Topological Superconductivity

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Materials Theory

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Introduction to Superconductivity

What is it?

How do we describe it?

Contents

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- Introduction to superconductivity
  - BCS theory
  - BdG formulation
- Unconventional superconductivity
- Topological matter
- Topological superconductivity
  - Chiral superconductors
  - “Spinless” superconductors – Majorana fermions

What is Superconductivity?

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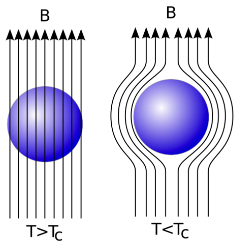
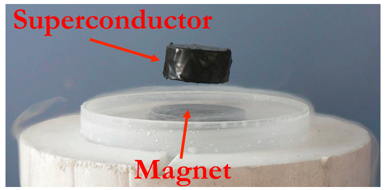
- What is superconductivity?
  - Electric transport without resistance

  - Meissner effect





History of Superconductivity

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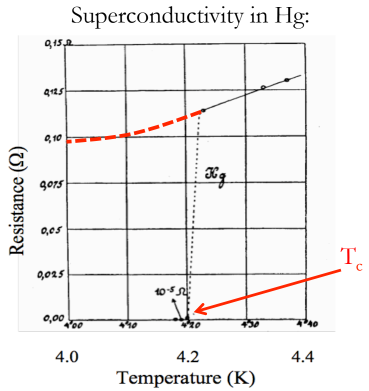
Heike Kammerlingh Onnes



Nobel Prizes

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Year	Subject	Laureates
1972	Superconductivity (BCS-Theory)	J. Bardeen L. N. Cooper J. R. Schrieffer
1973	Josephson Effects + Tunneling Phenomena	B. D. Josephson L. Esaki I. Giaever
1987	High Temperature Superconductors	J. G. Bednorz K. A. Mueller
1996	Superfluidity in ^{3}He	D. M. Lee D. D. Osheroff R. C. Richardson
2003	Contributions to Superconductivity	A. A. Abrikosov V. L. Ginzburg A. J. Legget
2008	Spontaneous Symmetry Breaking	Y. Nambu

Superconductors

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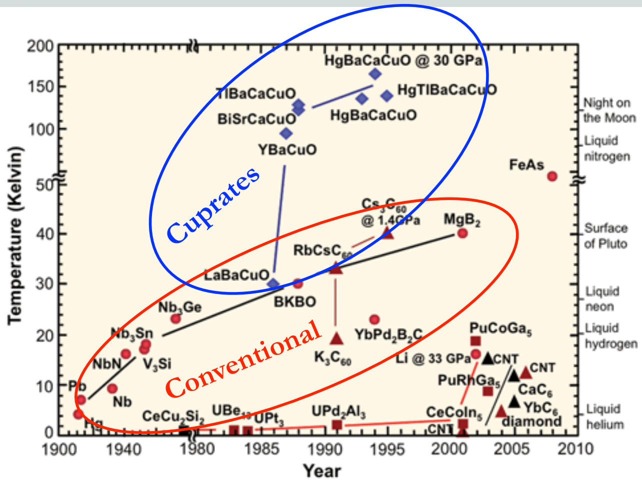

Department of Energy

How?

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- But how do the electrons move without resistance?
  - The electrons are all in a coherent quantum state with a fixed phase (condensate)

$$\Psi = \Delta_0 e^{i\varphi}$$

  - One of the few macroscopic manifestations of QM
  - Spontaneous gauge symmetry breaking – Higgs mechanism (discovered by P. W. Anderson before Higgs et al.)

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Higgs Mechanism

- In the Standard Model:
  - Interactions with the Higgs field (Higgs bosons) give masses to the $W^{+,-}$ and Z bosons due to electroweak (gauge) symmetry breaking
- In superconductors:
  - The superconducting pairs give mass to the electromagnetic field (photons) due to spontaneous symmetry breaking of the gauge symmetry (fixed phase on Ψ)
  - Explored by P.W. Anderson for superconductivity 2 years before Higgs et al.

