Unconventional superconducting pairing: Theoretical mechanisms and spectroscopic probes

Andreas Kreisel

Niels Bohr Institute, University of Copenhagen





Outline

- Unconventional superconductivity
 - What is it?
 - Some material candidates
- Superconducting pairing: mean-field theory
- Spin fluctuation pairing mechanism
- (selected) spectroscopic probes
 - Quasiparticle tunneling
 - Neutron scattering: resonance
 - Spin relaxation rate: Hebel-Slichter peak

Introduction

- Superconductivity (main phenomenology)
 - Zero resistance
 - Persistent currents in rings
 - Perfect diamagnetism
 - Energy gap opens in the SC state

Superconductivity

• Instability of Fermi sea due to interactions



T>T_c: normal metal, filled Fermi sea



 $T < T_c$ gas of Cooper pairs: zero resistivity, Meissner effect, excitation gap

• Order parameter $\Delta_{\mathbf{k}} \sim \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$ generically complex-valued

Conventional superconductivity

Origin of pairing interaction: Phonons

Conventional



Retarted interaction: electrons avoid repulsive part of Coulomb interaction in time: Effective attractive interaction in energy shell around E_{r}

• Order parameter (local)



Unconventional superconductivity

Pairing interaction momentum dependent



Electrons avoid repulsive part of Coulomb interaction in space rather than time! (Kohn-Luttinger, 1965)

• Order parameter non-local (momentum-dependent)



Possible materials (1)

Cuprates



Electronic structure at low energy: single Cu-d orbital (hybridized with O-p orbitals) Michael R. Norman Physics **13**, 85 (2020)





Sketch of model often discussed to represent phenomenology



Single band model

Band structure/density of states



• Fermi surface



Possible materials (2)

Nickelates



Electronic structure at low energy: two Ni d orbitals







Multiband model?!



Possible materials (3)

Fe-based superconductors



Chi, et al., PRB 94, 134515 (2016) [LiFeAs]

1111, 111, 122, 1122...



-

 d_{xu}

Possible materials (4)

Kagome superconductors



Simplistic electronic structure: single orbital model: sublattice structure



3 band model Interactions: Onsite and nearest neighbor Coulomb interactions

Mean field theory

Generic Hamiltonian including interaction term

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}^{\prime}\uparrow} c_{\mathbf{k}\downarrow} + \frac{1}{2N} \sum_{\mathbf{k},\mathbf{k}^{\prime}} [V(\mathbf{k},\mathbf{k}^{\prime}) c^{\dagger}_{\mathbf{k}^{\prime}\uparrow} c^{\dagger}_{-\mathbf{k}^{\prime}\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + \mathrm{H.c.}]$$

- Mean field theory H = AB $H \to H_{MF} = \langle A \rangle B + A \langle B \rangle - \langle A \rangle \langle B \rangle$
- Here: superconducting channel

$$A = c^{\dagger}_{\mathbf{k}^{\prime}\uparrow}c^{\dagger}_{-\mathbf{k}^{\prime}\downarrow} \qquad B = c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}$$

$$H_{MF} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} V(\mathbf{k},\mathbf{k}') \Big[\langle c^{\dagger}_{\mathbf{k}'\uparrow} c^{\dagger}_{-\mathbf{k}'\downarrow} \rangle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c^{\dagger}_{\mathbf{k}'\uparrow} c^{\dagger}_{-\mathbf{k}'\downarrow} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle - \langle c^{\dagger}_{\mathbf{k}'\uparrow} c^{\dagger}_{-\mathbf{k}'\downarrow} \rangle \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle + \mathrm{H.c.} \Big].$$

BCS theory

• **Define**
$$\Delta_{\mathbf{k}}^{s/t} = -\frac{1}{N} \sum_{\mathbf{k}'} V^{s/t}(\mathbf{k}, \mathbf{k}') \langle c_{\mathbf{k}'\uparrow}^{\dagger} c_{-\mathbf{k}'\downarrow}^{\dagger} \rangle \qquad V^{s/t}(\mathbf{k}, \mathbf{k}') = \frac{1}{2} [V(\mathbf{k}, \mathbf{k}') \pm V(-\mathbf{k}, \mathbf{k}')]$$
$$H_{MF} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^{s/t*} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \mp \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^{s/t} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} + \text{const.}$$

