1. Antiferromagnetism and quantum criticality in insulators

2. Onset of antiferromagnetism in metals, and d-wave superconductivity

3. Competing density wave order, and the pseudogap of the cuprate superconductors

4. Non-Fermi liquids
1. Antiferromagnetism and quantum criticality in insulators

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4. Non-Fermi liquids
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 \( \alpha = \uparrow, \downarrow \)

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

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

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

Will study on the square lattice
Fermi surfaces in electron- and hole-doped cuprates

Effective Hamiltonian for quasiparticles:

\[ H_0 = - \sum_{i<j} t_{ij} c_{i\alpha}^\dagger c_{j\alpha} \equiv \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha} \]

with \( t_{ij} \) non-zero for first, second and third neighbor, leads to satisfactory agreement with experiments. The area of the occupied electron states, \( \mathcal{A}_e \), from Luttinger’s theory is

\[ \mathcal{A}_e = \begin{cases} 2\pi^2(1 - x) & \text{for hole-doping } x \\ 2\pi^2(1 + p) & \text{for electron-doping } p \end{cases} \]

The area of the occupied hole states, \( \mathcal{A}_h \), which form a closed Fermi surface and so appear in quantum oscillation experiments is \( \mathcal{A}_h = 4\pi^2 - \mathcal{A}_e \).
The electron spin polarization obeys

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

where \( \vec{K} \) is the ordering wavevector.
We use the operator equation (valid on each site $i$):

$$U \left( n_{\uparrow} - \frac{1}{2} \right) \left( n_{\downarrow} - \frac{1}{2} \right) = -\frac{2U}{3} S^x_i + \frac{U}{4}$$

Then we decouple the interaction via

$$\exp \left( \frac{2U}{3} \sum_i \int d\tau \vec{S}_i^2 \right) = \int \mathcal{D} \vec{J}_i(\tau) \exp \left( -\sum_i \int d\tau \left[ \frac{3}{8U} \vec{J}_i^2 - \vec{J}_i \vec{S}_i \right] \right)$$

We now integrate out the fermions, and look for the saddle point of the resulting effective action for $\vec{J}_i$. At the saddle-point we find that the lowest energy is achieved when the vector has opposite orientations on the A and B sublattices. Anticipating this, we look for a continuum limit in terms of a field $\vec{\varphi}_i$ where

$$\vec{J}_i = \vec{\varphi}_i e^{i\mathbf{K} \cdot \mathbf{r}_i}$$
Fermi surface+antiferromagnetism

In this manner, we obtain the “spin-fermion” model

\[ Z = \int Dc_\alpha D\varphi \exp (-S) \]

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

\[ - \lambda \int d\tau \sum_i c_i^\dagger \varphi_i \cdot \vec{\sigma} c_i e^{i\vec{K} \cdot \vec{r}_i} \]

\[ + \int d\tau d^2r \left[ \frac{1}{2} (\nabla_r \varphi)^2 + \frac{1}{2} (\partial_\tau \varphi)^2 + \frac{s}{2} \varphi^2 + \frac{u}{4} \varphi^4 \right] \]
Fermi surface + antiferromagnetism

In the Hamiltonian form (ignoring, for now, the time dependence of $\varphi$), the coupling between $\varphi$ and the electrons takes the form

$$H_{\text{sdw}} = \lambda \sum_{k,q,\alpha,\beta} \varphi_q \cdot c_{k+q,\alpha} \bar{\sigma}_{\alpha\beta} c_{k+K,\beta}$$

where $\bar{\sigma}$ are the Pauli matrices, the boson momentum $q$ is small, while the fermion momentum $k$ extends over the entire Brillouin zone. In the antiferromagnetically ordered state, we may take $\varphi \propto (0, 0, 1)$, and the electron dispersions obtained by diagonalizing $H_0 + H_{\text{sdw}}$ are

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

This leads to the Fermi surfaces shown in the following slides as a function of increasing $|\varphi|$. 
Metal with “large” Fermi surface
Fermi surfaces translated by $\mathbf{K} = (\pi, \pi)$. 
Fermi surface + antiferromagnetism