Meissner effect = The “Higgs mass” of the electromagnetic field expels it from the superconductor

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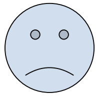
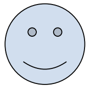
Statistics

- Fermions (half-integer spin):
  - Electrons, quarks, neutrinos
  - Only one electron per quantum state



- Bosons (integer spin):
  - Photons, gauge, and Higgs boson
  - As many particles as you wish in one quantum state (Bose-Einstein condensate, BEC)



Maybe two electrons can form an electron pair!?

Sort of, but not the whole story….

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But Wait!

- All electrons in one state: a superconducting condensate
  - Pauli exclusion principle??

How do electrons end up in the same state?

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Electron Pairing

- Electrons are negatively charged, how can they possibly pair?
  - In fact, they can pair pretty easily (at least at very, very low temperatures)
- The only instability of a Fermi Liquid is to attractive interactions
  - Any attractive interaction destroys the Fermi Liquid and creates electron pairs: Cooper pairs

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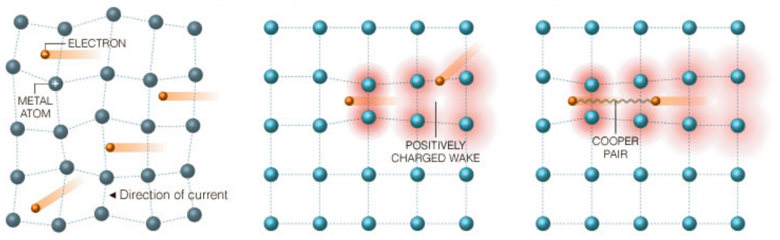
Attractive Interaction

- Where is attractive interaction coming from?



Normal state — At T_c — In the superconducting state

Electron-lattice vibration (phonon) interactions gives an effective attractive potential between two electrons

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BCS Theory

- How do the Cooper pairs condense (superconduct)?
- Bardeen-Cooper-Schrieffer (BCS) theory:
  – Condensation of Cooper pairs (with a fermionic wave function)
  – Truly many-body state (not a two-body bound state condensing)

(Higher temperatures than BECs)

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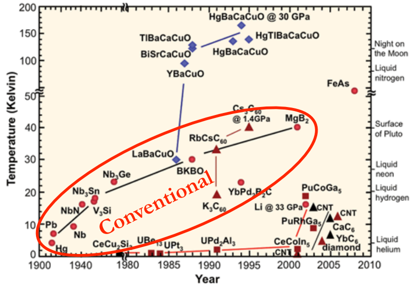
Conventional Superconductors

- Superconductivity from electron-phonon interactions
  – Superconductivity in "normal" metals
  – Low temperatures, $T_c < 40$ K



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Cooper Pairs

Pair of electrons above the Fermi surface (FS) with no net momentum:

$$|\Psi\rangle = \Lambda^\dagger |FS\rangle$$

$$\Lambda^\dagger = \int d^3x d^3x' \phi(\mathbf{x}-\mathbf{x}') \psi^\dagger_\downarrow(\mathbf{x}) \psi^\dagger_\uparrow(\mathbf{x}') \qquad |FS\rangle = \prod_{k<k_F} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} |0\rangle$$

Fourier transform ($\psi^\dagger_\sigma(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_\mathbf{k} c^\dagger_{\mathbf{k}\sigma} e^{-i\mathbf{k}\cdot\mathbf{x}}$):

$$\Lambda^\dagger = \sum_\mathbf{k} \phi_\mathbf{k} c^\dagger_{\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\uparrow}$$

spatial property of the Cooper pair

attractive

For $H = \sum_\mathbf{k} \epsilon_\mathbf{k} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \hat{V}$ the energy of a Cooper pair is < 0

→ FS is unstable to Cooper pair formation for any V<0

(see e.g. Tinkham: Introduction to superconductivity)

BCS Wave Function

Coherent state of Cooper pairs (ansatz):

$$|\psi_{BCS}\rangle = \prod_{\mathbf{k}} \exp[\phi_{\mathbf{k}} c^{\dagger}{}_{\mathbf{k}\uparrow} c^{\dagger}{}_{-\mathbf{k}\downarrow}]|0\rangle = \prod_{\mathbf{k}} (1 + \phi_{\mathbf{k}} c^{\dagger}{}_{\mathbf{k}\uparrow} c^{\dagger}{}_{-\mathbf{k}\downarrow})|0\rangle$$

$$= \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^{\dagger}{}_{-\mathbf{k}\downarrow} c^{\dagger}{}_{\mathbf{k}\uparrow} \right)|0\rangle$$

with $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$

- Ill-defined number of particles:

$$\Delta\varphi \Delta N \gtrsim 1$$

phase of order parameter: fixed (but same energy for all phases)

