Superconductivity from repulsive interactions

Heidelberger Graduate Days
April 2022

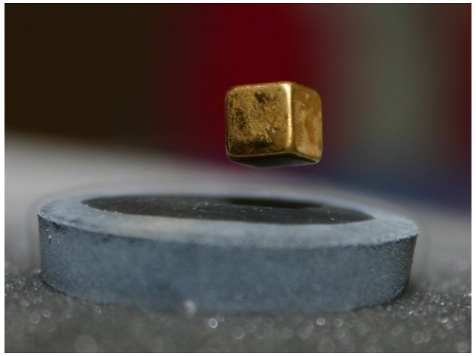
Laura Classen

1. Introduction

1.1 Superconductivity in short

▷ Superconductivity is one of the most fascinating states of interacting electrons:

- Dissipationless electric current ("perfect conductor") and expulsion of magnetic fields ("perfect diamagnetism")



https://commons.wikimedia.org/wiki/File:Magnet_4.jpg

- Associated with macroscopic condensate: quantum state of $\sim 10^{23}$ particles in lowest energy level
  ↳ known from bosons: Bose-Einstein condensate
  but impossible for electrons (fermions) due to Pauli principle
  ↳ How is superconducting state possible?

▷ Electronic pairing as solution?

- <u>If</u> electrons form pairs, pairs have spin 0 or 1, i.e. pairs are bosons
  ↳ bosons can condense ✓
  ↳ need explanation why electrons form pairs

- But Coulomb interaction is repulsive & does not allow pair formation ✗

▷ How to get attractive interaction?

- Bardeen, Cooper, Schrieffer (BCS): phonons, i.e. quanta of lattice vibrations, can mediate attractive interaction
  - ↳ happens in many metals ✓
  - ↳ pairs have high symmetry ("s-wave pairing")
  - ↳ "conventional" superconductivity

- Unconventional superconductivity:

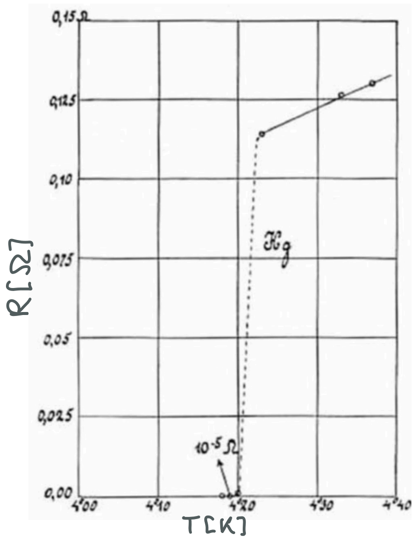
  This lecture

  any deviation from BCS-type pairing state
  - ↳ electron-phonon interaction too weak
  - ↳ Coulomb repulsion too strong (strongly correlated materials)
  - ↳ high-temperature superconductors
  - ↳ mediation via magnetic fluctuations, quantum-critical fluctuations ...
  - ↳ pairs have different symmetry (⇒ different response)

1.2 Brief history

- Electric current in a metal given by voltage-current relation $V = R\,I$
- Resistance R is temperature-dependent
  - ↪ What happens at lowest temperatures?
- 1911: discovery of superconductivity by Kamerlingh Onnes

Resistance of mercury drops to zero at 4.2 K



enabled by liquefaction of Helium

<https://www.nobelprize.org/prizes/physics/1913/onnes/facts/>

Heike Kamerlingh Onnes
Facts

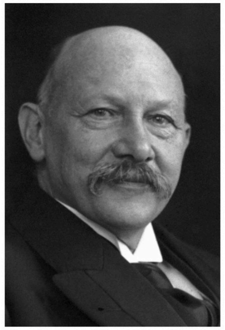


Photo from the Nobel Foundation archive.

Heike Kamerlingh Onnes
The Nobel Prize in Physics 1913

Born: 21 September 1853, Groningen, the Netherlands

Died: 21 February 1926, Leiden, the Netherlands

Affiliation at the time of the award: Leiden University, Leiden, the Netherlands

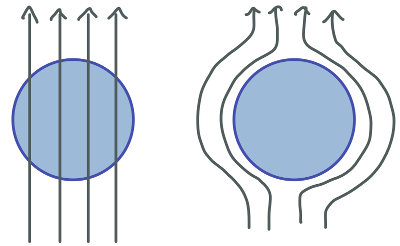
Prize motivation: "for his investigations on the properties of matter at low temperatures which led, inter alia, to the production of liquid helium."

Prize share: 1/1

Work

When different substances are cooled to very low temperatures, their properties change. In 1908 Heike Kamerlingh Onnes used an ingenious apparatus to cool helium to liquid form. Fluid helium was carefully studied and also became an important aid for the cooling of different substances and charting their properties at low temperatures. In 1911 Heike Kamerlingh Onnes discovered that the electrical resistance of mercury completely disappeared at temperatures a few degrees above absolute zero. The phenomenon became known as superconductivity.

▷ 1933: Meissner & Ochsenfeld: magnetic fields are expelled inside of a superconductor



$T > T_c$ $\qquad$ $T < T_c$

& effect is reversible

→ phenomenological description by London equations (1935)

$\partial_t \vec{j}_s = \frac{n_s e^2}{m}\vec{E}$, $\nabla\times\vec{j}_s = -\frac{n_s e^2}{m}\vec{B}$

Maxwell: $\mu_0 \vec{j} = \nabla\times\vec{B}$

$\Rightarrow \nabla\times\frac{1}{\mu_0}(\nabla\times\vec{B}) = -\frac{n_s e^2}{m}\vec{B}$

$\Rightarrow \nabla^2\vec{B} = \frac{1}{\lambda_L^2}\vec{B}$

$\Rightarrow$ e.g. $B_z(x) = B_0 e^{-x/\lambda_L}$

$\lambda_L = \sqrt{\frac{m}{\mu_0 n_s e^2}}$ London penetration depth

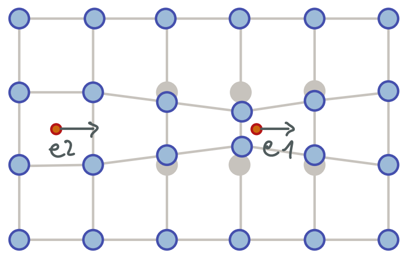
▷ 1956: "Cooper instability": arbitrarily weak attraction would give rise to superconductivity

▷ 1957: Microscopic explanation of superconductivity by Bardeen, Cooper & Schrieffer

Effective electron-electron interaction mediated by phonons is attractive at energies

$E < \omega_D$

Debye frequency: characteristic phonon frequency



Very successful for many materials (metals)

e.g. Hg (4.2 K), Al (1.2 K), MgB_2 (39 K),

fast forward 2018: hydrides as LaH_{10} (260 K @ 180 GPa)

https://www.nobelprize.org/prizes/physics/1972/summary/

The Nobel Prize in Physics 1972

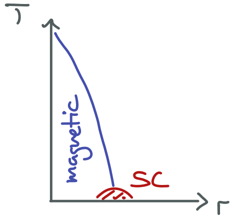
Photo from the Nobel Foundation archive.
John Bardeen
Prize share: 1/3

Photo from the Nobel Foundation archive.
Leon Neil Cooper
Prize share: 1/3

Photo from the Nobel Foundation archive.
John Robert Schrieffer
Prize share: 1/3

The Nobel Prize in Physics 1972 was awarded jointly to John Bardeen, Leon Neil Cooper and John Robert Schrieffer "for their jointly developed theory of superconductivity, usually called the BCS-theory."

▷ 1979 & 80's: superconductivity in heavy fermions $CeCu_2Si_2$ Steglich et al 1979
UBe_{13} Ott et al 1983
UPt_3 Stewart et al 1984



↳ at odds with BCS theory:
- strongly correlated materials, Coulomb repulsion too strong
- e.g. power-law instead of exponential behavior in London penetration depth (→ Cooper pairs w/ different symmetry?)

▷ 1986: discovery of "high-temperature" superconductivity by Bednorz & Müller in $(La,Sr)_2CuO_4$ (35 K) previous record Nb_3Ge (23 K) → "cuprates" material family

The Nobel Prize in Physics 1987

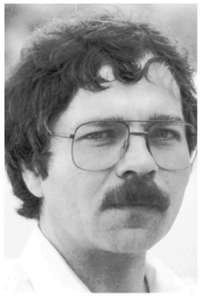


Photo from the Nobel Foundation archive.
J. Georg Bednorz
Prize share: 1/2

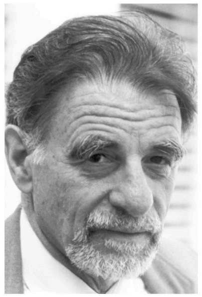


Photo from the Nobel Foundation archive.
K. Alexander Müller
Prize share: 1/2

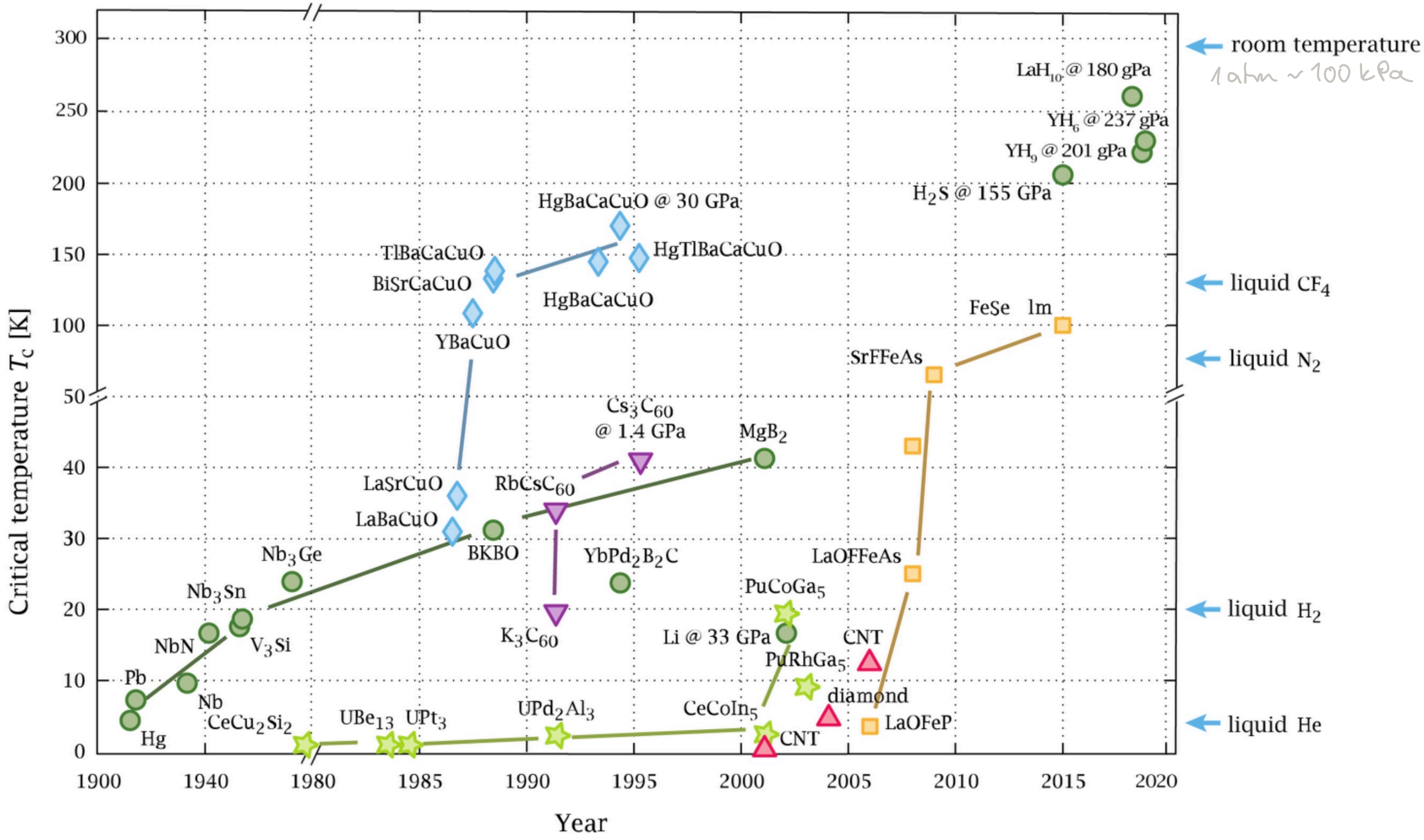
The Nobel Prize in Physics 1987 was awarded jointly to J. Georg Bednorz and K. Alexander Müller "for their important break-through in the discovery of superconductivity in ceramic materials."

https://www.nobelprize.org/prizes/physics/1987/summary/

▷ 2008: new class of materials with unconventional superconductivity: iron-pnictides (& later iron-chalcogenides)
LaOFeAs (26 K)

▷ 2014: new record in H_2S: 190 K @ 150 GPa by Eremets et al
- conventional superconductivity