Bogoliubov transformation to quasiparticle operators

$$\begin{pmatrix} \gamma_{\mathbf{k}\uparrow} \\ \gamma^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}}^{*} & -v_{\mathbf{k}} \\ v_{\mathbf{k}}^{*} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix}$$

• Want: diagonal Hamiltonian

$$H_{BCS} = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} \gamma_{\mathbf{k}\sigma}^{\dagger} \gamma_{\mathbf{k}\sigma} \qquad \qquad E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}^{s/t}|^2}.$$

Self-consistency condition

$$\Delta_{\mathbf{k}}^{s/t} = -\frac{1}{N} \sum_{\mathbf{k}'} V^{s/t}(\mathbf{k}, \mathbf{k}') \frac{\Delta_{\mathbf{k}'}^{s/t}}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}'}}{2}\right)$$

Unconventional superconductivity: Pairing from spin fluctuations

• Electrons avoid repulsive part of Coulomb interaction in space rather than time! (Kohn-Luttinger, 1965)



• channels $\Delta_{\mathbf{k}}^{s/t} = -\frac{1}{N} \sum_{\mathbf{k}'} V^{s/t}(\mathbf{k}, \mathbf{k}') \frac{\Delta_{\mathbf{k}'}^{s/t}}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}'}}{2}\right)$

Note: order parameter (matrix) needs to be antisymmetric in all quantum numbers (Pauli principle)

- singlet $\Delta^s_{\mathbf{k}} = \Delta^s_{-\mathbf{k}}$
- triplet $\Delta^t_{\mathbf{k}} = -\Delta^t_{-\mathbf{k}}$

Rømer, et al., PRB 92, 104505 (2015)



Pairing glue from spin fluctuations

• Spin susceptibility $\vec{S}(\mathbf{r},\tau) = \frac{1}{2}c^{\dagger}_{\mathbf{r},\alpha}(\tau)\vec{\sigma}_{\alpha\beta}c_{\mathbf{r},\beta}(\tau)$

$$\begin{split} \chi_{0}^{+-}(\mathbf{q},\tau) &= \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} \langle T_{\tau} S^{+}(\mathbf{q},\tau) S^{-}(-\mathbf{q},0) \rangle \\ &= \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} \langle T_{\tau} c_{\mathbf{k}+\mathbf{q},\uparrow}^{\dagger}(\tau) c_{\mathbf{k},\downarrow}(\tau) c_{\mathbf{k}'-\mathbf{q},\downarrow}^{\dagger}(0) c_{\mathbf{k}',\uparrow}(0) \rangle \end{split}$$

• Evaluate in band basis

$$\chi_0^{+-}(\mathbf{q}, i\nu_n) = -\frac{1}{\beta N} \sum_{\mathbf{k}, i\omega_m} G_0^{\uparrow}(\mathbf{k} + \mathbf{q}, i\omega_m + i\nu_n) G_0^{\downarrow}(\mathbf{k}, i\omega_m)$$
$$= -\frac{1}{N} \sum_{\mathbf{k}} \frac{n_F(\epsilon_{\mathbf{k}+\mathbf{q}}) - n_F(\epsilon_{\mathbf{k}})}{i\nu_n + \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}$$

Hubbard interaction

$$H_{\rm int} = U \sum c^{\dagger}_{\mathbf{r},\uparrow} c_{\mathbf{r},\uparrow} c^{\dagger}_{\mathbf{r},\downarrow} c_{\mathbf{r},\downarrow}$$

$$\chi_{\rm s}(\mathbf{k} - \mathbf{k}') = \frac{\chi_0 (\mathbf{k} - \mathbf{k})}{1 - U\chi_0^{zz}(\mathbf{k} - \mathbf{k}')}$$
$$\chi_{\rm c}(\mathbf{k} - \mathbf{k}') = \frac{\chi_0^{zz}(\mathbf{k} - \mathbf{k}')}{1 + U\chi_0^{zz}(\mathbf{k} - \mathbf{k}')}$$

• Longitudinal and transverse contributions $V(\mathbf{k}, \mathbf{k}') = U + V_{lo}^{RPA}(\mathbf{k} - \mathbf{k}') + V_{tr}^{RPA}(\mathbf{k} + \mathbf{k}')$ $V_{lo}^{RPA}(\mathbf{k} - \mathbf{k}') = \frac{U^{3}\chi_{0}^{zz}(\mathbf{k} - \mathbf{k}')^{2}}{1 - U^{2}\chi_{0}^{zz}(\mathbf{k} - \mathbf{k}')^{2}} \qquad V_{tr}^{RPA}(\mathbf{k} + \mathbf{k}') = \frac{U^{2}\chi_{0}^{+-}(\mathbf{k} + \mathbf{k}')}{1 - U\chi_{0}^{+-}(\mathbf{k} + \mathbf{k}')} \qquad \mathbf{k}^{+}$