- Breaks gauge invariance: $c^{\dagger}{}_{\mathbf{k}\sigma} \to e^{i\alpha} c^{\dagger}{}_{\mathbf{k}\sigma}$

BCS Hamiltonian

Pairing Hamiltonian:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^{\dagger}{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}{}_{\mathbf{k}\uparrow} c^{\dagger}{}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}$$

kinetic (band) energy

$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -g_0/V, & (|\epsilon_{\mathbf{k}}| < \omega_D) \\ 0 & \text{(otherwise)} \end{cases}$$

We can determine u_k, v_k in ψ_{BCS} by minimizing $<\psi_{BCS}|H\text{-}\mu N|\psi_{BCS}>$ but it is a bit clumsy (see e.g. Tinkham: Introduction to superconductivity)

Instead we use mean-field theory with the order parameter

$$F_{\mathbf{k}} = \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$$

pair amplitude at **k** (off-diagonal long-range order)

Mean-Field Treatment

$$\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} [(c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} - F^{\dagger}_{\mathbf{k}}) + F^{\dagger}_{\mathbf{k}}][(c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} - F_{\mathbf{k}'}) + F_{\mathbf{k}'} \approx$$

$$\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} (F_{\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} + F^{\dagger}_{\mathbf{k}} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} - F^{\dagger}_{\mathbf{k}} F_{\mathbf{k}'}]$$

ignore fluctuations (mean-field approximation) $(c^{\dagger}c^{\dagger} - F^{\dagger})(cc - F)$

Set the order parameter $\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} F_{\mathbf{k}'} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle$

$$\rightarrow \quad H_{MFT} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \left[\bar{\Delta} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c^{\dagger}{}_{\mathbf{k}\uparrow} c^{\dagger}{}_{-\mathbf{k}\downarrow} \Delta\right] + \frac{V}{g_0} \bar{\Delta}\Delta$$

Matrix Formulation (BdG)

Define the Nambu spinor $\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}{}_{-\mathbf{k}\downarrow} \end{pmatrix}$ $\quad \psi^{\dagger}{}_{\mathbf{k}} = \left(c^{\dagger}{}_{\mathbf{k}\uparrow},\ c_{-\mathbf{k}\downarrow}\right)$

$$\rightarrow \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (c^{\dagger}{}_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} - c_{-\mathbf{k}\downarrow} c^{\dagger}{}_{-\mathbf{k}\downarrow} + 1) = \left(c^{\dagger}{}_{\mathbf{k}\uparrow},\ c_{-\mathbf{k}\downarrow}\right) \begin{bmatrix} \epsilon_{\mathbf{k}} & 0 \\ 0 & -\epsilon_{\mathbf{k}} \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}{}_{-\mathbf{k}\downarrow} \end{pmatrix} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}$$

TRS: $\varepsilon_{\mathbf{k}} = \varepsilon_{-\mathbf{k}}$ constant

$$\rightarrow \epsilon_{\mathbf{k}} \sum_{\sigma} c^{\dagger}{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \left[\bar{\Delta} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c^{\dagger}{}_{\mathbf{k}\uparrow} c^{\dagger}{}_{-\mathbf{k}\downarrow} \Delta\right] = \left(c^{\dagger}{}_{\mathbf{k}\uparrow},\ c_{-\mathbf{k}\downarrow}\right) \begin{bmatrix} \epsilon_{\mathbf{k}} & \Delta \\ \bar{\Delta} & -\epsilon_{\mathbf{k}} \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}{}_{-\mathbf{k}\downarrow} \end{pmatrix}$$

$$= \psi^{\dagger}{}_{\mathbf{k}} \begin{bmatrix} \epsilon_{\mathbf{k}} & \Delta_1 - i\Delta_2 \\ \Delta_1 + i\Delta_2 & -\epsilon_{\mathbf{k}} \end{bmatrix} \psi_{\mathbf{k}}$$

$$= \psi^{\dagger}{}_{\mathbf{k}} [\epsilon_{\mathbf{k}} \tau_3 + \Delta_1 \tau_1 + \Delta_2 \tau_2] \psi_{\mathbf{k}},$$