▷ Critical temperatures over the years

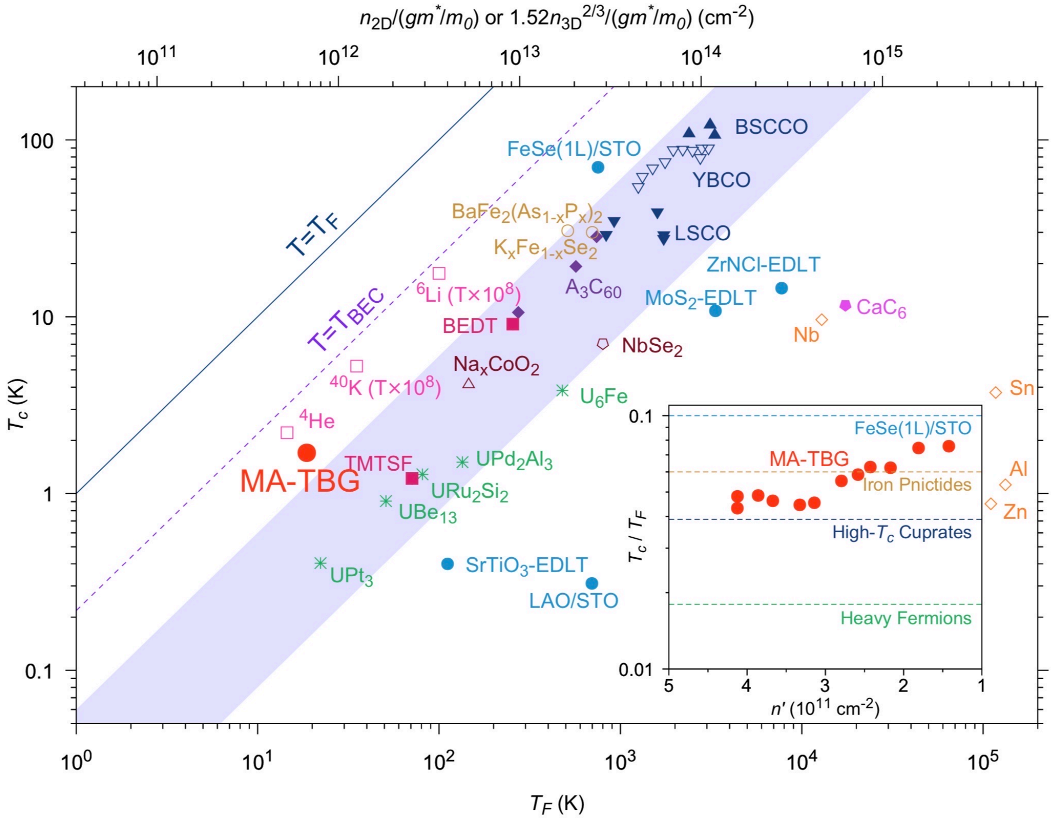


Pia Jensen Ray, Master's thesis (2015)

DOI:10.6084/M9.FIGSHARE.2075680.V2

- Absolute vs. relative critical temperatures
  - See in relation to available carriers
  - $T_c/T_F \ll 1$ for conventional superconductors
  - $T_c/T_F \lesssim 1$ for unconventional ones

- 2018: discovery of superconductivity in magic-angle twisted bilayer graphene with large T_c/T_F, pairing mechanism not yet clear

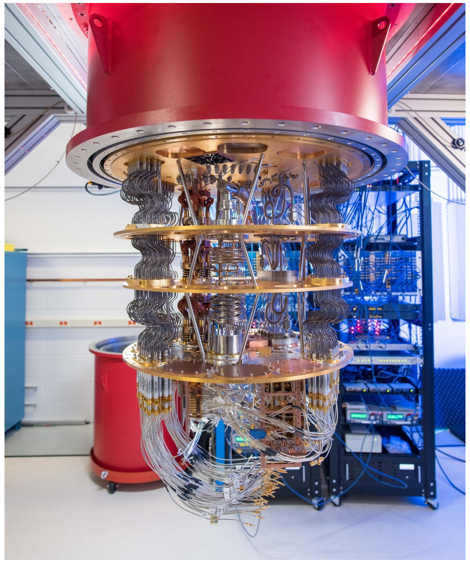


Cao et al Nature 556, 43 (2018)

1.3 Applications

- ▷ Creation of strong, stable magnetic fields
  - current flows dissipationless in coil
  - conventional superconductors used, e.g. Nb, because long, thin cables needed
  - used, e.g., in MRI/NMR or particle colliders

- ▷ Precise measurement of magnetic fields
  - e.g. Josephson effect & SQUID (superconducting quantum interference device)



https://commons.wikimedia.org/wiki/File:QuantumAI.jpg

- ▷ Quantum computation
  - Perhaps most popular qubit technology at the moment (Google, IBM, Intel, ...)
    ~ 50 qubits
  - Different types of superconducting qubits:
    charge, flux, transmon qubit
    based on # Cooper pairs or quantized flux

- ▷ Possible efficiency & size advantages for
  - electric power transmission (pilot project in Essen)
  - generators in wind turbines (prototype from Bremerhaven tested in Denmark)
  - power storage devices in superconducting coils
  - magnetic levitation devices

1.4 Summary

Superconductivity is a fascinating quantum many-body state with important technological applications.

For it to occur, electrons need to form pairs and overcome Coulomb repulsion.

Conventional pairing mechanism: effective attraction mediated by phonons yields high-symmetry pairs

Unconventional pairing mechanism: everything else
E.g.: magnetic fluctuations
Superconductors with some of the highest T_c's (absolute & relative)

Outline

$\hbar = k_B = 1$ troughout

Literature and credit

- S. Maiti, A. Chubukov, AIP Conference Proceedings 1550, 3 (2013) "Superconductivity from repulsive interaction" https://arxiv.org/abs/1305.4609
- M. Sigrist, AIP Conference Proceedings 789, 165 (2005) "Introduction to unconventional superconductivity" http://edu.itp.phys.ethz.ch/2007b/ws0506/us/summer_school.pdf
- G. Mahan, Springer Science+Business Media New York "Many-particle physics" https://link.springer.com/book/10.1007/978-1-4757-5714-9
- M. Sigrist and K. Uedao, Rev. Mod. Phys 63, 239 (1991), "Phenomenological theory of unconventional superconductivity" https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.63.239
- A. Black-Schaffer and C. Honerkamp, J. Phys.: Condens. Matter 26, 423201 (2014) "Chiral d-wave superconductivity in doped graphene" https://arxiv.org/abs/1406.0101

2. Technical background

2.1. Recap Fermi liquid

- Out of which state does superconductivity develop?
  ↳ Fermi liquid if metallic

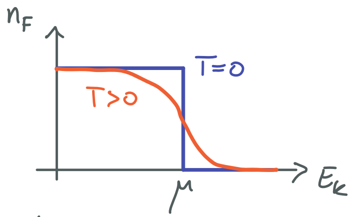
- First: Fermi gas → free (non-interacting) gas of fermions
  - Quantum statistics important at low enough temperatures: (de Broglie wavelength $\lambda_T \sim \frac{\hbar}{\sqrt{mT}}$ comparable to interparticle distance)
    average number of particles at energy E_k:

fermions: $n_F(k) = \dfrac{1}{e^{(E_k-\mu)/T}+1}$

here: electrons with spin 1/2

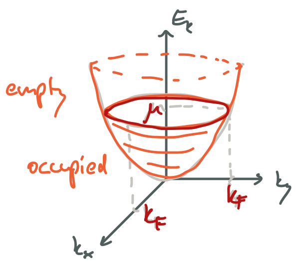
bosons $n_B(k) = \dfrac{1}{e^{(E_k-\mu)/T}-1}$

  - Free electrons: $E_k = \frac{k^2}{2m}$



At $T=0$: $n_F(k) = 1$ for $E_k < \mu$

$n_F(k) = 0$ for $E_k > \mu$



⇒ sharp boundary in k-space up to which states are occupied: Fermi surface

$\mu = E_k = \frac{k_F^2}{2m}$ ↳ defines Fermi wavevector

$k_F = \sqrt{2m\mu}$

  - Close to k_F: $E_k \approx \mu + \frac{k_F}{m}(k-k_F) = \mu + v_F(k-k_F)$

▷ Fermi liquid: "weakly" interacting fermions
↪ see below

- Collective excitations behave almost like free fermions → quasiparticles
- Well-defined excitations with momentum k & dispersion near k_F

$$\varepsilon_k = \mu + v_F^*(k-k_F)$$

renormalized $v_F^* = \frac{k_F}{m^*}$ and quasiparticle mass m^*

"feel" other fermions around, properties get "dressed" by interaction

- Lifetime for quasiparticle with momentum k becomes finite

near k_F: $\mathrm{Im}\,\varepsilon_k \propto (k-k_F)^\alpha$

interactions enable change of energy state ε_k

- Quasiparticles well defined / Fermi liquid stable if $\mathrm{Re}\,\varepsilon_k > \mathrm{Im}\,\varepsilon_k$ ($\Rightarrow$ if $\alpha > 1$)

$\alpha = 2$ in 3D
log. corrections in 2D
$\mathrm{Im}\,\varepsilon_k \propto (k-k_F)\ln|k-k_F|$

▷ Many superconducting states manifest as "Fermi surface instabilities", where Fermi liquid description breaks down

2.2 Green's function approach

▷ Interacting many-body system described by space- and/or time-dependent correlation functions of the form

$$\langle \hat{O}(\vec{x},t)\,\hat{O}(\vec{x}',t')\rangle = \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H}\,\hat{O}(\vec{x},t)\,\hat{O}(\vec{x}',t')\right] \qquad t > t'$$

↪ thermodynamic average, trace over complete set of states

$\hat{O}(x,t)$: operator in Heisenberg picture $\hat{O}(\vec{x},t) = e^{iHt}\,\hat{O}(x)\,e^{-iHt}$
includes chemical potential $H = \hat{H} - \mu N$

statistical physics
$\langle \hat{O} \rangle = \mathrm{Tr}[\rho\,\hat{O}]$
↪ density matrix

▷ Convenient to use Matsubara formalism

- interaction $H = H_0 + V$ appears in two instances $e^{\pm iHt}$ and $e^{-\beta H}$
- to treat on equal footing in perturbative expansion: consider complex time $\tau = it$, τ & β appear formally in the same way

▷ Here: single- and two-particle Green's function

$\mathcal{O}(x,\tau) = e^{H\tau} \mathcal{O}_x e^{-H\tau}$

$\mathcal{O}(p,\omega) = \int d\tau \int d^d x \, e^{i\omega\tau \mp ipx} \mathcal{O}(x,\tau)$

$$G_{\alpha\beta}(X_1; X_2) = - \langle T \, \psi_\alpha(X_1) \, \psi^+_\beta(X_2) \rangle$$

$$G_{\alpha\beta,\gamma\delta}(X_1, X_2, X_3, X_4) = \langle T \psi_\alpha(X_1) \psi_\beta(X_2) \psi^+_\gamma(X_3) \psi^+_\delta(X_4) \rangle$$

with $X = (\vec{x}, \tau)$: space & (imaginary) time variables

T: time ordering in imaginary time

$\psi_\alpha(X)$: space- & time dependent electron operator in Heisenberg picture

$$\psi_\alpha(\vec{x}, \tau) = e^{H\tau} \psi_\alpha(\vec{x}) e^{-H\tau}$$

α, β: spin (or any other quantum number)

▷ Single-particle Green's function

- In translational invariant system: $G_{\alpha\beta}(X_1, X_2) = G_{\alpha\beta}(X_1 - X_2) =: G_{\alpha\beta}(X)$

Fourier transform $G_{\alpha\beta}(\vec{k}, \omega_n) = \int d\tau \int d^d x \; e^{i\omega_n \tau + i\vec{k}\cdot\vec{x}} \, G_{\alpha\beta}(\vec{x}, \tau)$

ω_n: Matsubara frequency, real frequency via analytic continuation $i\omega_n \to \omega + i\delta$ & $\delta \to 0^+$ for retarded Green's function

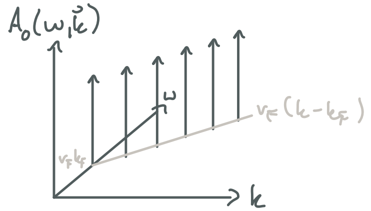
- Examples: Green's function of free fermions near Fermi surface

$$G_0 = (\vec{k}, \omega_n) = \frac{1}{i\omega - v_F(k-k_F)}$$

or with real frequency

$$G_0^R = \frac{1}{\omega - v_F(k-k_F) + i\delta} \qquad (\delta \to 0^+)$$

↪ spectral function $A_0(\vec{k},\omega) = -2\,\mathrm{Im}\, G_0^R(\vec{k},\omega) = 2\pi\,\delta(\omega - v_F(\vec{k}-\vec{k}_F))$

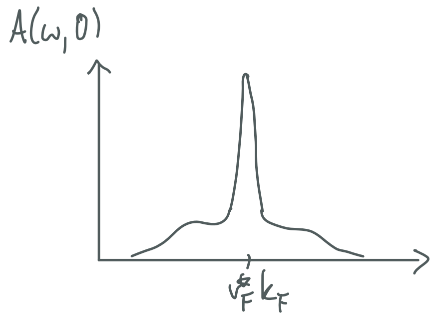


Green's function of Fermi liquid

$$G^R(\vec{k},\omega) = \frac{Z}{\omega - v_F^*(k-k_F) + i\delta} + G_{inc}$$

↪ broadening due to finite lifetime

quasiparticle residue $0 < Z < 1$

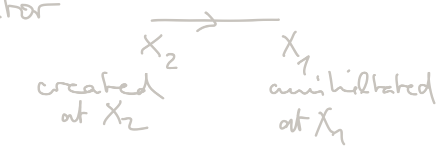


- Define self-energy for interacting system

$$G^{-1}(\vec{k},\omega) = G_0^{-1}(\vec{k},\omega) + \Sigma(\vec{k},\omega)$$

relates full Green's function G (dressed by interactions) to non-interacting one in diagrams