22(1- 1r/)

Pairing from spin fluctuations

• Back to example

$$\Gamma^s(\mathbf{q}) \sim \frac{3}{2} (U + U^2 \chi(\mathbf{q})) \text{ spin surprise} \quad (\text{RPA}) = 0 \quad \text{ momental spin surprise} \quad (\text{RPA$$

Spin susceptibility RPA): peaked at nomentum q_o

$$H = \sum_{ij,\sigma} t_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow}$$

$$\Gamma^t(\mathbf{q}) \sim -\frac{U^2}{2}\chi(\mathbf{q}) = -\tilde{\Gamma}^s(\mathbf{q})/3$$

Superconducting gap function from linearized gap equation

$$\Delta_{\mathbf{k}}^{s/t} = -\frac{1}{N} \sum_{\mathbf{k}'} V^{s/t}(\mathbf{k}, \mathbf{k}') \frac{\Delta_{\mathbf{k}'}^{s/t}}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}'}}{2}\right)$$

Linearize: on r.h.s. $E_{\mathbf{k}} = \epsilon_{\mathbf{k}}$

 \rightarrow only contributions from FS

$$-\frac{1}{V_G} \int_{FS} dS' \ \Gamma(\mathbf{k} - \mathbf{k}') \frac{g_i(\mathbf{k}')}{|v_F(\mathbf{k}')|} = \lambda_i g_i(\mathbf{k}) - \operatorname{Eigenvalue} \text{ and gap symmetry function}$$

Rømer, et al., PRB **92**, 104505 (2015)

Connection to critical temperature (in principle)



Singlet pairing

- Spin susceptibility in single band models
 - Onsite interaction: RPA enhancement

$$\chi_0^{+-}(\mathbf{q}, i\nu_n) = -\frac{1}{N} \sum_{\mathbf{k}} \frac{n_F(\epsilon_{\mathbf{k}+\mathbf{q}}) - n_F(\epsilon_{\mathbf{k}})}{i\nu_n + \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}$$
$$\chi_s(\mathbf{k} - \mathbf{k}') = \frac{\chi_0^{zz}(\mathbf{k} - \mathbf{k}')}{1 - U\chi_0^{zz}(\mathbf{k} - \mathbf{k}')}$$

• Examples



Singlet pairing

- Ingredients:
 - Repulsive pairing interaction
 - Fermi surface geometry (nesting): solve for eigenvalues/eigenvectors to

$$\Gamma^{s}(\mathbf{q}) \sim \frac{3}{2} (U + U^{2} \chi(\mathbf{q}))$$
$$M_{\mathbf{k},\mathbf{k}'}^{s/t} = -\frac{1}{V_{G}} \frac{l_{\mathbf{k}'}}{|v_{F}(\mathbf{k}')|} V^{s/t}(\mathbf{k},\mathbf{k}')$$

Examples



Triplet pairing

A. Layzer and D. Fay, Int. J. Magn. **1**, 135 (1971)

- Pairing dominated by small q₀ interactions
 - susceptibility peaked at q=0 (close to ferromagnetic instability) $\Gamma^t(\mathbf{q}) \sim -\frac{U^2}{2}\chi(\mathbf{q}) = -\tilde{\Gamma}^s(\mathbf{q})/3$
- Odd parity state $\Delta_{\mathbf{k}}^t = -\Delta_{-\mathbf{k}}^t$



Triplet pairing: large momentum spin fluctuations

Square lattice Hubbard model close to quarter filling

 $\xi_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)]$

Susceptibility



• Pairing (from linearized gap equation)





Rømer, et al., Phys. Rev. Research **2**, 013108 (2020) Roig, et al., in preparation