Bogliubov-de Gennes (BdG) formulation:
2x2 matrix problem
→ Solve by finding eigenvalues and vectors

$$\vec{\tau} = (\tau_1, \tau_2, \tau_3) = \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right)$$

$$\rightarrow H = \sum_{\mathbf{k}} \psi^{\dagger}{}_{\mathbf{k}} (\vec{h}_{\mathbf{k}} \cdot \vec{\tau}) \psi_{\mathbf{k}} + V \frac{\bar{\Delta}\Delta}{g_0} \qquad (\ \vec{h}_{\mathbf{k}} = (\Delta_1, \Delta_2, \epsilon_{\mathbf{k}})\ )$$

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Eigenstates = Quasiparticles

QP energy (eigenvalue): $E_{\mathbf{k}} = \pm\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$

QP operators (eigenvector):

$$\begin{cases} a^\dagger{}_{\mathbf{k}\uparrow} = \psi^\dagger{}_{\mathbf{k}} \cdot \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = c^\dagger{}_{\mathbf{k}\uparrow} u_{\mathbf{k}} + c_{-\mathbf{k}\downarrow} v_{\mathbf{k}} \\ a_{-\mathbf{k}\downarrow} = \psi^\dagger{}_{\mathbf{k}} \cdot \begin{pmatrix} -v_{\mathbf{k}}^* \\ u_{\mathbf{k}}^* \end{pmatrix} = c_{-\mathbf{k}\downarrow} u_{\mathbf{k}}^* - c^\dagger{}_{\mathbf{k}\uparrow} v_{\mathbf{k}}^* \end{cases}$$

Bogoliubov tranformation

$$u_{\mathbf{k}} = \sqrt{\frac{1}{2}\left[1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right]} \qquad v_{\mathbf{k}} = \sqrt{\frac{1}{2}\left[1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right]}$$

(Same coefficients as in the BCS wave fcn)

Diagonal Hamiltonian: $H = \sum_{\mathbf{k}} E_{\mathbf{k}}(a^\dagger{}_{\mathbf{k}\uparrow} a_{\mathbf{k}\uparrow} - a_{-\mathbf{k}\downarrow} a^\dagger{}_{-\mathbf{k}\downarrow}) + V\frac{\bar{\Delta}\Delta}{g_0}$

$$H = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}}(a^\dagger{}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} - \frac{1}{2}) + V\frac{\bar{\Delta}\Delta}{g_0}$$

QP excitations — Condensation energy

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Quasiparticle Properties II

- Excitation $a^\dagger{}_{\mathbf{k}\uparrow} = \psi^\dagger{}_{\mathbf{k}} \cdot \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = c^\dagger{}_{\mathbf{k}\uparrow} u_{\mathbf{k}} + c_{-\mathbf{k}\downarrow} v_{\mathbf{k}}$

  creates electron with momentum k and spin up,

  destroys electron with momentum –k and spin down
- At E = 0: $|u_{\mathbf{k}}|^2 = |v_{\mathbf{k}}|^2 = \frac{1}{2}$ → QP is equal parts electron and hole

  → Can become its own antiparticle (Majorana fermion)

- $a_{\mathbf{k}\uparrow}|\psi_{BCS}\rangle = 0$ annihilates ground state

  $a^\dagger_{-\mathbf{k}\downarrow}|\psi_{BCS}\rangle = c^\dagger_{-\mathbf{k}\downarrow} \prod_{\mathbf{k}'\neq\mathbf{k}} (u_{\mathbf{k}'} + v_{\mathbf{k}'} c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow})|0\rangle$ puts 1 electron in state **–k,↓** and prevents a Cooper pair at momentum **k**

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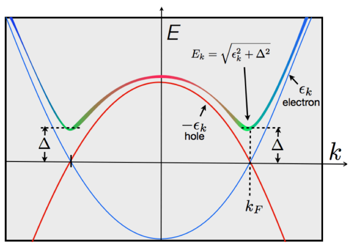
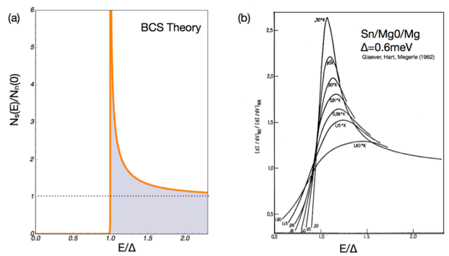
Quasiparticle Properties