“Hot” spots
Fermi surface + antiferromagnetism

Electron and hole pockets in antiferromagnetic phase with $\langle \bar{\phi} \rangle \neq 0$
Increasing SDW order


Square lattice Hubbard model with hole doping
Square lattice Hubbard model with hole doping

Increasing SDW order


Square lattice Hubbard model with hole doping

Increasing SDW order

Hot spots

where $\varepsilon_k = \varepsilon_{k+K}$

Fermi surface breaks up at hot spots into electron and hole “pockets”

Fermi surface breaks up at hot spots into electron and hole “pockets”

Square lattice Hubbard model with hole doping
Square lattice Hubbard model with hole doping

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

and large

Metal with hole pockets

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

and small

Metal with electron and hole pockets

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

Metal with “large” Fermi surface

\( h \sim i = 0 \)
Square lattice Hubbard model with electron doping

\[ \langle \varphi \rangle \neq 0 \quad \text{and large} \]

\[ \langle \varphi \rangle \neq 0 \quad \text{and small} \]

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

Metal with electron pockets

Metal with electron and hole pockets

Metal with “large” Fermi surface
Square lattice Hubbard model with no doping

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

and large

Insulator

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

and small

Metal with electron and hole pockets

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

Metal with “large” Fermi surface
Fermi surfaces translated by $K = (\pi, \pi)$. 

**Fermi surface + antiferromagnetism**
“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 $\lambda$

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

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

“Hot spot”

“Cold” Fermi surfaces

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

Order parameter: \[ \mathcal{L}_\varphi = \frac{1}{2} (\nabla_r \varphi)^2 + \frac{1}{2} (\partial_\tau \varphi)^2 + \frac{s}{2} \varphi^2 + \frac{u}{4} \varphi^4 \]
\[ L_f = \psi_{1\alpha}^\dagger (\partial_\tau - i \mathbf{v}_1 \cdot \nabla_r) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\partial_\tau - i \mathbf{v}_2 \cdot \nabla_r) \psi_{2\alpha} \]

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

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

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

Fermion dispersions: \( \varepsilon_{k1} = \mathbf{v}_1 \cdot \mathbf{k} \) and \( \varepsilon_{k2} = \mathbf{v}_2 \cdot \mathbf{k} \)
\[ \mathcal{L}_f = \psi_{1\alpha}^\dagger (\partial_\tau - i \mathbf{v}_1 \cdot \nabla_{\mathbf{r}}) \psi_{1\alpha} + \psi_{2\alpha}^\dagger (\partial_\tau - i \mathbf{v}_2 \cdot \nabla_{\mathbf{r}}) \psi_{2\alpha} - \lambda \bar{\varphi} \cdot \left( \psi_{1\alpha}^\dagger \sigma_{\alpha\beta} \psi_{2\beta} + \psi_{2\alpha}^\dagger \sigma_{\alpha\beta} \psi_{1\beta} \right) \]

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 \( \langle \bar{\varphi} \rangle \neq 0 \)
Hertz action.

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

![Fermion Loop Diagram](attachment:fermion_loop_diagram.png)

$$\Pi(q, \omega_n) = \int \frac{d^d k}{(2\pi)^d} \int \frac{d\epsilon_n}{2\pi} \frac{1}{[-i(\epsilon_n + \omega_n) + v_1 \cdot (k + q)][-i\epsilon_n + v_2 \cdot k]}.$$

We define oblique co-ordinates $p_1 = v_1 \cdot k$ and $p_2 = v_2 \cdot k$. It is then clear that the integrand 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

$$
\Pi(q, \omega_n) = \frac{\Lambda^{d-2}}{|v_1 \times v_2|} \int \frac{dp_1 dp_2 d\epsilon_n}{8\pi^3} \frac{1}{[-i(\epsilon_n + \omega_n) + p_1][-i\epsilon_n + p_2]}.
$$

Next, we evaluate the frequency integral to obtain

$$
\Pi(q, \omega_n) = \frac{\Lambda^{d-2}}{\zeta |v_1 \times v_2|} \int \frac{dp_1 dp_2}{4\pi^2} \frac{[\text{sgn}(p_2) - \text{sgn}(p_1)]}{-i\zeta \omega_n + p_1 - p_2} = -\frac{|\omega_n| \Lambda^{d-2}}{4\pi |v_1 \times v_2|}.
$$