$\langle \psi(x_1)\psi^{+}(x_2)\rangle$ as propagator

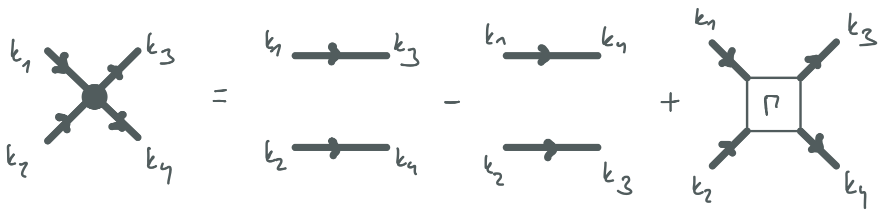


e.g. $\frac{1}{Z} = 1 + \frac{\partial \Sigma}{\partial \omega}$ and $v_F^* = Z\left(v_F^* - \frac{\partial \Sigma}{\partial k}\right)$

▷ Two-particle Green's function:

$$G^{(4)}_{\alpha\beta,\gamma\delta}(x_1,x_2,x_3,x_4) = \langle T\, \psi_\alpha(x_1)\psi_\beta(x_2)\,\psi^{+}_\gamma(x_3)\psi^{+}_\delta(x_4)\rangle$$

Diagrams



$k = (\omega, \vec{k})$

- For free fermions: $G^{(4)}_{\alpha\beta,\gamma\delta}(k_1,k_2,k_3,k_4) = G_{\alpha\gamma}(k_1,k_3)G_{\beta\delta}(k_2,k_4) - G_{\alpha\delta}(k_1,k_4)G_{\beta\gamma}(k_2,k_3)$
  ↳ no new information compared to single-particle Green's function
- For interacting fermions: one-particle irreducible vertex function $\Gamma_{\alpha\beta\gamma\delta}(k_1,k_2,k_3,k_4)$
  ↳ cannot be obtained from single-particle properties
- Vertex Γ can be viewed as effective interaction, i.e. "dressed" interaction that particles feel due to multiple scattering processes
- Singularity of effective interaction describes collective excitations/potential bound states (see e.g. next section)

- E.g. spin SU(2) symmetric Hamiltonian: $H = H_0 + V$

$$H_0 = \sum_{\sigma k} \psi^+_\sigma(k) \frac{k^2}{2m} \psi_\sigma(k) \qquad V = \frac{1}{\Omega} \sum_{\substack{k_1 \dots k_4 \\ \sigma\sigma'}} V(k_1,k_2,k_3,k_4)\, \delta(k_1+k_2-k_3-k_4)\, \psi^+_\sigma(k_3)\psi^+_{\sigma'}(k_4)\psi_{\sigma'}(k_2)\psi_\sigma(k_1)$$

Expand 2-particle Green's function in interaction

$e^{H\tau}\psi e^{-H\tau}$ $\qquad \tilde{\psi}(\tau_i) = e^{H_0\tau_i}\psi e^{-H_0\tau_i}$

$$\langle T \psi_1\psi_2\psi_3^+\psi_4^+ \rangle = \frac{1}{Z} \mathrm{Tr}\, T e^{-\beta H} \psi_1\psi_2\psi_3^+\psi_4^+ = \frac{\mathrm{Tr}\, T e^{-\beta H_0 - \beta V} \psi_1\psi_2\psi_3^+\psi_4^+}{\mathrm{Tr}\, e^{-\beta H_0 - \beta V}} = \frac{\langle T e^{-\int_0^\beta d\tau V} \tilde{\psi}_1\tilde{\psi}_2\tilde{\psi}_3^+\tilde{\psi}_4^+ \rangle_0}{\langle T e^{-\int_0^\beta d\tau V} \rangle_0}$$

↳ average w.r.t H_0

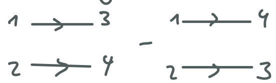
$$= \frac{\sum_n \frac{1}{n!} \langle T (-\int_0^\beta d\tau V)^n \tilde{\psi}_1\tilde{\psi}_2\tilde{\psi}_3^+\tilde{\psi}_4^+ \rangle_0}{\sum_n \frac{1}{n!} \langle T (-\int_0^\beta d\tau V)^n \rangle_0}$$

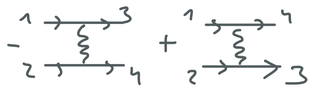
↳ see as expectation value of free system with $e^{-\beta H_0}$ & expand in V

$\sim \sum_n \frac{1}{n!} \langle (-\int d\tau V)^n \psi_1\psi_2\psi_3^+\psi_4^+ \rangle_{0,C}$

↳ connected, no vaccuum contractions like 

contains all possibilities how to connect two incoming (1,2) & two outgoing (3,4) electrons with n interactions

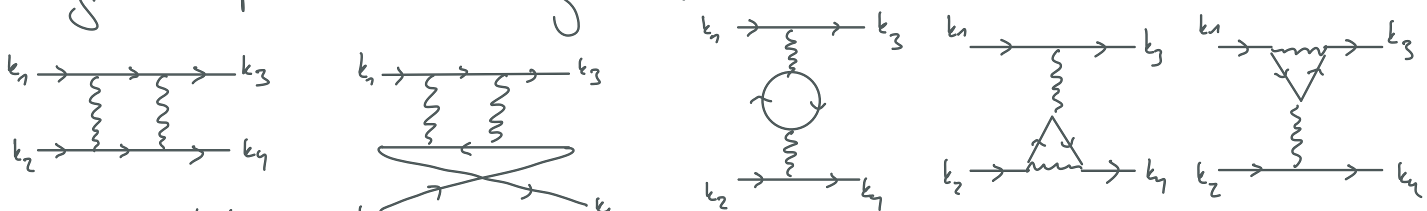
↳ $n=0$: no interaction in $\langle \psi_1\psi_2\psi_3^+\psi_4^+ \rangle_0$: 

↳ $n=1$: to leading order in interaction: one interaction in between 

in formulas vertex is anti-symmetrized interaction

$$\Gamma^0_{\alpha\beta\gamma\delta}(k_1,k_2,k_3,k_4) = -V(k_1-k_3)\,\delta_{\alpha\gamma}\delta_{\beta\delta} + V(k_1-k_4)\,\delta_{\alpha\delta}\delta_{\beta\gamma}$$

↳ $n=2$: diagrams of next-to-leading order



particle-particle $\qquad$ crossed particle-hole $\qquad$ direct particle-hole

$-\ (3 \Leftrightarrow 4)$

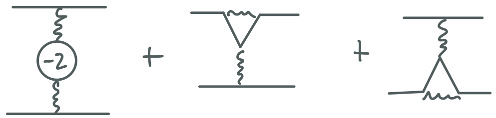
- Diagrams differ in momentum dependence of internal lines (Green's functions) and interactions

- Consider constant interaction $H = H_0 + V$

$$V = U \sum_i \sum_{\sigma\sigma'} \psi^+_{i\sigma} \psi_{i\sigma} \psi^+_{i\sigma'} \psi_{i\sigma'} = \frac{1}{\Omega} U \sum_{\substack{k_1 .. k_4 \\ \sigma\sigma'}} \delta(k_1 + k_2 - k_3 - k_4)\, \psi^+_{k_3\sigma} \psi^+_{k_4\sigma'} \psi_{k_2\sigma'} \psi_{k_1\sigma}$$

and write down expressions for diagrams

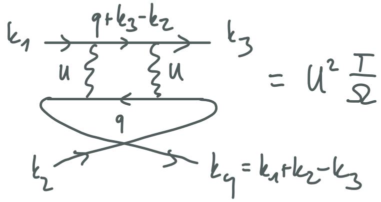
↪ direct particle-hole:



$= 0$

↪ crossed particle hole:

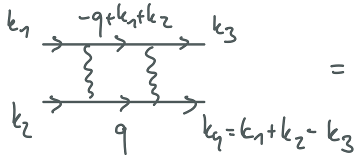
already use momentum conservation



$$= U^2 \frac{T}{\Omega} \sum_{i\omega} \int d^d q \; G_0(\vec{q}, \omega)\, G_0(\vec{q} + \vec{k}_3 - \vec{k}_2, \omega + \omega_3 - \omega_2) = -U^2 \Pi_{ph}(k_3 - k_2) \quad (2.1)$$

loop is function of transferred momentum and frequency $k_3 - k_2$

↪ particle-particle:



$$= U^2 \frac{T}{\Omega} \sum_{i\omega} \int d^d q \; G_0(\vec{q}, \omega)\, G_0(-\vec{q} + \vec{k}_1 + \vec{k}_2, -\omega + \omega_1 + \omega_2) = U^2 \Pi_{pp}(k_1 + k_2) \quad (2.2)$$

loop is function of total momentum & frequency $k_1 + k_2$

- Evaluation of frequency sums: $T \sum_{i\omega} \frac{1}{i\omega - \varepsilon_1} \frac{1}{i\omega - \varepsilon_2}$

Consider $I_R = \oint \frac{dz}{2\pi i} n_F(z) \frac{1}{(z-\varepsilon_1)(z-\varepsilon_2)} \xrightarrow[R\to\infty]{} 0$

circle of radius R

Fermi function $n_F = \frac{1}{e^{z/T}+1}$ has poles at $z = i\omega_n = i(2n+1)\pi T$ with residue $(-T)$

$$\Rightarrow 0 = I_\infty = \sum_n \mathrm{Res}\left[n_F(z)\frac{1}{(z-\varepsilon_1)(z-\varepsilon_2)}\right] = -T\sum_n \frac{1}{(i\omega_n-\varepsilon_1)(i\omega_n-\varepsilon_2)} + \frac{n_F(\varepsilon_1)}{\varepsilon_1-\varepsilon_2} + \frac{n_F(\varepsilon_2)}{\varepsilon_2-\varepsilon_1}$$

$$\Rightarrow T\sum_{i\omega}\frac{1}{(i\omega-\varepsilon_1)(i\omega-\varepsilon_2)} = \frac{n_F(\varepsilon_1)-n_F(\varepsilon_2)}{\varepsilon_1-\varepsilon_2} \qquad (2.3)$$

3. Pairing mechanisms

3.1. Cooper instability

▷ Consider constant, attractive interaction $V = \frac{U}{\Omega}\sum_{\substack{k_1\dots k_4\\ \sigma\sigma'}} \psi^\dagger_{k_3\sigma}\psi^\dagger_{k_4\sigma'}\psi_{k_2\sigma'}\psi_{k_1\sigma}$

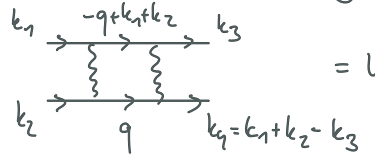
$U<0$ within some energy range around Fermi energy $[\varepsilon_F-\varepsilon_c, \varepsilon_F+\varepsilon_c]$

▷ Leading-order vertex $\Gamma^0_{\alpha\beta\gamma\delta} = -U(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})$

- note that $(\delta_{\alpha\gamma}\delta_{\beta\delta}-\delta_{\alpha\delta}\delta_{\beta\gamma}) = (i\sigma_y)_{\alpha\beta}(i\sigma_y)_{\gamma\delta}$ has the form of a spin singlet: it is odd under exchange of two particles, respectively (i.e. either $\alpha \Leftrightarrow \beta$ or $\gamma \Leftrightarrow \delta$)

▷ Second order: pp and ph diagram

- Calculate pp diagram for special case with total incoming $k_1+k_2=0$

(2.2): 

$$= U^2\frac{T}{\Omega}\sum_{i\omega}\int d^dq\, G_0(\vec q, \omega)\, G_0(-\vec q+\vec k_1+\vec k_2, -\omega+\omega_1+\omega_2) = U^2\Pi_{pp}(k_1+k_2)$$

$$\Pi_{pp}(\omega_1+\omega_2=0, \vec k_1+\vec k_2=0) = \frac{T}{(2\pi)^d}\sum_{i\omega}\int d^dq\, G_0(\vec q,\omega)\, G_0(-\vec q,-\omega)$$

$\Omega = (2\pi)^d$

$$= \frac{T}{(2\pi)^d}\sum_{i\omega}\int d^dq \frac{1}{i\omega-\varepsilon_{\vec q}}\frac{1}{-i\omega-\varepsilon_{-\vec q}}$$

with $\varepsilon_{\vec q} = v_F(|\vec q|-k_F)$

$\varepsilon_{-\vec q} = \varepsilon_{\vec q}$

$$= -\frac{T}{(2\pi)^d}\sum_{i\omega}\int d^dq \;\frac{1}{i\omega-\varepsilon_{\vec q}}\;\frac{1}{i\omega+\varepsilon_{\vec q}}$$

$$\overset{(2.3)}{=} -\frac{1}{(2\pi)^d}\int d^dq \;\frac{n_F(\varepsilon_{\vec q})-n_F(-\varepsilon_{\vec q})}{2\varepsilon_q}$$

$n_F(-\varepsilon) = 1 - n_F(\varepsilon)$

$$= \frac{1}{(2\pi)^d}\int d^dq \;\frac{1-2n_F(\varepsilon_q)}{2\varepsilon_q}$$

$$= \frac{1}{(2\pi)^d}\int d^dq \;\frac{1}{2\varepsilon_q}\tanh\frac{\varepsilon_q}{2T}$$

$$= \frac{1}{2}\int_{-\varepsilon_c}^{\varepsilon_c} du\; \rho(u)\,\frac{1}{u}\tanh\frac{u}{2T} \quad \text{with density of states } \rho(u) = \int\frac{d^dq}{(2\pi)^d}\,\delta(u-\varepsilon_q)$$

$$\approx \frac{\rho_0}{2}\int_{-\varepsilon_c}^{\varepsilon_c} du\;\frac{1}{u}\tanh\frac{u}{2T} \quad \text{with DOS at Fermi level } \rho_0$$