- Excitations out of the condensate, always positive energy



Band structure



Density of states (DOS)

P. Coleman: Introduction to Many Body Physics

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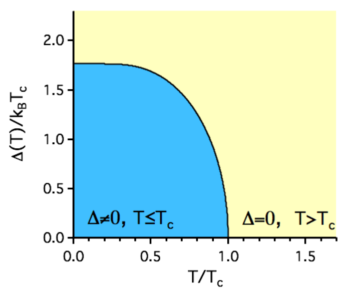
Self-Consistent Equation

Having found the diagonal Hamiltonian we can determine the superconducting order parameter self-consistently:

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}\rangle = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'}^* \langle a^\dagger_{\mathbf{k}'\uparrow} a_{\mathbf{k}'\uparrow} + a^\dagger_{-\mathbf{k}'\downarrow} a_{\mathbf{k}'\downarrow} - 1\rangle$$

$$\langle a^\dagger_{\mathbf{k}'\sigma} a_{\mathbf{k}'\sigma}\rangle = (1 + e^{E_{\mathbf{k}'}/k_B T})^{-1}$$ Fermi-Dirac distribution



$$\Delta_{\mathbf{k}} = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} \tanh[E_{\mathbf{k}'}/(2k_B T)]$$

At T = 0: $\Delta_{\mathbf{k}} = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}}$

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Summary BCS Theory

BCS wave function: $|\mathrm{BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} \underbrace{c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}}_{\text{Cooper pair}}) |\phi_0\rangle$

Hamiltonian with kinetic energy $\varepsilon_{\mathbf{k}}$ and a pairing potential $V_{\mathbf{kl}}$:

Quasiparticle energy: $E_{\mathbf{k}} = \sqrt{\varepsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}$

Energy gap = order parameter

Quasiparticles: $\begin{cases} a_{\mathbf{k}\uparrow} = u^*_{\mathbf{k}} c_{\mathbf{k}\uparrow} + v^*_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow} \\ a^\dagger_{-\mathbf{k}\downarrow} = -v_{\mathbf{k}} c_{\mathbf{k}\uparrow} + u_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow} \end{cases}$ $\left(|v_{\mathbf{k}}|^2 = 1 - |u_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \right)$

Order parameter (Ψ before): $\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} V_{\mathbf{k},\mathbf{k}'}$

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Unconventional Superconductivity

What is unconventional?

How do we handle unconventional superconductivity?

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Introduction to Superconductivity

What is it?

A charged superfluid of Cooper pairs (2 electrons) with fermionic character

Cooper pairs formed by effective attractive interaction

How do we describe it?

BCS theory for the condensation

BdG matrix formalism

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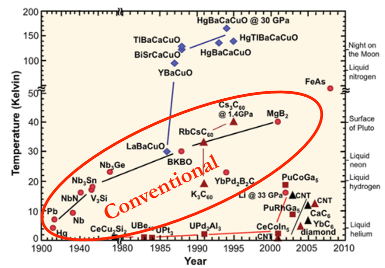
Conventional Superconductors

- Superconductivity from electron-phonon interactions
  - Superconductivity in "normal" metals
  - Low temperatures, $T_c < 40$ K
  - Isotropic pairing ($\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{l}} \frac{\Delta_{\mathbf{l}}}{E_{\mathbf{l}}} V_{\mathbf{kl}} = \Delta$)



Superconducting Symmetries

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Superconducting order parameter is fermionic i.e. odd under particle exchange:

$$\Psi_{\alpha\beta}(\mathbf{k}) = -\Psi_{\beta\alpha}(-\mathbf{k})$$

$$\Psi_{\alpha\beta}(\mathbf{k}) = \Delta e^{i\varphi}\eta(\mathbf{k})\chi_{\alpha\beta}$$

orbital ($\eta(\mathbf{k})$), spin ($\chi_{\alpha\beta}$)

$$\chi_{\alpha\beta} \rightarrow \begin{cases} \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) & (S=0) \\ |\uparrow\uparrow\rangle & (S=1, S_z=1) \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) & (S=1, S_z=0) \\ |\downarrow\downarrow\rangle & (S=1, S_z=-1) \end{cases}$$