Multiband generalization

- electronic structure $H_0 = \sum_{\mathbf{k}\sigma\ell\ell'} t_{\mathbf{k}}^{\ell\ell'} c_{\ell\sigma}^{\dagger}(\mathbf{k}) c_{\ell'\sigma}(\mathbf{k}) \qquad t_{\mathbf{k}}^{\ell\ell'} = \sum_{\delta} t_{\delta}^{\ell\ell'} \exp(i\mathbf{k}\cdot\delta)$
- Hubbard-Kanamouri interaction

$$H_{\text{int}} = U \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + U' \sum_{i,\ell'<\ell} n_{i\ell} n_{i\ell'} + J \sum_{i,\ell'<\ell} \sum_{\sigma,\sigma'} c^{\dagger}_{i\ell\sigma} c^{\dagger}_{i\ell'\sigma'} c_{i\ell\sigma'} c_{i\ell'\sigma} + J' \sum_{i,\ell'\neq\ell} c^{\dagger}_{i\ell\uparrow} c^{\dagger}_{i\ell\downarrow} c_{i\ell'\downarrow} c_{i\ell'\uparrow}$$

Generalized Lindhard function

$$\chi^{0}_{\ell_{1}\ell_{2}\ell_{3}\ell_{4}}(\mathbf{q},i\nu_{n}) = -\sum_{\mathbf{k},\mu,\nu} \frac{a^{\ell_{4}}_{\nu}(\mathbf{k})a^{\ell_{2},*}_{\nu}(\mathbf{k})a^{\ell_{1}}_{\mu}(\mathbf{k}+\mathbf{q})a^{\ell_{3},*}_{\mu}(\mathbf{k}+\mathbf{q})[n_{F}(\epsilon_{\mu,\mathbf{k}+\mathbf{q}}) - n_{F}(\epsilon_{\nu,\mathbf{k}})]}{i\nu_{n} + \epsilon_{\mu,\mathbf{k}+\mathbf{q}} - \epsilon_{\nu,\mathbf{k}}}$$

• Matrix equation for RPA

$$\chi^{\text{RPA}}_{s/c\,\ell_1\ell_2\ell_3\ell_4}(\mathbf{q},\omega) = \left\{\chi^0(\mathbf{q},\omega)\left[1\mp \bar{U}^{s/c}\chi^0(\mathbf{q},\omega)\right]^{-1}\right\}_{\ell_1\ell_2\ell_3\ell_4}$$

• Pairing interaction (orbital space)

$$\Gamma_{\ell_{1}\ell_{2}\ell_{3}\ell_{4}}(\mathbf{k},\mathbf{k}') = \frac{1}{2} \left[3\bar{U}^{s}\chi_{s}^{\text{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^{s} + \bar{U}^{s} - \bar{U}^{c}\chi_{c}^{\text{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^{c} + \bar{U}^{c} \right]_{\ell_{1}\ell_{2}\ell_{3}\ell_{4}}$$



 $-d_{x^2-y^2}$

- (bilayer) Nickelates
 - Bands, Fermi surface \rightarrow susceptibility, pairing





-0.5

 $\binom{0}{k_x/\pi}$

0.5

+ d_{z^2}

(d) Fe-based SC

 $+ d_{x^2 - y^2}$

+ d_{z^2}

dry.

- Fe-based materials: 111
 - Bands, Fermi surface \rightarrow susceptibility, pairing





(d) Fe-based SC

 $+ d_{x^2 - y^2}$

 $\uparrow \downarrow d_{z^2}$

drz.

- Fe-based materials: 122
 - Bands, Fermi surface \rightarrow susceptibility, pairing







- Sr₂RuO₄
 - Bands, Fermi surface \rightarrow susceptibility, pairing





(i) Sr₂RuO₄

 d_{xz}

Sublattice degree of freedom

Consider single band model in 1D



Susceptibility: Sublattice degree of freedom



(selected) spectroscopic probes

• Tunneling (density of states)



Tunnelling current:

$$I(V, x, y, z) = -\frac{4\pi e}{\hbar} \rho_t(0) |M|^2 \int_0^{e_V} \rho(x, y, z, \epsilon) d\epsilon$$

Local Density Of States (LDOS) of sample at given energy at the tip position

ARPES (spectral function)





Chi, et al. Nat. Commun (2017)

Z. X. Shen et al., PRL 70, 1553 (1993)



Density of states

• "electronic density of states"

 $\widehat{G}^{(0)}(\mathbf{k},\omega) = \left[(\omega + i\eta) \mathbb{1} - \widehat{H}_{\text{BdG}}(\mathbf{k}) \right]^{-1}$

$$\widehat{H}_{\rm BdG}(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & \Delta^{s/t}(\mathbf{k}) \\ \Delta(\mathbf{k})^{s/t \dagger} & -h(-\mathbf{k})^T \end{pmatrix}$$