- Limits of integration correspond to energy range, where U can be approximated as attractive constant
- Assume $\varepsilon_c \ll \varepsilon_F$, then in small energy window $[\varepsilon_F-\varepsilon_c, \varepsilon_F+\varepsilon_c]$: $\rho(\varepsilon) \approx \rho(\varepsilon_F) =: \rho_0$

For example in $d=3$

$$\frac{1}{(2\pi)^3}\int d^3q\;\frac{1}{2\varepsilon_q}\tanh\frac{\varepsilon_q}{2T}$$

$$= \frac{4\pi}{(2\pi)^3}\int_{k_F-q_c}^{k_F+q_c} dq\; q^2\,\frac{1}{2v_F(q-k_F)}\tanh\frac{v_F(q-k_F)}{2T}$$

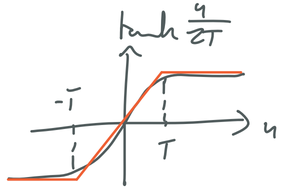
$$= \frac{1}{2\pi^2}\int_{-\varepsilon_c}^{\varepsilon_c}\frac{du}{v_F}\left(\frac{u}{v_F}+k_F\right)^2\frac{1}{2u}\tanh\frac{u}{2T}$$

$$= \frac{1}{4\pi^2 v_F^3}\int_{-\varepsilon_c}^{\varepsilon_c} du\;(u+v_Fk_F)^2\,\frac{\tanh\frac{u}{2T}}{u}$$

$$\overset{\varepsilon_c\ll\varepsilon_F}{\approx} \frac{mk_F}{4\pi^2}\int_{-\varepsilon_c}^{\varepsilon_c} du\;\frac{\tanh\frac{u}{2T}}{u}$$

- To solve integral analytically, approximate

$$\tanh\frac{u}{2T} \approx \begin{cases} -1 & u<-T \\ u/T & -T<u<T \\ 1 & u>T \end{cases}$$



$$\hookrightarrow \Pi_{pp}(0) \approx \frac{\rho_0}{2}\left[\int_{-\varepsilon_c}^{-T} du\,\frac{-1}{u} + \int_{-T}^{T} du\,\frac{u/T}{u} + \int_{T}^{\varepsilon_c} du\,\frac{1}{u}\right]$$

$$= \rho_0 \int_{T}^{\varepsilon_c} du\,\frac{1}{u} + \text{const}$$

$\hookrightarrow$ neglible for small T

$$\approx \rho_0 \ln\frac{\varepsilon_c}{T}$$

numerical estimate gives
$\Pi_{pp}(0) \approx \rho_0 \ln\frac{1.14\varepsilon_c}{T}$

- Π_{ph} is regular for generic frequency- or momentum transfer
  $\rightarrow$ negligible compared to Π_{pp}

▷ Vertex up to second order $\Gamma_{\alpha\beta,\gamma\delta} = -U[1-U\Pi_{pp}(0)](\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})$

▷ At every order in U, number of diagrams increases, but all are small in U^n except the ones which are powers of $U\Pi_{pp}$

So that Γ can be approximated by "particle-particle ladder":

$$\Gamma_{\alpha\beta\gamma\delta} = -U\left[1 - U\Pi_{pp} + (U\Pi_{pp})^2 - (U\Pi_{pp})^3 + \dots\right](\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})$$

$\hookleftarrow$ geometric series

$$= -U\,\frac{1}{1+U\Pi_{pp}(0)}\,(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})$$

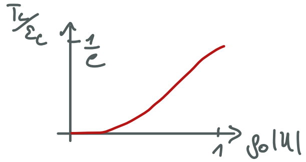
▷ For negative (i.e. attractive) U, Γ has a singularity when $1 + U\Pi_{pp}(0) = 0$

note that it is perfectly regular for repulsive $U>0$

$$\Rightarrow \quad 1 - |U|\rho_0 \ln \frac{\varepsilon_c}{T_c} = 0$$

$$\Rightarrow \quad T_c = \varepsilon_c \, e^{-\frac{1}{\rho_0 |U|}}$$

▷ This means that the Fermi liquid, which we started from, is unstable at temperatures $T \leq T_c$



- No threshold: happens for arbitrarily weak interaction

  but T_c can become arbitrarily small

- Intuitively, effective interaction between two particles with $k_1 + k_2 = 0$ grows infinitely strong so that a bound pair is formed with total spin $S=0$ (due to singlet structure $\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma}$)
- Our description breaks down and we should switch to a description in terms of these pairs
- Note that beyond weak coupling, formation of pairs and condensation can appear at different temperatures $T_{pair} > T_{cond}$ (BCS - BEC crossover)

3.2 BCS idea

▷ Retarded interaction between electrons, mediated by phonons is attractive at energies smaller than Debye frequency

$$V_{eph} \propto \frac{\omega_q^2}{\omega^2 - \omega_q^2}$$

(ω: real frequency, Matsubara: $-\frac{\omega_q^2}{\omega^2 + \omega_q^2}$)

acoustic phonons $\omega_q = c|\vec{q}| \leq \omega_D$

▷ Still needs to overcome Coulomb repulsion

- help: Coulomb repulsion screened at small energies

$$V_c \propto \frac{4\pi e^2}{q^2 + q_{TF}^2}$$

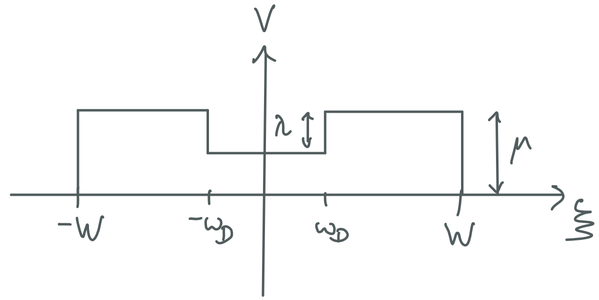
$\Rightarrow V(r) = \frac{e^{-q_{TF} r}}{r}$

↳ if ω_D small enough compared to bandwidth W, Coulomb interaction can be sufficiently reduced

▷ Minimal model by Anderson and Morel

$$H = \sum_{k\sigma} \xi_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{1}{2\Omega} \sum_{kk'} V_{kk'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

$$V_{kk'} = V^{ee}_{kk'} + V^{eph}_{kk'}$$



$$V^{ee}_{kk'} = \mu \quad \text{for} \quad -W \leq \xi_k, \xi_{k'} \leq W$$

$$V^{eph}_{kk'} = -\lambda \quad \text{for} \quad -\omega_D \leq \xi_k, \xi_{k'} \leq \omega_D$$

- Interaction is repulsive overall, but reduced around Fermi energy $\quad \xi_k = \varepsilon_k - \varepsilon_F$
- Mean-field solution gives $\quad T_c = \omega_D \, e^{-\frac{1}{\rho_0(\lambda - \mu^*)}} \qquad \mu^* = \dfrac{\mu}{1 + \mu \rho_0 \ln \frac{W}{\omega_D}}$

  ↳ effect of attraction diminished by "screened" μ^*

  ↳ pairing possible as long as $\lambda > \mu^*$

  ↳ Mean-field gab $\Delta \propto \langle cc \rangle$ changes sign as fuction of energy (frequency) at ω_D to optimize pairing energy
- Similar form obtained by full solution within self-consistent Eliashberg formalism

  ↳ Isotope effect: $\omega_D \propto M_{ion}^{-1/2} \rightarrow T_c \propto M_{ion}^{-1/2}$

3.3 Kohn – Luttinger mechanism

- In strongly correlated electron systems, electron-phonon interaction cannot overcome Coulomb repulsion via retardation effect
  - Electrons considerably slower (E_{kin} small)
  - Coulomb repulsion considerably larger ($U \gtrsim E_{kin}$)

- Consider pair wave-function $\phi(\vec{x},\sigma;\vec{x}',\sigma') = f(|\vec{x}-\vec{x}'|)\,\chi_{\sigma\sigma'}$ with orbital part f and spin part χ
  - for BCS: $f = \text{const}$ and $\chi_{\sigma\sigma'} = (i\sigma_y)_{\sigma\sigma'}$ spin singlet
  - What if f describes higher angular momentum: $f(r) \propto r^{\ell}$ for $r \to 0$?

    ↳ pair wave-function vanishes for electrons at the same place

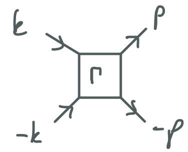
    ↳ if screened Coulomb repulsion is sufficiently short-ranged, it can be avoided with $\ell > 0$

- Can we get this with momentum-dependent interaction?

- Log-singularity in Π_{pp} from states near Fermi surface

  → consider incoming & outgoing particles on Fermi surface

  → interaction is a function of the angle between $\vec{k}$ & $\vec{p}$



$$U(q = |\vec{k}-\vec{p}|) = U(\theta)$$

- Expand $U(\theta)$ into angular momentum harmonics

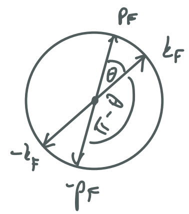
$$U(\theta) = \sum_{\ell} P_\ell(\theta)\, U_\ell$$

$$\int_{-1}^{1} dx\, P_\ell(x) P_{\ell'}(x) = \frac{2}{2\ell+1}\delta_{\ell\ell'}$$

P_ℓ: Legendre polynomials

$$u_\ell = \frac{2\ell+1}{2} \int_{-1}^{1} dx \; u(x) P_\ell(x)$$

- Leading order vertex $\Gamma^0_{\alpha\beta\gamma\delta}(k_1,k_2,k_3,k_4) = -V(k_1-k_3)\,\delta_{\alpha\gamma}\delta_{\beta\delta} + V(k_1-k_4)\,\delta_{\alpha\delta}\delta_{\beta\gamma}$



$$\Rightarrow \quad \Gamma^0_{\alpha\beta\gamma\delta}(\vec{k}_F, -\vec{k}_F, \vec{p}_F, -\vec{p}_F) = -u(|\vec{k}_F - \vec{p}_F|)\,\delta_{\alpha\gamma}\delta_{\beta\delta} + u(|\vec{k}_F + \vec{p}_F|)\,\delta_{\alpha\delta}\delta_{\beta\gamma}$$

$$= -u(\theta)\,\delta_{\alpha\gamma}\delta_{\beta\delta} + u(\pi-\theta)\,\delta_{\alpha\delta}\delta_{\beta\gamma}$$

$$= -\frac{1}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})\,[u(\theta) + u(\pi-\theta)] \quad \leftarrow \text{singlet component}$$

$$-\frac{1}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})\,[u(\theta) - u(\pi-\theta)] \quad \leftarrow \text{triplet component}$$

Legendre polynomials $P_\ell(\cos(\pi-\theta)) = P_\ell(-\cos\theta) = \pm P_\ell(\cos\theta)$ for $\ell \begin{Bmatrix} \text{even} \\ \text{odd} \end{Bmatrix}$

$$\Rightarrow \quad \Gamma^0_s = \frac{1}{2}[u(\theta) + u(\pi-\theta)] = \sum_\ell P_{2\ell}(\theta)\, u_{2\ell} \quad \leftarrow \text{only even } \ell$$

$$\Gamma^0_t = \frac{1}{2}[u(\theta) - u(\pi-\theta)] = \sum_\ell P_{2\ell+1}(\theta)\, u_{2\ell+1} \quad \leftarrow \text{only odd } \ell$$

- Within particle-particle channel, spin structure reproduced at every order

$$\hookrightarrow \quad \Gamma_{\alpha\beta\gamma\delta}(\vec{k}_F, -\vec{k}_F, \vec{p}_F, -\vec{p}_F) = -(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})\,\Gamma_s - (\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})\,\Gamma_t$$

with Γ_s even & Γ_t odd

- In $\Gamma^{(2)}_{pp}(0)$: $\displaystyle\int \frac{d^3q}{(2\pi)^3}\, u(\theta_{kq})\, u(\theta_{qp})\, \underbrace{G(\omega,\vec{q})\,G(-\omega,-\vec{q})}_{\text{function of } \varepsilon_{\vec{q}}\text{, i.e. of } |\vec{q}|}$

↳ angular integral decouples

$$\Gamma^{(2)}_{pp}(0) = \sum_{\ell\ell'} \frac{1}{4\pi} \int d\Omega_q \, P_\ell(\cos\theta_{kq}) P_{\ell'}(\cos\theta_{qp}) \, U_\ell U_{\ell'} \; \Pi^c_{pp}(0)$$

↳ from calculation with const. U

$$= \sum_{\ell\ell'} \frac{\delta_{\ell\ell'}}{2\ell+1} P_\ell(\cos\theta_{kp}) \, U_\ell U_{\ell'} \; \Pi^c_{pp}(0)$$

$$= \sum_\ell U_\ell^2 \, P_\ell(\cos\theta_{kp}) \; \Pi^c_{pp}(0)$$

↳ Project onto $\Gamma^{(2)}_m = \frac{2m+1}{2} \int dx \; P_m(x) \, \Gamma^{(2)}$

$$= U_m^2 \, \Pi^c_{pp}(0)$$

↳ Similarly $\Gamma^{(n)}_m = U_m^n \left(\Pi^c_{pp}\right)^{n-1}$

- Components with different orbital momentum ℓ do not mix

$$\Gamma_\ell = \frac{U_\ell}{1 + U_\ell \Pi^c_{pp}} \qquad \text{with } \Pi^c_{pp} = \rho_0 \ln\frac{\varepsilon_c}{T}$$

- There is a pairing instability if any of U_ℓ is attractive even if bare, constant interaction $U_{\ell=0}$ is (strongly) repulsive

▷ Kohn - Luttinger: renormalized Coulomb interaction has a long-range oscillatory tail due to sharp Fermi edge: "Friedel oscillations"