→ η even function in $\mathbf{k}$ (for $S=0$)

→ η odd function in $\mathbf{k}$ (for $S=1$)

$$\Delta_{\mathbf{k}} = -\frac{1}{2}\sum_{\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}}V_{\mathbf{k},\mathbf{k}'}$$

Superconducting Symmetries

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$V_{\mathbf{k,k'}}$ (and the band structure) determines the pairing symmetry, but it often very hard to determine

- Lattice fluctations: spin-singlet *s*-wave
- Antiferromagnetic spin fluctuations: spin-singlet *d*-wave (extended s-wave)
- Ferromagnetic spin fluctuations: spin-triplet *p*-wave
- Strong on-site repulsion (Heisenberg interaction): spin-singlet *d*-wave

Is there a way to determine the possible pairing symmetries in a material without knowledge of $V_{\mathbf{k,k'}}$?

Yes, we can do a general symmetry group analysis

See e.g. Sigrist and Ueda, RMP **63**, 239 (1991)

Spatial Symmetries

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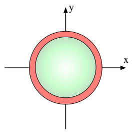
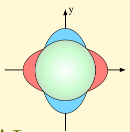
- Conventional superconductors:
  - Spin-singlet, *s*-wave (η k-independent)

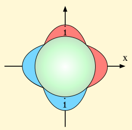


- Cuprate (high-Tc) superconductors:
  - Spin-singlet, *d*-wave (η = k_x^2 - k_y^2)



UNCONVENTIONAL

- Exotic superconductors:
  - Spin-triplet, *p*-wave (^3He, Sr_2RuO_4?)
  - Topological "spinless" superconductors with Majorana fermions



$k_x + ik_y$

General Pairing Hamiltonian

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General pairing Hamiltonian: $\mathcal{H} = \sum_{\mathbf{k},s}\varepsilon(\mathbf{k})a^\dagger_{\mathbf{k}s}a_{\mathbf{k}s}$

$$+\frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',s_1,s_2,s_3,s_4} V_{s_1s_2s_3s_4}(\mathbf{k},\mathbf{k}')a^\dagger_{-\mathbf{k}s_1}a^\dagger_{\mathbf{k}s_2}a_{\mathbf{k}'s_3}a_{-\mathbf{k}'s_4}$$

Mean-field order parameter: $\Delta_{ss'}(\mathbf{k}) = -\sum_{\mathbf{k}',s_3,s_4} V_{s'ss_3s_4}(\mathbf{k},\mathbf{k}')\langle a_{\mathbf{k}'s_3}a_{-\mathbf{k}'s_4}\rangle$

$$\rightarrow \tilde{\mathcal{H}} = \sum_{\mathbf{k},s}\varepsilon(\mathbf{k})a^\dagger_{\mathbf{k}s}a_{\mathbf{k}s} + \frac{1}{2}\sum_{\mathbf{k},s_1,s_2}[\Delta_{s_1s_2}(\mathbf{k})a^\dagger_{\mathbf{k}s_1}a^\dagger_{-\mathbf{k}s_2}$$

$$-\Delta^*_{s_1s_2}(-\mathbf{k})a_{-\mathbf{k}s_1}a_{\mathbf{k}s_2}]$$

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Matrix Formulation

4-component notation (Nambu): $\mathbf{a}_\mathbf{k} = (a_{\mathbf{k}\uparrow}, a_{\mathbf{k}\downarrow}, a^\dagger_{-\mathbf{k}\uparrow}, a^\dagger_{-\mathbf{k}\downarrow})^T$

$$\rightarrow \tilde{\mathcal{H}} = \mathbf{a}^\dagger_\mathbf{k} \begin{pmatrix} \varepsilon(\mathbf{k})\sigma_0 & \hat{\Delta}(\mathbf{k}) \\ \hat{\Delta}^\dagger(\mathbf{k}) & -\varepsilon(\mathbf{k})\sigma_0 \end{pmatrix} \mathbf{a}_\mathbf{k}$$