 $\rho(\omega) = -\frac{1}{\pi} \operatorname{Tr} \operatorname{Im} G_{11}^{(0)}(\mathbf{k}, \omega) = -\frac{1}{2\pi} \operatorname{Tr} \operatorname{Im} \left[G_{11}^{(0)}(\mathbf{k}, \omega) + G_{\bar{1}\bar{1}}^{(0)}(\mathbf{k}, -\omega) \right]$

• Sensitive to saddle points and nodal behavior, but not to the sign of the order parameter



Disorder in superconductors

- Conventional superconductor $\Delta(\mathbf{k}) = \Delta_0$
 - Nonmagnetic impurity \rightarrow no bound states
 - Magnetic impurity \rightarrow Yu-Shiba-Rusinov bound states
- Unconventional superconductor, sign change: $\Delta({\bf k})=-\Delta(\tilde{{\bf k}})$
 - Nonmagnetic impurity \rightarrow in-gap bound states



Iron-based SC: s_{+-} order parameter

0 (¥)



S. Chi, *et al.* Phys. Rev. B **94**, 134515 (2016)

A. V. Balatsky, I. Vekhter, and Jian-Xin Zhu Rev. Mod. Phys. **78**, 373 (2006)

Disorder in superconductors

- Non-magnetic impurity $\widehat{H}_{imp} = S_z \tau^0 \otimes M$
- **T-matrix approximation** $\widehat{G}(\mathbf{r}, \mathbf{r}', \omega) = \widehat{G}^{(0)}(\mathbf{r} - \mathbf{r}', \omega) + \widehat{G}^{(0)}(\mathbf{r}, \omega)\widehat{T}(\omega)\widehat{G}^{(0)}(-\mathbf{r}', \omega)$ $\widehat{T}(\omega) \equiv \left[\mathbb{1} - \widehat{H}_{imp}\widehat{G}^{(0)}(\mathbf{0}, \omega)\right]^{-1}(\omega)\widehat{H}_{imp}$
- Local density of states* $\rho_{\alpha}(\mathbf{r},\omega) = -\frac{1}{\pi} \operatorname{Im} \left[G_{\alpha\alpha}(\mathbf{r},\mathbf{r},\omega) + G_{\bar{\alpha}\bar{\alpha}}(\mathbf{r},\mathbf{r},-\omega) \right]$







Resonances: if Re(HG)=1, Im(G)~0

 $G^{(0)}_{1\bar{1}}(\omega) \; = \; 0$

*here only lattice DOS is discussed, for STM tunneling "continuum" LDOS important S. Chi, et al. Phys. Rev. B 94, 134515 (2016)

(selected) spectroscopic probes

- Neutron scattering (spin susceptibility)
 - Enhancement of scattering below 2Δ in the SC state

C. Stock, et al., Phys. Rev. Lett. 100, 087001 (2008)

- Nuclear spin resonance (NMR)
 - Screening from external field due to SC (Knight shift)
 - Low energy spin fluctuations (relaxation rate)



T (K)



Spin susceptibility in the superconducting state

Convolution of normal and anomalous GF

$$\chi_0^{+-}(\mathbf{q},\tau) = -\frac{1}{N} \sum_{\mathbf{k}} \left(G_{11}^0(\mathbf{k}+\mathbf{q},-\tau) G_{\bar{1}\bar{1}}^0(\mathbf{k},\tau) + G_{\bar{1}1}^0(\mathbf{k}+\mathbf{q},-\tau) G_{1\bar{1}}^0(\mathbf{k},\tau) \right)$$

 Contribution of magnitude and sign of order parameter

$$\begin{split} \chi_{0}^{+-}(\mathbf{q},\omega) &= \frac{1}{\mathcal{N}} \sum_{\mathbf{k},E>0} \left[\left(1 - \frac{\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{1 - f(E_{\mathbf{k}}) - f(E_{\mathbf{k}+\mathbf{q}})}{\omega + E_{\mathbf{k}+\mathbf{q}} + E_{\mathbf{k}} + i\eta} \right) \\ &+ \left(1 - \frac{\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) + f(E_{\mathbf{k}+\mathbf{q}}) - 1}{\omega - E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} \\ &+ \left(1 + \frac{\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}+\mathbf{q}})}{\omega - E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} \\ &+ \left(1 + \frac{\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}+\mathbf{q}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} \\ &+ \left(1 + \frac{\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}+\mathbf{q}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{q}} + i\eta} \\ \end{bmatrix} \end{split}$$