- This has attractive component

- Compute vertex in pp-channel using "bare" interaction from ph-channel:

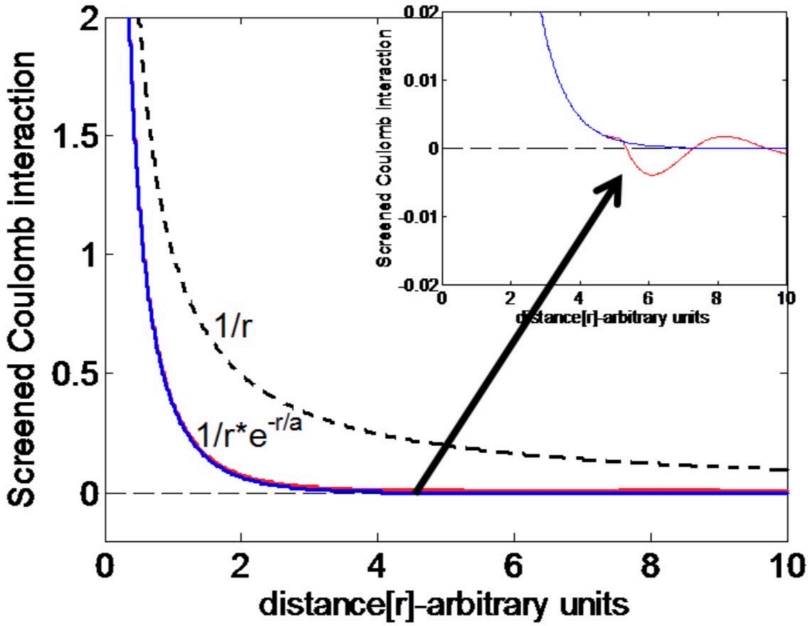
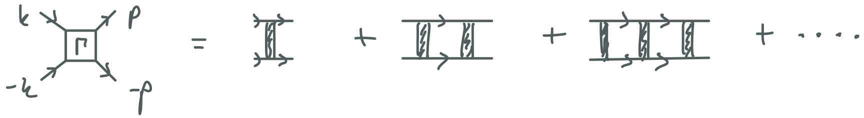
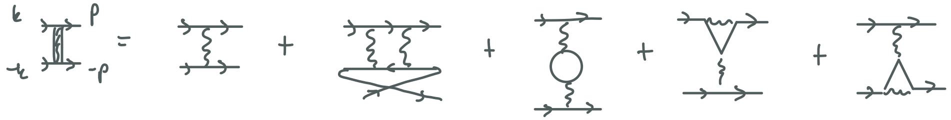


FIGURE 5. The screened coulomb potential as a function of r. $\frac{1}{r}$ (dashed line) is the bare coulomb potential. $\frac{1}{r}e^{-r/a}$ (blue line) is the Yukawa potential which includes regular screening and dies of exponentially (a is some characteristic screening length). The fully screened potential (red line) includes the contribution from the $2k_F$ scattering which gives rise to Friedel oscillations at large r. These oscillations are responsible for the attraction in large angular momentum channels. The inset is a zoomed in version, which shows the oscillations.

Maiti, Chubukov, AIP Conf. Proc. 1550, 3 (2013)



$- (p \leftrightarrow -p)$



- Static particle-hole bubble is non-analytic at $q = 2k_F$

in 3D: $\Pi_{ph}(q, \omega=0) = \frac{m k_F}{2\pi^2}\left(\frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|\right) \qquad x = \frac{q}{2k_F}$

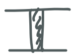
calculated for free fermions with spherical Fermi surface

$\propto (1-x)\ln|1-x| \quad \text{for } x \to 1$

approximate for $q = \vec{k}_F \pm \vec{p}_F$ and $\theta \approx \pi$: $\Pi_{ph}(\theta) \approx -\frac{m k_F}{16\pi^2}(1+\cos\theta)\ln(1+\cos\theta)$

$q = k_F\sqrt{2 - 2\cos(\varphi_k - \varphi_p)}$
$= 2k_F\left|\sin\frac{\theta_{kp}}{2}\right|$
$\Rightarrow x = \left|\sin\frac{\theta}{2}\right| = \sqrt{1-\cos^2\frac{\theta}{2}}$
$1 - x = 1 - \sqrt{1-\cos^2\frac{\theta}{2}}$
$\approx 1 - \left(1 - \frac{1}{2}\cos^2\frac{\theta}{2}\right) \quad \theta \approx \pi$
$\approx \frac{1}{2}(1+\cos\theta)$

- To second order in interaction

 $\Big|_{\ell, q\approx 2k_F} = U_\ell^0 + \left[2U^2(\pi) - 2U(0)U(\pi) \mp U^2(0)\right] S_\ell$

ℓ even (singlet)
ℓ odd (triplet)

with $S_\ell = -\int \frac{d\Omega_q}{4\pi}\,\Pi_{ph}(\theta) P_\ell(\cos\theta) \approx \frac{m k_F}{8\pi^2}\frac{(-1)^\ell}{\ell^4}$

↳ U_ℓ can be attractive (is always attractive for ℓ large & odd, for ℓ even: $U(0)/U(\pi)$ needs to be large enough)

- Naming: $\ell = 0$ "s-wave", $\ell = 1$ "p-wave", $\ell = 2$ "d-wave" pairing etc. according to orbitals
- Critical temperature very small $T_c \sim T_F\, e^{-(2\ell)^4}$ with $\ell > 0$

▷ Main important principles from Kohn-Luttinger mechanism

1. Pairing with higher angular momentum can circumvent (strong) Coulomb repulsion
2. Fluctuations in particle-hole channel (renormalization due to Π_{ph}) can yield attractive pairing components for higher angular momentum

3.4 Generalized BCS mean-field theory

▷ Consider extended form of attractive pairing interaction

$$H = \sum_{ks} \xi_k c^\dagger_{ks} c_{ks} + \frac{1}{2} \sum_{kk'} \sum_{s_1..s_4} V_{s_1..s_4}(k,k')\, c^\dagger_{ks_1} c^\dagger_{-ks_2} c_{-k's_3} c_{k's_4}$$

$$V_{s_1..s_4}(k,k') = \langle -ks_1, ks_2 | V | -k's_3, k's_4 \rangle$$

due to fermionic anticommutation : $V_{s_1s_2s_3s_4}(k,k') = -V_{s_2s_1s_3s_4}(-k,k') = -V_{s_1s_2s_4s_3}(k,-k') = V_{s_2s_1s_4s_3}(-k,-k')$

$V_{s_1..s_4}(k,k')$ attractive in energy range $-\varepsilon_c < \xi_k, \xi_{k'} < \varepsilon_c$

▷ Mean-field decoupling: $c^\dagger_{ks_1} c^\dagger_{-ks_2} c_{-k's_3} c_{k's_4}$

$$= \left[\left(c^\dagger_{ks_1} c^\dagger_{-ks_2} - \langle c^\dagger_{ks_1} c^\dagger_{-ks_2}\rangle\right) + \langle c^\dagger_{ks_1} c^\dagger_{-ks_2}\rangle\right]\left[\left(c_{-k's_3} c_{k's_4} - \langle c_{-k's_3} c_{k's_4}\rangle\right) + \langle c_{-k's_3} c_{k's_4}\rangle\right]$$

$$= \left(c^\dagger_{ks_1} c^\dagger_{-ks_2} - \langle c^\dagger_{ks_1} c^\dagger_{-ks_2}\rangle\right)\left(c_{-k's_3} c_{k's_4} - \langle c_{-k's_3} c_{k's_4}\rangle\right)$$ ← fluctuations around mean value squared ↳ small

$$+ \left(c^\dagger_{ks_1} c^\dagger_{-ks_2} - \langle c^\dagger_{ks_1} c^\dagger_{-ks_2}\rangle\right)\langle c_{-k's_3} c_{k's_4}\rangle + \langle c^\dagger_{ks_1} c^\dagger_{-ks_2}\rangle\left(c_{-k's_3} c_{k's_4} - \langle c_{-k's_3} c_{k's_4}\rangle\right)$$

$$+ \langle c^\dagger_{ks_1} c^\dagger_{-ks_2}\rangle\langle c_{-k's_3} c_{k's_4}\rangle$$

$$\approx c^\dagger_{ks_1} c^\dagger_{-ks_2}\langle c_{-k's_3} c_{k's_4}\rangle + \langle c^\dagger_{ks_1} c^\dagger_{-ks_2}\rangle c_{-k's_3} c_{k's_4} - \underbrace{\langle c^\dagger_{ks_1} c^\dagger_{-ks_2}\rangle\langle c_{-k's_3} c_{k's_4}\rangle}_{\hookrightarrow \text{ const.}}$$

$$V^*_{s_1..s_4}(k,k') = \langle -k's_4, k's_3 | V | -ks_2\, ks_1\rangle = V_{s_4...s_1}(k',k)$$

$$\hookrightarrow H \approx \sum_{ks} \xi_k c^\dagger_{ks} c_{ks} + \frac{1}{2}\sum_{kk'}\sum_{s_1..s_4} V_{s_1..s_4}(k,k')\left[c^\dagger_{ks_1} c^\dagger_{-ks_2}\langle c_{-k's_3} c_{k's_4}\rangle + \langle c^\dagger_{ks_1} c^\dagger_{-ks_2}\rangle c_{-k's_3} c_{k's_4}\right]$$
$$+ \text{ const. } + \text{ small}$$

$$= \sum_{ks} \xi_k c^\dagger_{ks} c_{ks} + \frac{1}{2}\sum_{ks_1s_2}\left[\Delta_{s_1s_2}(k)\, c^\dagger_{ks_1} c^\dagger_{-ks_2} + \Delta^*_{s_2s_1}(k)\, c_{-ks_1} c_{ks_2}\right] + \text{const} + \text{small} \qquad (3.1)$$

with $\Delta_{ss'}(k) = \sum_{k'} \sum_{\sigma\sigma'} V_{ss'\sigma\sigma'}(k,k') \langle c_{-k'\sigma} c_{k'\sigma'} \rangle$

↳ self-consistent equation due to $\langle \dots \rangle$

▷ The gap $\Delta_{ss'}(k)$ depends on momentum and spin !

- Viewed as a matrix in spin space

$$\Delta(k) = \begin{pmatrix} \Delta_{\uparrow\uparrow}(k) & \Delta_{\uparrow\downarrow}(k) \\ \Delta_{\downarrow\uparrow}(k) & \Delta_{\downarrow\downarrow}(k) \end{pmatrix}$$

▷ The gap function is antisymmetric under exchange of fermions

$$\Delta_{ss'}(k) = -\sum_{k'\sigma\sigma'} V_{ss'\sigma\sigma'}(k,k') \langle c_{k'\sigma'} c_{-k'\sigma} \rangle = -\sum_{k'\sigma\sigma'} V_{s's\sigma'\sigma}(-k,-k') \langle c_{k'\sigma'} c_{-k'\sigma} \rangle = -\Delta_{s's}(-k)$$

or as a matrix $\hat{\Delta}(k) = -\hat{\Delta}^T(-k)$

▷ Two options : spin singlet : odd under $s \leftrightarrow s'$, even under $k \leftrightarrow -k$

spin triplet : even under $s \leftrightarrow s'$, odd under $k \leftrightarrow -k$

commonly used convenient parameterization

$$\hat{\Delta}(k) = \underbrace{\Psi(k)\, i\sigma_y}_{\text{singlet}} + \underbrace{(\vec{d}(k)\cdot\vec{\sigma})\, i\sigma_y}_{\text{triplet}} = \begin{pmatrix} 0 & \Psi(k) \\ -\Psi(k) & 0 \end{pmatrix} + \begin{pmatrix} -d_x(k) + i d_y(k) & d_z(k) \\ d_z(k) & d_x(k) + i d_y(k) \end{pmatrix}$$

with $\Psi(-k) = \Psi(k)$ & $\vec{d}(-k) = -\vec{d}(k)$

▷ Self-consistent gap equation and Bogoliubov quasiparticles

- To diagonalize mean-field Hamiltonian (Eq. (3.1)), rewrite in terms of Nambu spinor: $\mathcal{C}_k = (c_{k\uparrow}, c_{k\downarrow}, c^+_{-k\uparrow}, c^+_{-k\downarrow})^T$

$$H = \sum_k \mathcal{C}_k^+ h_k \mathcal{C}_k \quad \text{with} \quad h_k = \frac{1}{2}\begin{pmatrix} \xi_k \mathbb{1} & \hat{\Delta}_k \\ \hat{\Delta}_k^+ & -\xi_{-k}\mathbb{1} \end{pmatrix} \quad \& \text{ use } \xi_{-k} = \xi_k$$

- h_k is diagonalized by unitary transformation (Bogoliubov transformation)

$$U_k = \begin{pmatrix} u_k & v_k \\ v_{-k}^* & u_{-k}^* \end{pmatrix} \quad \text{so that} \quad H = \sum_k \mathcal{C}_k^+ U_k U_k^+ h_k U_k \underbrace{U_k^+ \mathcal{C}_k}_{\psi_k} = \sum_k \psi_k^+ \mathcal{E}_k \psi_k$$

Matrix of eigenvalues $\mathcal{E}_k = \begin{pmatrix} E_k & & & \\ & E_k & & \\ & & -E_k & \\ & & & -E_k \end{pmatrix}$ with $E_k = \sqrt{\xi_k^2 + |\Delta_k|^2}$, $|\Delta_k|^2 = \mathrm{Tr}(\hat{\Delta}_k^+ \hat{\Delta}_k)$

and U_k contains eigenvectors $u_k = \dfrac{E_k + \xi_k}{\sqrt{2E_k(E_k+\xi_k)}}\mathbb{1}$, $v_k = \dfrac{-\hat{\Delta}_k}{\sqrt{2E_k(E_k+\xi_k)}}$