Spin-singlet pairing: $\hat{\Delta}(\mathbf{k}) = i\hat{\sigma}_y \psi(\mathbf{k}) = \begin{bmatrix} 0 & \psi(\mathbf{k}) \\ -\psi(\mathbf{k}) & 0 \end{bmatrix}$ — ψ even function of **k**

$\left[\psi(\mathbf{k})[c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} - c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}]\right]$

Spin-triplet pairing: $\hat{\Delta}(\mathbf{k}) = i(\mathbf{d}(\mathbf{k})\cdot\hat{\boldsymbol{\sigma}})\hat{\sigma}_y$ — **d** vectorial odd function of **k**

$$= \begin{bmatrix} -d_x(\mathbf{k}) + id_y(\mathbf{k}) & d_z(\mathbf{k}) \\ d_z(\mathbf{k}) & d_x(\mathbf{k}) + id_y(\mathbf{k}) \end{bmatrix}$$

$m_z = 0$: $d_z(\mathbf{k})[c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} + c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}]$

$m_z = 1$: $[-d_x(\mathbf{k}) + id_y(\mathbf{k})]c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\uparrow}$

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Solution

- The largest eigenvalue gives T_c
- The eigenfunction spaces (Δ) form a basis of an irreducible representation (irrep) of the symmetry group of the equation (V)

→ Possible SC symmetries belong to irreps of the symmetry group of H

→ SC state always breaks U(1) but can also break
  - Crystal lattice symmetry
  - Spin-rotation symmetry
  - Time-reversal symmetry

Below T_c:
  - 2nd SC transition from same V → new Δ belongs to same irrep
  - 2nd SC transition from other V

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Solution Equations

QP energy (eigenvalue): $E_\mathbf{k} = \sqrt{\varepsilon(\mathbf{k})^2 + |\psi(\mathbf{k})|^2}$

$$E_\mathbf{k} = \sqrt{\varepsilon(\mathbf{k})^2 + |\mathbf{d}(\mathbf{k})|^2 \pm \mathbf{q}(\mathbf{k})|}$$

$\hat{\Delta}\hat{\Delta}^\dagger = |\mathbf{d}|^2\hat{\sigma}_0 + \mathbf{q}\cdot\hat{\boldsymbol{\sigma}}$

$\mathbf{q} = i(\mathbf{d}\times\mathbf{d}^*)$

Finite **q** = non-unitary

Self-consistency: $\Delta_{ss'}(\mathbf{k}) = -\sum_{\mathbf{k}', s_3, s_4} V_{s'ss_3s_4}(\mathbf{k},\mathbf{k}')\mathcal{F}_{s_3s_4}(\mathbf{k}',\beta)$

$$\hat{\mathcal{F}}(\mathbf{k},\beta) = \frac{\hat{\Delta}(\mathbf{k})}{2E_\mathbf{k}}\tanh\left[\frac{\beta E_\mathbf{k}}{2}\right] \quad \text{(unitary states)}$$

Linearize close to T_c: $v\Delta_{s_1s_2}(\mathbf{k}) = -\sum_{s_3s_4}\langle V_{s_2s_1s_3s_4}(\mathbf{k},\mathbf{k}')\Delta_{s_3s_4}(\mathbf{k}')\rangle_{\mathbf{k}'}$

$$\frac{1}{v} = N(0)\int_0^{\varepsilon_c} d\varepsilon \frac{\tanh\left[\frac{\beta_c\varepsilon(k)}{2}\right]}{\varepsilon(\mathbf{k}} = \ln(1.14\beta_c\varepsilon_c)$$

Linear eigenvalue equation

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Basis gap functions: D_{4h}

- D_{4h} = tetragonal symmetry (cuprates with $k_z = 0$)