• UNIVERSITY OF COPENHAGEN

Hebel-Slichter peak

Single band square lattice model

$$\mathcal{H}_0 = \sum_{\mathbf{k}\sigma} \left[-2t \left(\cos k_x + \cos k_y \right) - \mu \right] c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

• Spin relaxation rate $\alpha \equiv \frac{1}{T_1T} \propto \lim_{\omega \to 0} \frac{1}{N} \sum_{\mathbf{q}} \operatorname{Im} \frac{\chi_0^{+-}(\mathbf{q},\omega)}{\omega}$

$$\begin{split} \chi_{0}^{+-}(\mathbf{q},\omega) &= \frac{1}{\mathcal{N}} \sum_{\mathbf{k},E>0} \left[\left(1 - \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{1 - f(E_{\mathbf{k}}) - f(E_{\mathbf{k}+\mathbf{q}})}{\omega + E_{\mathbf{k}+\mathbf{q}} + E_{\mathbf{k}} + i\eta} + \left(1 - \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) + f(E_{\mathbf{k}+\mathbf{q}}) - 1}{\omega - E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} \\ &+ \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}+\mathbf{q}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}+\mathbf{q}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}+\mathbf{q}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}+\mathbf{q}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}+\mathbf{q}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}+\mathbf{q}} + i\eta} \end{bmatrix}, \end{split}$$

• Relevant quantity

$$\left(1 + \frac{\Delta_{\mathbf{k}+\mathbf{q}}\Delta_{\mathbf{k}}}{|\Delta_{\mathbf{k}}||\Delta_{\mathbf{k}+\mathbf{q}}|}\right) \approx \begin{cases} 2 & \text{same sign} \\ 0 & \text{different sign} \end{cases}$$

$$B(\mathbf{q}, \mathbf{k}_n) = \frac{\Delta^*_{\mathbf{k}_n + \mathbf{q}} \Delta_{\mathbf{k}_n}}{E_{\mathbf{k}_n} E_{\mathbf{k}_n + \mathbf{q}}}$$

Hebel-Slichter peak

• Relevant quantity $B(\mathbf{q}, \mathbf{k}_n) = \frac{\Delta_{\mathbf{k}_n + \mathbf{q}}^* \Delta_{\mathbf{k}_n}}{E_{\mathbf{k}_n} E_{\mathbf{k}_n + \mathbf{q}}}$

Fixed kn

 $\left(1 + \frac{\Delta_{\mathbf{k}+\mathbf{q}}\Delta_{\mathbf{k}}}{|\Delta_{\mathbf{k}}||\Delta_{\mathbf{k}+\mathbf{q}}|}\right) \approx \begin{cases} 2 & \text{same sign} \\ 0 & \text{different sign} \end{cases}$

Summary (1)

- A number of material candidates for unconventional superconductivity
- Momentum dependent interaction allows for momentum dependent order parameter and different symmetries

$$\Delta_{\mathbf{k}} \sim \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$$

- Experimental probes sensitive to the sign of the order parameter are rare
 - Impurity resonances in LDOS
 - Neutron resonance
 - Hebel-Slichter peak in NMR relaxation rate

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}^{s/t}|^2}.$$

Frontiers in materials: Kagome superconductors

2.76Å

Hexagonal system

• Electronic structure dominated by V states

KV₃Sb₅

B. Ortiz *et al.*, Phys. Rev. Lett **125**, 247002 (2020) (b)

3.16Å

Kagome superconductors

• CDW at high temperature

superconductivity at ~3K

B. Ortiz *et al.*, Phys. Rev. Lett **125**, 247002 (2020)

>2500

3.5

Kagome systems

to

• Basics: electronic structure

$$\mathcal{H}_0 = \sum_{\mathbf{k},\sigma} \psi_{\mathbf{k}\sigma}^{\dagger} H_0(\mathbf{k}) \psi_{\mathbf{k}\sigma} \qquad \psi_{\mathbf{k}\sigma} = \begin{pmatrix} c_{\mathbf{k}\sigma A} & c_{\mathbf{k}\sigma B} & c_{\mathbf{k}\sigma C} \end{pmatrix}^T$$