- Rewrite gap equation with quasiparticle operators $\psi_k = U_k^+ \mathcal{C}_k$ $\Rightarrow \mathcal{C}_k = \begin{pmatrix} c_{ks} \\ c^+_{-ks} \end{pmatrix} = U_k \psi_k = U_k^{ss'}\begin{pmatrix} \psi_{ks'} \\ \psi^+_{-ks'} \end{pmatrix} = \begin{pmatrix} u_{k\,ss'}\psi_{ks'} + v_{k\,ss'}\psi^+_{-ks'} \\ v^*_{-k\,ss'}\psi_{ks'} + u^*_{-k\,ss'}\psi^+_{-ks'} \end{pmatrix}$

$$\Delta_{ss'}(k) = \sum_{k'}\sum_{\sigma\sigma'} V_{ss'\sigma\sigma'}(k,k')\langle c_{-k'\sigma} c_{k'\sigma'}\rangle$$

$$\sum_{tt'} (u_{-k'\sigma t}\psi_{-k't} + v_{-k'\sigma t}\psi^+_{k't})(u_{k'\sigma' t'}\psi_{k't'} + v_{k'\sigma' t'}\psi^+_{-k't'})$$

$$= \sum_{k'}\sum_{\sigma\sigma'} V_{ss'\sigma\sigma'}(k,k')\sum_t \Big[\underbrace{u_{-k'\sigma t}v_{k'\sigma' t}}_{-\frac{1}{2E_{k'}}\delta_{\sigma t}\hat{\Delta}_{k'\sigma' t}}\underbrace{\langle\psi_{-k't}\psi^+_{-k't}\rangle}_{1-n_F(E_{k'})} + \underbrace{v_{-k'\sigma t}u_{k'\sigma' t}}_{-\frac{1}{2E_{k'}}\delta_{\sigma' t}\hat{\Delta}_{-k'\sigma t}}\underbrace{\langle\psi^+_{k't}\psi_{k't}\rangle}_{n_F(E_{k'})}\Big] \quad \leftarrow \text{only diagonal } \langle\ \rangle \neq 0$$

$$= \sum_{k'}\sum_{\sigma\sigma'} V_{ss'\sigma\sigma'}(k,k')\frac{1}{2E_{k'}}\Delta_{\sigma'\sigma}(k)\big(-1+2n_F(E_{k'})\big)$$

$$= -\sum_{k'}\sum_{\sigma\sigma'} V_{ss'\sigma\sigma'}(k,k')\frac{1}{2E_{k'}}\Delta_{\sigma'\sigma}(k)\tanh\frac{E_{k'}}{2T} \qquad (3.2)$$

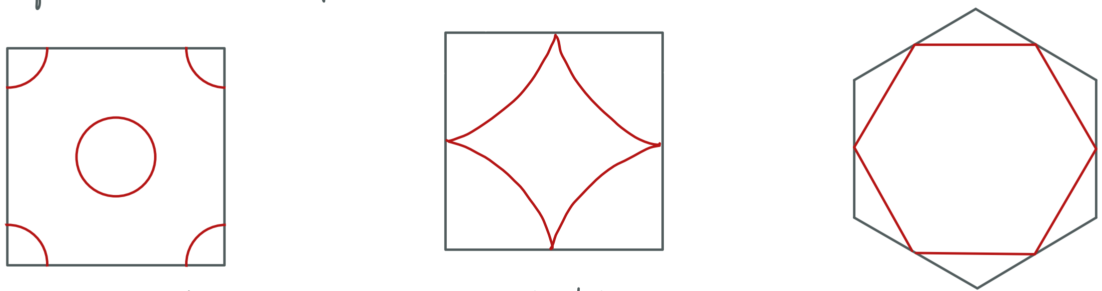
4. Superconductivity in 2D lattice materials

4.1 Symmetry considerations

▷ Consider systems with inversion & SU(2) spin symmetry
↳ pairing instability for pairs with k and -k in spin singlet or triplet channel

▷ Real materials are lattice systems
↳ symmetry is not isotropic but discrete
↳ Fermi surface not necessarily a circle (2D) or a sphere (3D) as considered in previous Sec.

Example Fermi surfaces

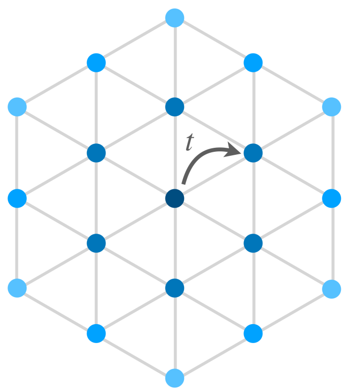


iron-pnictides   cuprates   graphene / twisted TMDs

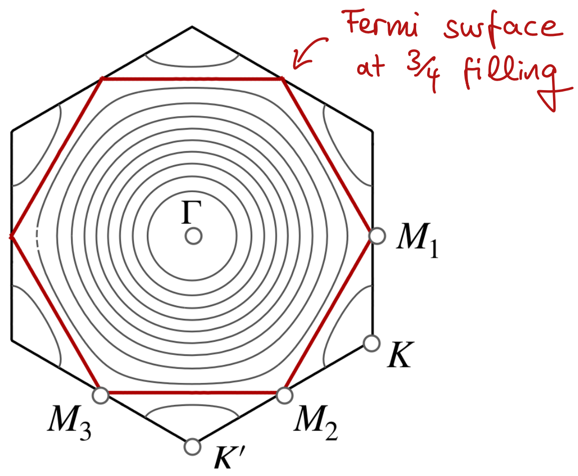
↳ In expansion into eigenfunctions of isotropic system, different angular components do not decouple (not all are independent eigenfunctions of Hamiltonian)

▷ "Partial" decoupling according to symmetries of lattice
↳ determined by irreducible representations of lattice symmetry group

▷ Example: triangular lattice



real space



Brillouin zone

- lattice symmetry group is C_{6v}: it is invariant under 12 operations:

  1 identity (E)

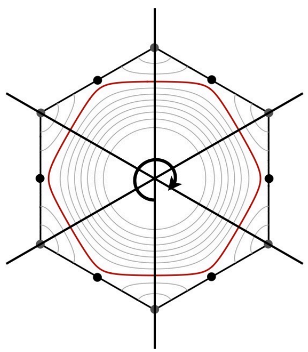
  2 rotations by $\frac{2\pi}{6}$ $(2C_6)$

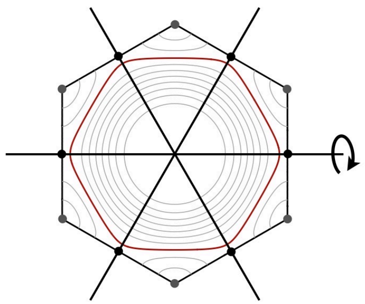
  2 rotations by $\frac{2\pi}{3}$ $(2C_3)$

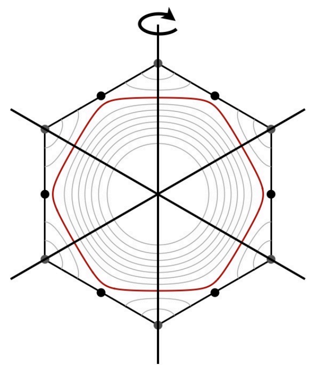
  1 rotation by π (C_2)

  3 vertical mirrors (σ_v)

  3 diagonal mirrors (σ_d)







- irreducible representations classify behavior under these operations

  see figure on next page for examples of each irrep in C_{6v}

  e.g. A_1 is invariant under all rotations and reflections (s-wave)

  A_2 is invariant under rotations, but odd under reflections (i-wave)

  B_1 & B_2 are odd under C_6, C_2 and one of the reflections (f-wave)

  E_1 & E_2 are two-dimensional, i.e. they contain two independent eigenfunctions, which transform into each other under rotations (p- & d-wave)

  E_1 is odd & E_2 is even under inversion (C_2)

▷ Pairing solutions are eigenfuctions of symmetry group and decouple between different representation

- Within the same representation, infinite set of functions remains coupled

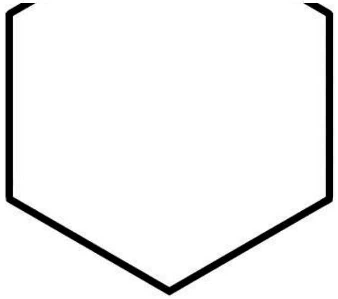
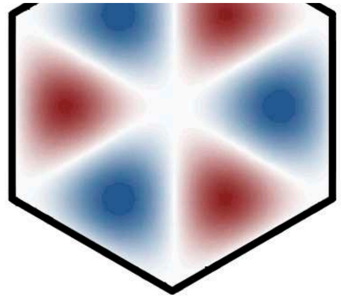
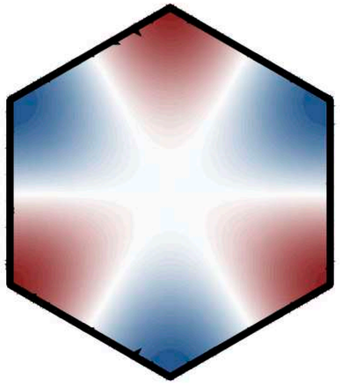
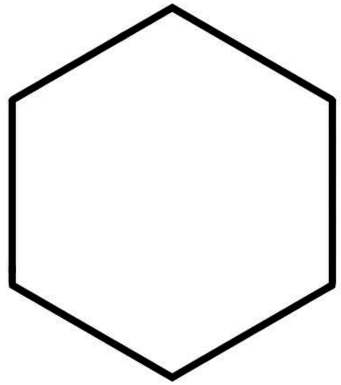
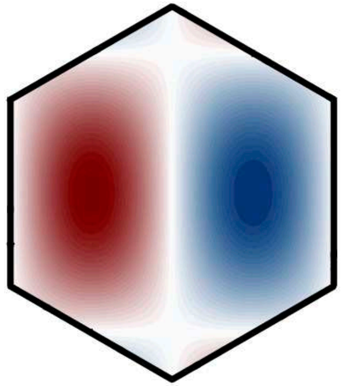
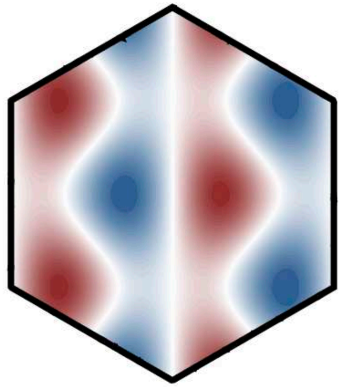
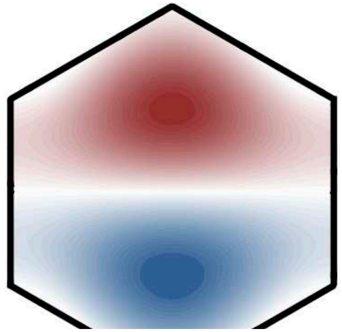
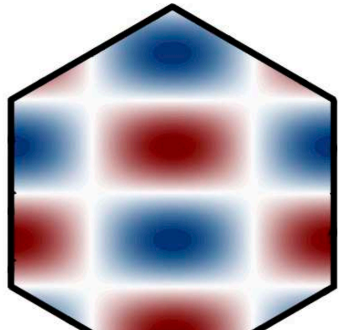
  (e.g. in A_1: $\underset{l=0}{1}$, $\underset{l=6}{\cos(6\theta)}$, $\underset{l=12}{\cos(12\theta)}$ ...)