Irreducible representation Γ	Basis function	
	(a) Spin-singlet	
Γ_1^+	$\psi(\Gamma_1^+;\mathbf{k}) = 1,\ k_x^2+k_y^2,\ k_z^2$	*s*-wave, extended *s*-wave
Γ_2^+	$\psi(\Gamma_2^+;\mathbf{k}) = k_xk_y(k_x^2-k_y^2)$	
Γ_3^+	$\psi(\Gamma_3^+;\mathbf{k}) = k_x^2-k_y^2$	$d(x^2\text{-}y^2)$-wave
Γ_4^+	$\psi(\Gamma_4^+;\mathbf{k}) = k_xk_y$	d(xy)-wave
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k}) = k_xk_z$	
	$\psi(\Gamma_5^+,2;\mathbf{k}) = k_yk_z$	
	(b) Spin-triplet	
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k}) = \hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y,\ \hat{\mathbf{z}}k_z$	
Γ_2^-	$\mathbf{d}(\Gamma_2^-;\mathbf{k}) = \hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$	
Γ_3^-	$\mathbf{d}(\Gamma_3^-;\mathbf{k}) = \hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_x$	
Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k}) = \hat{\mathbf{x}}k_y+\hat{\mathbf{y}}k_x$	
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k}) = \hat{\mathbf{x}}k_z,\ \hat{\mathbf{z}}k_x$	*p*(x)- and *p*(y)-wave degenerate
	$\mathbf{d}(\Gamma_5^-,2;\mathbf{k}) = \hat{\mathbf{y}}k_z,\ \hat{\mathbf{z}}k_y$	

Sigrist and Ueda, RMP **63**, 239 (1991)

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Basis gap functions: D_{6h}

- D_{6h} = hexagonal symmetry (graphene, Bi_2Se_3 TIs with $k_z = 0$,)

Irreducible representation Γ	Basis functions	
	(a) Spin-singlet	
Γ_1^+	$\psi(\Gamma_1^+;\mathbf{k})=1,\ k_x^2+k_y^2,\ k_z^2$	s-wave, extended s-wave
Γ_2^+	$\psi(\Gamma_2^+;\mathbf{k})=k_xk_y(k_x^2-3k_y^2)(k_y^2-3k_x^2)$	
Γ_3^+	$\psi(\Gamma_3^+;\mathbf{k})=k_zk_x(k_x^2-3k_y^2)$	
Γ_4^+	$\psi(\Gamma_4^+;\mathbf{k})=k_zk_y(k_y^2-3k_x^2)$	
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k})=k_xk_z$ $\psi(\Gamma_5^+,2;\mathbf{k})=k_yk_z$	
Γ_6^+	$\psi(\Gamma_6^+,1;\mathbf{k})=k_x^2-k_y^2$ $\psi(\Gamma_6^+,2;\mathbf{k})=2k_xk_y$	d(x^2-y^2)-wave and d(xy)-wave degenerate
	(b) Spin-triplet	
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k})=\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y,\hat{\mathbf{z}}k_z$	
Γ_2^-	$\mathbf{d}(\Gamma_2^-;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$	
Γ_3^-	$\mathbf{d}(\Gamma_3^-;\mathbf{k})=\hat{\mathbf{z}}k_x(k_x^2-3k_y^2),$ $k_z[(k_x^2-k_y^2)\hat{\mathbf{x}}-2k_xk_y\hat{\mathbf{y}}]$	
Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k})=\hat{\mathbf{z}}k_y(k_y^2-3k_x^2),$ $k_z[(k_y^2-k_x^2)\hat{\mathbf{y}}-2k_xk_y\hat{\mathbf{x}}]$	
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k})=\hat{\mathbf{x}}k_z,\hat{\mathbf{z}}k_x$ $\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{y}}k_z,\hat{\mathbf{z}}k_y$	
Γ_6^-	$\mathbf{d}(\Gamma_6^-,1;\mathbf{k})=\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_y$ $\mathbf{d}(\Gamma_6^-,2;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$	

Sigrist and Ueda, RMP **63**, 239 (1991)

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Unconventional Superconductivity

What is unconventional?

Any SC state which is does not have spin-singlet *s*-wave order

How do we handle unconventional superconductivity?

Generalized formalism using a 4 x 4 BdG equation

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Multiple Order Parameters

The superconducting state especially interesting if it has multiple components

- Two-dimensional irreps gives Δ_1+iΔ_2
  - singlet $d(x^2-y^2)$+id(xy)-wave for hexagonal lattices (graphene?)
  - triplet (m_z = 0) p(x)+ip(y)-wave for square lattices (Sr_2RuO_4)

  Break time-reversal symmetry (TRS)

  Topological superconductors

- Subdominant pairing
  - singlet $d(x^2-y^2)$+is-wave (cuprates with small s-wave component)

  Breaks TRS but not a topological superconductor