Band structure and susceptibility

• Strategy: use periodic Hamiltonian to calculate

$$\tilde{H}_{0}(\mathbf{k}) = -\begin{pmatrix} \mu & t(1+e^{2ik_{3}}) & t(1+e^{-2ik_{1}}) \\ t(1+e^{-2ik_{3}}) & \mu & t(1+e^{-2ik_{2}}) \\ t(1+e^{2ik_{1}}) & t(1+e^{2ik_{2}}) & \mu \end{pmatrix}$$

$$\begin{pmatrix} e^{-ik_{1}} & 0 & 0 \end{pmatrix}$$

$$T(\mathbf{k}) = \begin{pmatrix} e^{-ik_1} & 0 & 0\\ 0 & e^{-ik_2} & 0\\ 0 & 0 & 1 \end{pmatrix}$$

Then, unitary transformation to express in other basis

$$\chi_{0,\alpha\beta}^{+-}(\mathbf{q},\omega) = \begin{pmatrix} \tilde{\chi}_{0,AA}^{+-} & e^{i(q_2-q_1)}\tilde{\chi}_{0,AB}^{+-} & e^{-iq_1}\tilde{\chi}_{0,AC}^{+-} \\ e^{i(q_1-q_2)}\tilde{\chi}_{0,BA}^{+-} & \tilde{\chi}_{0,BB}^{+-} & e^{-iq_2}\tilde{\chi}_{0,BC}^{+-} \\ e^{iq_1}\tilde{\chi}_{0,CA}^{+-} & e^{iq_2}\tilde{\chi}_{0,CB}^{+-} & \tilde{\chi}_{0,CC}^{+-} \end{pmatrix}$$

Spin-fluctuation pairing

- Band structure+onsite/NN interactions

Morten Holm Christenser

Astrid

Tranum

Rømer

• What are the leading superconducting instabilities? Main ingredients:

$$-\frac{\sqrt{3}}{2(2\pi)^2}\oint_{\mathrm{FS}} d\mathbf{k}'_f \frac{1}{|v(\mathbf{k}'_f)|} \Gamma_{s/t}(\mathbf{k}_f, \mathbf{k}'_f) \Delta(\mathbf{k}'_f) = \lambda \Delta(\mathbf{k}_f)$$

$$\Gamma_{s/t}(n_1\mathbf{k}, n_2\mathbf{k}') = \sum_{\{s\}} [\mathcal{V}(n_1\mathbf{k}, n_2\mathbf{k}')]_{\overline{s}\,\overline{s}\,\overline{s}}^{s\,\overline{s}} \mp [\mathcal{V}(n_1\mathbf{k}, n_2\mathbf{k}')]_{\overline{s}\,\overline{s}\,\overline{s}}^{s\,\overline{s}}$$

Spin and charge susceptibilities: dominated by v. Hove singularities and sublattice interference

Perfect nesting, but sublattice mismatch

Phase diagram

- Which state is realized?
- Experimental verifications?
 - TRSB in SC state (two component order parameter?)
 - Sign change from disorder effects?

k-dependence Lowest order lattice harmonics Irrep Singlet A_1 $k_y(3k_x^2 - k_y^2) \times$ Singlet $k_x(k_x^2 - 3k_y^2)$ $k_x(k_x^2 - 3k_y^2)$ Triplet B_1 $k_y(3k_x^2 - k_y^2)$ B_2 Triplet $\binom{k_x}{k_y}$ Triplet E_1 $\binom{k_x^2 - k_y^2}{2k_x k_y}$ Singlet E_2

Hanbin Deng, et al., arXiv:2408.02898 (2024)

Kagome materials: Conventional or unconventional?

• T_c suppression due to disorder?

Zhang, et al., Nano Lett. 23, 872 (2023)

• Bound states at nonmagnetic impurities?

Are kagome superconductors conventional?