- Instability due to Kohn-Luttinger mechanism as in isotropic system not guaranteed because components with large l mix with components with small l and small-l components can be stronger + repulsive

- Kohn-Luttinger-like pairing instability still possible if bare, repulsive interaction is small in some pairing channel

  ↳ e.g. if only on-site repulsion U considered: bare repulsion in A_1 channel

  bare interaction is zero in other channels

B_1	$x(x^2 - 3y^2)$		
B_2	$y(y^2 - 3x^2)$		
E_1	x		
	y		

4.2 Superconductivity in 2D hexagonal systems

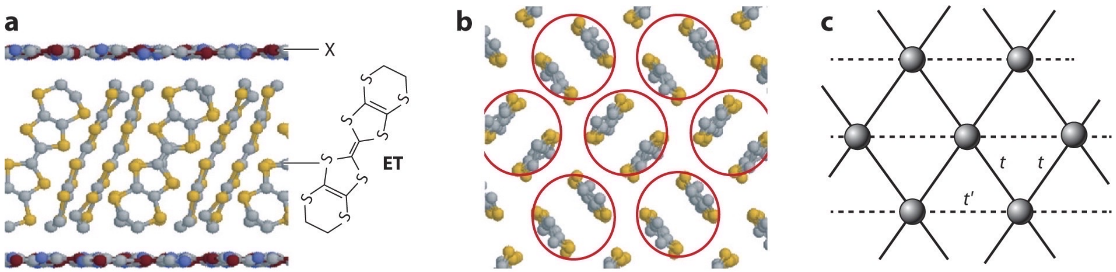
4.2.1 Examples

▷ Triangular, honeycomb or Kagome lattice
(Same Bravais lattice, different number of sites in unit cell)

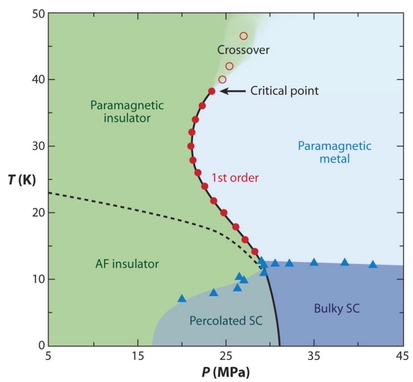
▷ Focus here on triangular lattice (some results generalizable to other examples)

▷ (Superconducting) systems described by triangular lattice

- Organic superconductors κ-$(ET)_2Cu_2(CN)_3$ ET: bis(ethylene-dithio)tetrathiafulvalene

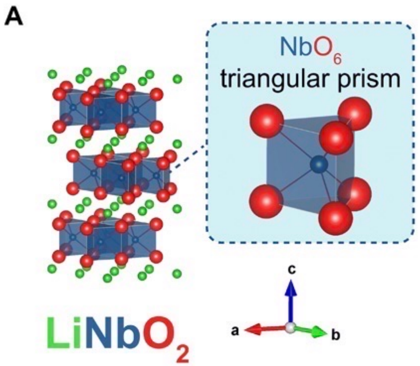


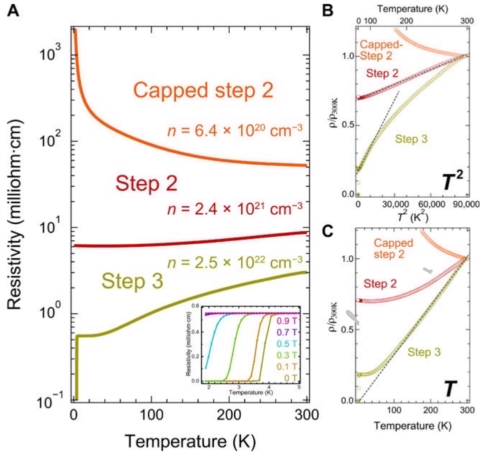
Kanoda K, Kato R. 2011.
Annu. Rev. Condens. Matter Phys. 2:167–88



Kanoda K, Kato R. 2011.
Annu. Rev. Condens. Matter Phys. 2:167–88

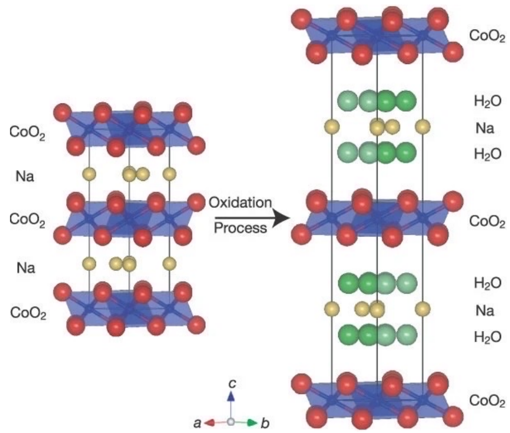
– Layered transition metal oxide $Li_x NbO_2$

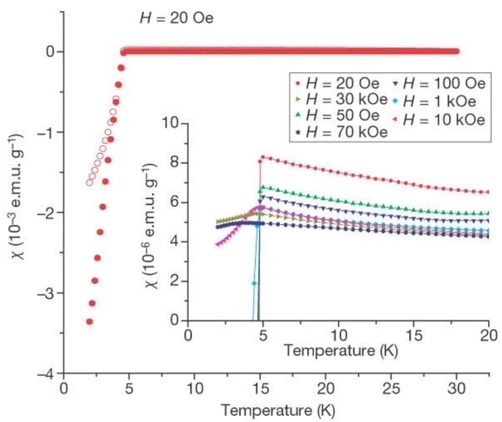




→ T. Soma et al
Sci. Adv. 6 (2020)

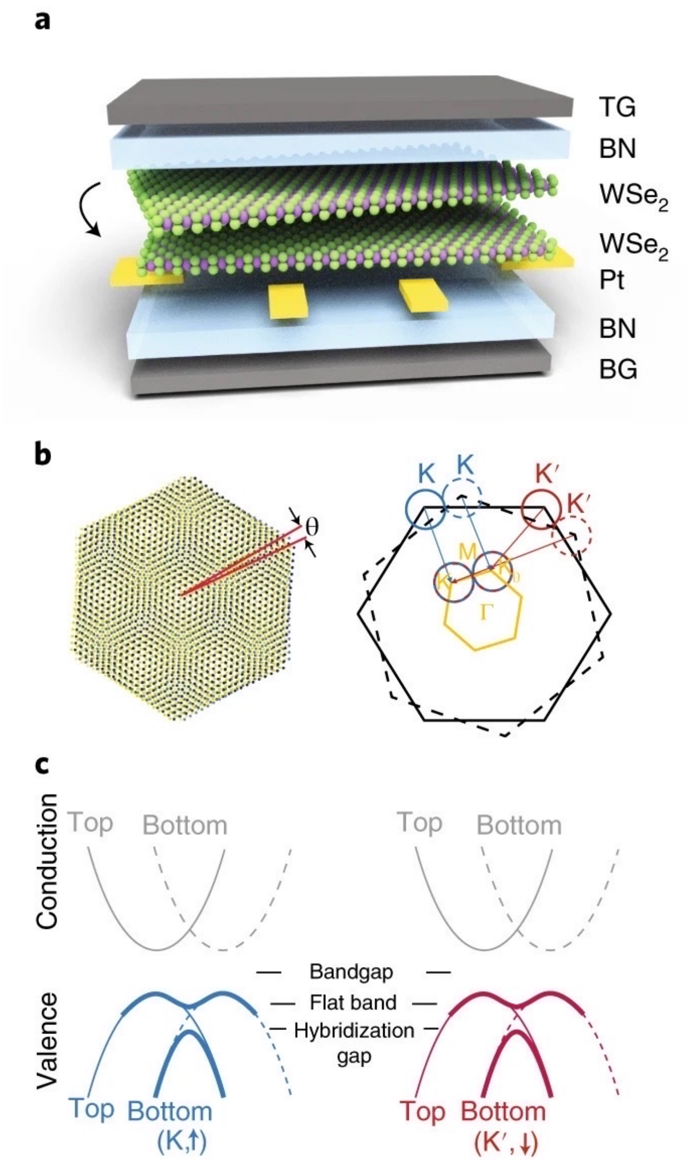
– (Intercalated) sodium cobaltides $Na_x CoO_2$

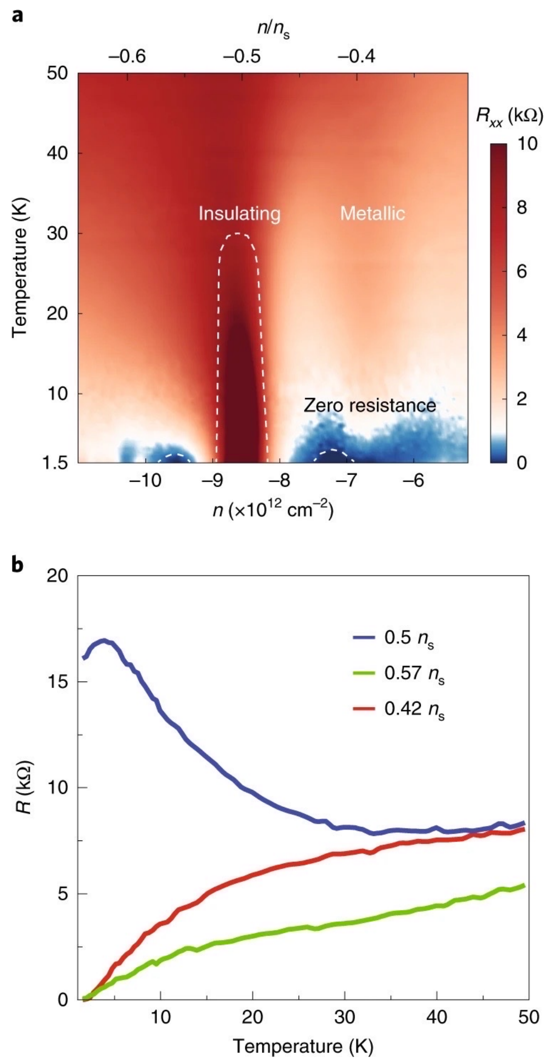




→ Takada et al
Nature 422, 53 (2003)

- Effective models for moiré transition metal dichalcogenides





→ Wang et al
Nat. mat. 19, 861 (2020)
(twisted tWSe$_2$)

- Different systems, important details & extensive literature
  - Appearance of superconductivity and pairing mechanisms not necessarily settled
  - Discuss minimal model and information we can get from electronic, Kohn–Luttinger-type pairing mechanism

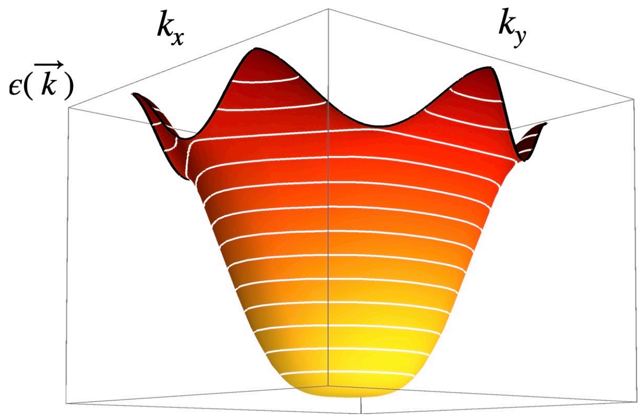
4.2.2 Triangular lattice at van Hove filling

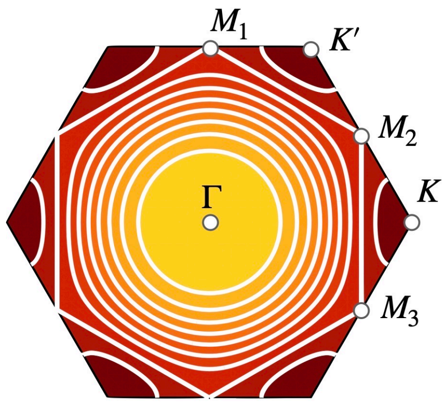
- Free Hamiltonian

$$H_0 = -t \sum_{\langle ij \rangle} \sum_{\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + h.c. \right) - \mu \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma}$$

$$= \sum_{k,\sigma} \xi_k c^\dagger_{k\sigma} c_{k\sigma} \qquad \text{with} \qquad \xi_k = \varepsilon_k - \mu \,, \quad \varepsilon_k = -t \sum_b e^{ibk} = -2t\left(\cos k_x + 2\cos\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}\right)$$

$\hookrightarrow$ 6 n.n. vectors





▷ Interesting point of dispersion $\varepsilon_k = 2t$

- Density of states $\rho(\varepsilon) = \int \frac{d^2k}{A_{BZ}} \delta(\varepsilon - \xi_k)$ has Van Hove singularity
- Fermi level at Van Hove energy for $3/4$ filling (or $1/4$ for holes) $\rightarrow$ set $\mu = 2t$
  - ↪ e.g. achievable via gating in moiré TMDs
- Due to saddle points in ε_k at M_i-points

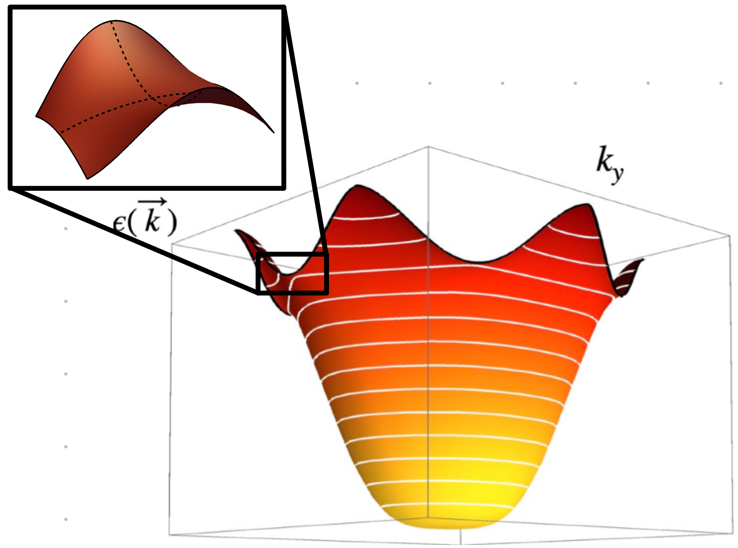
$$\xi_{M_1+k}(\mu=2t) = \varepsilon_{M_1+k} - 2t \approx \underbrace{\frac{t}{2}\left(k_x^2 - 3k_y^2\right)}_{=:\,\varepsilon_1(k)} + O(k^3)$$

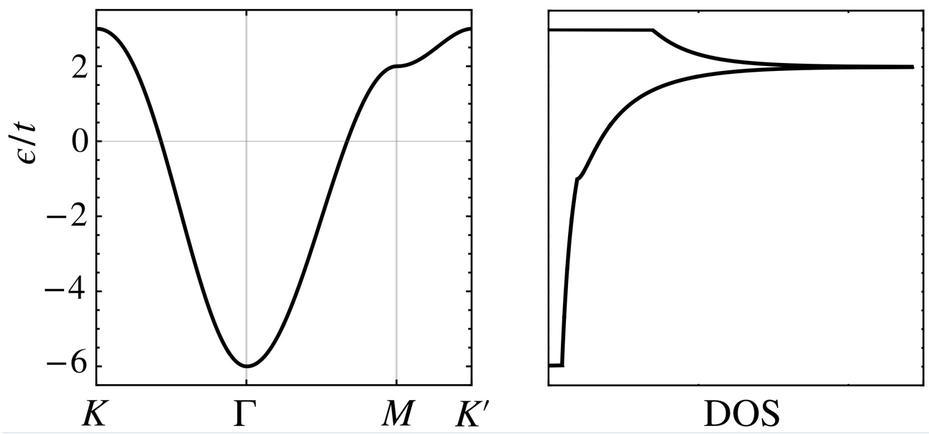
$$\xi_{M_{2,3}+k} \approx \underbrace{-t\left(k_x^2 \mp \sqrt{3}\, k_x k_y\right)}_{=:\,\varepsilon_{2,3}(k)} + O(k^3)$$