In the last step, we have dropped a frequency-independent, cutoff-dependent constant which can absorbed into a redefinition of $r$. 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.
$$
Exercise: Perform a tree-level RG rescaling on $S_H$. Now we rescale coordinates 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 $d \geq 2$. 
Spin-fluctuation exchange theory of d-wave superconductivity

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

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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.
Spin-fluctuation exchange theory of d-wave superconductivity

Increasing SDW order

\[ \Gamma \]
Spin-fluctuation exchange theory of d-wave superconductivity

Fermions at the large Fermi surface exchange fluctuations of the SDW order parameter $\vec{\phi}$.
Spin-fluctuation exchange theory of d-wave superconductivity

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

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

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

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

where the pairing interaction is

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

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 $p - k \approx K$. 
Unconventional pairing at \( \text{and near} \) hot spots
Pairing “glue” from antiferromagnetic fluctuations

The theory for the onset of antiferromagnetism in a metal flows to strong coupling in $d=2$. 
The theory for the onset of antiferromagnetism in a metal flows to strong coupling in $d=2$

- Pairing glue becomes stronger.
The theory for the onset of antiferromagnetism in a metal flows to strong coupling in $d=2$

- Pairing glue becomes stronger.
- There is stronger fermion-boson scattering, and fermionic quasi-particles lose their integrity.
The theory for the onset of antiferromagnetism in a metal flows to strong coupling in $d=2$

- Pairing glue becomes stronger. 😊
- There is stronger fermion-boson scattering, and fermionic quasi-particles lose their integrity. 😞
- Other instabilities can appear *e.g.* to density waves (next lecture). 😊
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 \textit{generic} universal low energy theory for the onset of antiferromagnetism.

Hot spots in a two band model

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

Hot spots in a two band model

QMC for the onset of antiferromagnetism

Requires only time-reversal symmetry. Particle-hole or point-group symmetries or commensurate densities not required!


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

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

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

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

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

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

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

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

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

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

\[
- \lambda \int d\tau \sum_i \bar{\varphi}_i \cdot (-1)^x_i c^\dagger_{i\alpha} \bar{\sigma}_{\alpha\beta} c^{}_{i\beta} + \text{H.c.}
\]

QMC for the onset of antiferromagnetism

No sign problem!

QMC for the onset of antiferromagnetism

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

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

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

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

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

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

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

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

$$
S = \int d\tau \sum_k c^{(x)}_{k\alpha} \left( \frac{\partial}{\partial \tau} - \varepsilon^{(x)}_k \right) c^{(x)}_{k\alpha} 
+ \int d\tau \sum_k c^{(y)}_{k\alpha} \left( \frac{\partial}{\partial \tau} - \varepsilon^{(y)}_k \right) c^{(y)}_{k\alpha} 
+ \int d\tau d^2x \left[ \frac{1}{2} (\nabla_x \bar{\varphi})^2 + \frac{r}{2} \bar{\varphi}^2 + \ldots \right] 
- \lambda \int d\tau \sum_i \bar{\varphi}_i \cdot (-1)^{x_i} c^{(x)}_{i\alpha} \bar{\sigma}_{\alpha\beta} c^{(y)}_{i\beta} + \text{H.c.}
$$

Can integrate out $\bar{\varphi}$ 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

QMC for the onset of antiferromagnetism


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

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 $r$

Quantum phase transition with onset of antiferromagnetism in a metal

Metal with electron and hole pockets

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

Metal with “large” Fermi surface

$\langle \bar{\phi} \rangle = 0$
Quantum phase transition with onset of antiferromagnetism in a metal

Metal with electron and hole pockets

$\langle \phi \rangle \neq 0$

Find new instabilities upon approaching critical point

Metal with "large" Fermi surface

$r$
Quantum phase transition with onset of antiferromagnetism in a metal

Metal with electron and hole pockets

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

Metal with “large” Fermi surface

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

d-wave superconductivity