals.

Obtained \textit{(first ?)} convincing evidence for the presence of unconventional superconductivity at strong coupling and near SDW quantum criticality.

Good prospects for studying competing charge orders, and non-Fermi liquid physics at non-zero temperature.