Xu, et al, PRL **127**, 187004 (2021)

The case of the Kagome SC

- Open question: How does disorder affect SC in the Kagome system?
- Answer depends on
 - Nature of the defects ("symmetry")
 - Superconducting phase

No subgap states if
$$\left\{\hat{h}_0^{\rm BdG} + \hat{h}_{\rm imp}^{\rm BdG}, \hat{h}_\Delta^{\rm BdG}\right\} = 0$$

Generalized Anderson's theorem: M. Scheurer PhD thesis (2016)

$$H_{\rm imp} = V\tau^{z} \otimes \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

A bit of theory details

T-matrix approach

$$\begin{split} \widehat{G}(\mathbf{r}, \mathbf{r}', \omega) &= \widehat{G}^{(0)}(\mathbf{r} - \mathbf{r}', \omega) + \widehat{G}^{(0)}(\mathbf{r}, \omega)\widehat{T}(\omega)\widehat{G}^{(0)}(-\mathbf{r}', \omega) \\ \widehat{T}(\omega) &\equiv \widehat{D}^{-1}(\omega)\widehat{H}_{imp} \end{split}$$

 $\widehat{D}(\omega) \equiv [\mathbb{1} - \widehat{H}_{imp}\widehat{G}^{(0)}(\mathbf{0}, \omega)].$

Multiband electronic structure

$$\widehat{H}_{BdG}(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) - \mu \mathbb{1} & -\Delta(\mathbf{k}) \\ -\Delta(\mathbf{k})^{\dagger} & -h(-\mathbf{k})^{T} + \mu \mathbb{1} \end{pmatrix}$$

Local anomalous Green function

$$\widehat{G}^{(0)}(\mathbf{k},\omega) = [(\omega + i\eta)\mathbb{1} - \widehat{H}_{\text{BdG}}(\mathbf{k})]^{-1}$$

$$\mathbf{d}_{xy} + i \mathbf{d}_{x^2 - y^2}$$

Results: d+id

• Denominator of T-matrix $det[\widehat{D}(\omega)] = 0$

 $V^{2} \Big[G^{(0)}_{AA}(\omega) G^{(0)}_{\bar{A}\bar{A}}(\omega) - G^{(0)}_{A\bar{A}}(\omega) G^{(0)}_{\bar{A}A}(\omega) \Big] + V \Big[G^{(0)}_{AA}(\omega) - G^{(0)}_{\bar{A}\bar{A}}(\omega) \Big] - 1 = 0,$

- Important quantity: $G_{A\bar{A}}^{(0)}(\omega) \neq 0$
- Absence of in-gap bound states!

What about T_{c} suppression?

Calculate T_c within Abrikosov-Gorkov theory

NMR spin relaxation rate?

Are kagome superconductors unconventional?

• What can we learn?

2) sign change in from Hebel Slichter peak

Hebel-Slichter peak

• Multiband system: sublattice interference

$$\chi_{0}^{+-}(\mathbf{q},\omega) = \frac{1}{\mathcal{N}} \sum_{\mathbf{k},E>0} \left[\left(1 - \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{1 - f(E_{\mathbf{k}}) - f(E_{\mathbf{k}+\mathbf{q}})}{\omega + E_{\mathbf{k}+\mathbf{q}} + E_{\mathbf{k}} + i\eta} + \left(1 - \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) + f(E_{\mathbf{k}+\mathbf{q}}) - 1}{\omega - E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}+\mathbf{q}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}}} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \left(1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{q}} + \Delta_{\mathbf{k}+\mathbf{q}}^{*}\Delta_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{q}} + i\eta} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} \right) \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \frac{f(E_{\mathbf{k}}) - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \frac{f(E_{\mathbf{k})} - f(E_{\mathbf{k}})}{\omega + E_{\mathbf{k}+\mathbf{q}} - E_{\mathbf{k}} + i\eta} + \frac{f(E$$

Relevant quantity

Unconventional superconductivity DOES exhibit Hebel-Slichter peak

 $|u_{\rm C}(\mathbf{k})|^2$

 $|u_{\rm B}(\mathbf{k})|^2$

 $|u_{\rm A}(\mathbf{k})|^2$

Summary (2)

- Unconventional pairing from spin fluctuations: Interplay of Fermi surface and structure of susceptibility
 - Fe-based superconductors: multiband, dominating s+- state
 - Kagome superconductors: rich phase diagram
- Unconventional Kagome
 superconductors: two surprises
 - Robust against disorder
 - Features Hebel-Slichter peak

A. Kreisel, et al. Phys. Rev. Lett. **129**, 077002 (2022)

A. T. Rømer *et al.*, Phys. Rev. B **106**, 174514 (2022)

S. C. Holbæk, et al., Phys. Rev. B **108**, 144508 (2023)

Yi Dai, et al., arXiv:2404.10835 (2024)