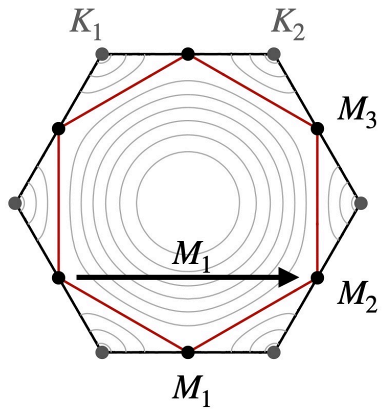
- At this filling, Fermi surface is nested.

$$\varepsilon(k + M_i) \approx -\varepsilon(k)$$

↪ similarities to cuprates







▷ High density of states boosts interaction effects

- Dimensionless interaction is $\bar{u} = \rho \cdot U$ "DOS × interaction" ⇒ if ρ increases, $\bar{u}$ increases

  $\bar{u}$ is exactly the quantity that appears in 'effective' vertex:

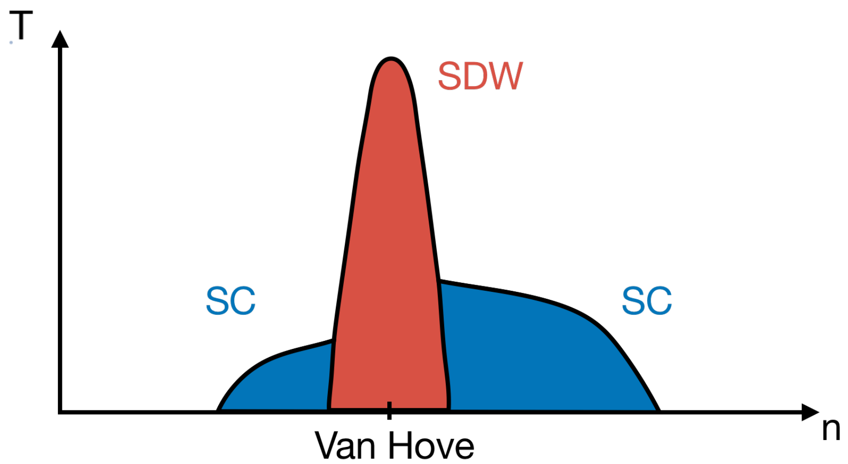
  see e.g. effective pairing vertex in Sec. 3.1 for 3D isotropic system:

  $$\Gamma(k,-k,p,-p) = \frac{U}{1+U\Pi_{pp}(0)} = \frac{U}{1+U\rho_0 \ln\frac{\varepsilon_c}{T}}$$

  also true for other channels

- Expect instability towards ordered states

  ↳ schematic phase diagram that was discussed



▷ Consider vicinity of Van Hove filling, i.e. set $\mu \approx 2t$

▷ Particle-particle diagram (Eq. 2.2) has stronger singularity: "Cooper + Van Hove"

$$\Pi_{pp}(0) = T\sum_{i\omega} \int \frac{d^2q}{A_{BZ}} \frac{1}{i\omega - \xi_q} \frac{1}{-i\omega - \xi_{-q}}$$

$$= \frac{1}{A_{BZ}} \int d^2q \, \frac{1}{2\xi_q} \tanh \frac{\xi_q}{2T} \qquad \text{(see Sec 3.1)}$$

- Calculate contribution from regions around Van Hove points M_i

$$\Pi_{pp}(0) \approx 3 \cdot \frac{1}{(2\pi)^2} \int d^2q \, \frac{1}{\varepsilon_1(q)} \tanh \frac{\varepsilon_1(q)}{2T}$$

3 pairs of patches

↪ restrict to circle of radius $\sqrt{\varepsilon_c}$ around M-point

rescale coordinates

$x = \sqrt{t/2}\, k_x \quad y = \sqrt{3t/2}\, k_y$

hyperbolic coordinates

$\xi = k^2 \cos 2\varphi \quad \eta = k^2 \sin 2\varphi \quad \xi^2 + \eta^2 = k^4 \leq \varepsilon_c^2$

$$= \frac{2\sqrt{3}}{t} \frac{1}{(2\pi)^2} \int dx \int dy \, \frac{1}{x^2 - y^2} \tanh \frac{x^2 - y^2}{2T}$$

$$= \frac{2\sqrt{3}}{t} \frac{1}{(2\pi)^2} \int d\xi \int_0^{\sqrt{\varepsilon_c^2 - \xi^2}} d\eta \, \frac{1}{2\sqrt{\xi^2 + \eta^2}} \frac{1}{\xi} \tanh \frac{\xi}{2T}$$

$$= \frac{\sqrt{3}}{2t} \frac{1}{(2\pi)^2} \int_{-\varepsilon_c}^{\varepsilon_c} d\xi \, \ln \frac{\varepsilon_c + \sqrt{\varepsilon_c^2 - \xi^2}}{\varepsilon_c - \sqrt{\varepsilon_c^2 - \xi^2}} \frac{1}{\xi} \tanh \frac{\xi}{2T}$$

$$\approx \frac{\sqrt{3}}{2t} \frac{1}{(2\pi)^2} \int d\xi \, \frac{\ln \left(\frac{\varepsilon_c}{\xi}\right)^2}{\xi} \tanh \frac{\xi}{2T}$$

approximate tanh as in Sec. 3.1

$$\approx \frac{\sqrt{3}}{2t} \frac{1}{(2\pi)^2} \int_T^{\varepsilon_c} d\xi \, \frac{2 \ln \frac{\varepsilon_c}{\xi}}{\xi} + \mathcal{O}(\ln \xi, 1)$$

$$= \frac{\sqrt{3}}{8\pi^2 t} \ln^2 \frac{\varepsilon_c}{T} =: \rho_0 \ln^2 \frac{\varepsilon_c}{T}$$

↪ double-logarithmic singularity

- Vertex in pp channel $\Gamma \propto \frac{U}{1 + U\Pi_{pp}(0)}$ has singularity at $T_c = \varepsilon_c \, e^{-\frac{1}{\sqrt{|U| g_0}}}$

  for attractive $U<0$

  ↪ T_c increased due to double-log

4.2.3 Patch model and Kohn-Luttinger mechanism

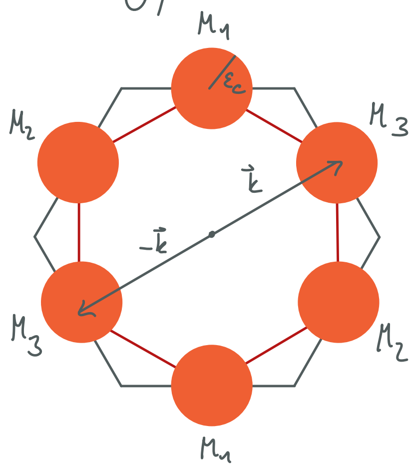
▷ Consider simple model to work out pairing mechanism analytically

- Fermi surface regions with largest density of states contribute most strongly

  ↪ they lead, the rest follows

  ↪ Consider only these regions: 6 patches

  ↪ $M_i = -M_i (+ \Gamma)$ → only 3 inequivalent patches
  ↪ reciprocal lattice vector

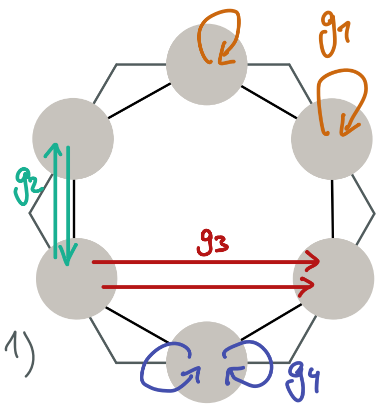


  ↪ Introduce fermion operators for states in patches
  $c^{(+)}_{p\sigma}(k) = c^{(+)}_{\sigma}(M_p + k)$

  ↪ Free Hamiltonian: $H_0 = \sum_{k,p,\sigma} \varepsilon_p(k) \, c^{+}_{p\sigma}(k) \, c_{p\sigma}$ $\quad k \leq \varepsilon_c$

- Symmetry-allowed intra- and interpocket interactions:

$$V = \sum_{k_1 \dots k_4} \sum_{\sigma\sigma'} \delta(k_1 + k_2 - k_3 - k_4) \Big[g_1 \sum_{p \neq p'} c^{+}_{p\sigma}(k_4) c^{+}_{p'\sigma'}(k_3) c_{p'\sigma'}(k_2) c_{p\sigma}(k_1)$$
$$+ g_2 \sum_{p \neq p'} c^{+}_{p\sigma}(k_4) \, c^{+}_{p'\sigma'}(k_3) \, c_{p\sigma'}(k_2) \, c_{p'\sigma}(k_1)$$
$$+ \tfrac{1}{2} g_3 \sum_{p \neq p'} c^{+}_{p\sigma}(k_4) c^{+}_{p\sigma'}(k_3) \, c_{p'\sigma'}(k_2) \, c_{p'\sigma}(k_1)$$
$$+ \tfrac{1}{2} g_4 \sum_{p} c^{+}_{p\sigma}(k_4) \, c^{+}_{p\sigma'}(k_3) \, c_{p\sigma'}(k_2) \, c_{p\sigma}(k_1) \Big] \qquad (4.1)$$



▷ Interested in effective pairing vertex $\Gamma(k_F, -k_F, p_F, -p_F)$

- Focus on singlet pairing: pair wave function even under $\vec{k} \Leftrightarrow -\vec{k}$, i.e. the same in opposite patches (Pairs with momentum $\vec{k}$ & $-\vec{k}$ connect opposite patches)
- Introduce intra- & inter-patch vertices $\Gamma_{pp'}$

↳ because of lattice symmetry and singlet pairing:

$$\Gamma_{pp'} = \Gamma_{p'p}$$

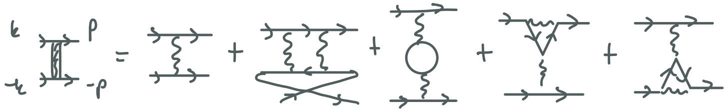
$$\Gamma_{11} = \Gamma_{22} = \Gamma_{33} =: \Gamma_u$$

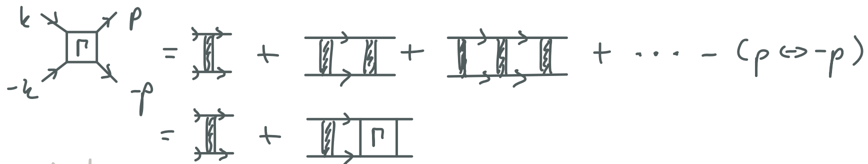
$$\Gamma_{12} = \Gamma_{13} = \Gamma_{23} =: \Gamma_v$$

▷ Reminder Kohn-Luttinger idea (Sec. 3.2):

(1) Calculate corrections due to particle-hole scattering

(2) Use result in particle-particle ladder

(1) 

(2) 

reminder:

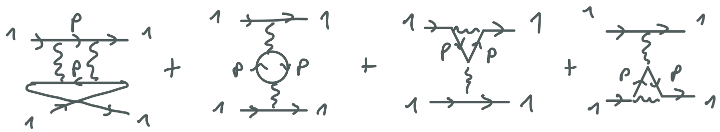
$\Gamma_{\alpha\beta\gamma\delta}(k_1 .. k_4) = -V(k_1-k_3)\delta_{\alpha\gamma}\delta_{\beta\delta} + V(k_1-k_4)\delta_{\alpha\delta}\delta_{\beta\gamma}$

$\rightarrow -V(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})$ for const. ia & spin-singlet

(1) To first order in interaction

$$\Gamma_u^0 = -g_4 \qquad \Gamma_v^0 = -g_3$$

- Second order in ph-channel

↳ diagrams for $\Gamma_u^{0,ph}$ 

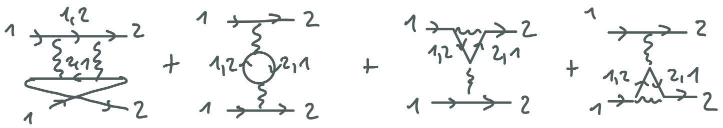
w.l.o.g. Γ_{11}

$$(\underbrace{g_4^2}_{p=1} + \underbrace{2g_2^2}_{p=2,3} \quad -2g_4^2 - 4g_1^2 \quad + g_4^2 + 2g_1g_2 \quad + g_4^2 + 2g_1g_2)\,\Pi_{ph}(0)$$

$k_1 = k_3$ (intrapatch Γ_{11})

↳ diagrams for $\Gamma_v^{0,ph}$

w.l.o.g. Γ_{12}



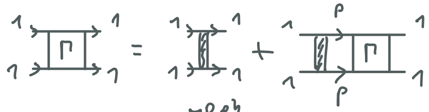
$$\left(2g_1g_3 \quad -4g_2g_3 \quad +g_1g_3+g_2g_3 \quad +g_1g_3+g_2g_3 \right) \Pi_{ph}(M)$$

↳ $k_1 = k_3 \pm M_i$ (interpatch Γ_v)

$$\Rightarrow \quad \Gamma_u^{0,ph} = -g_4 - \left(g_4^2 + 2g_2^2 - 4g_1^2 + 4g_1g_2 \right) \Pi_{ph}(0)$$

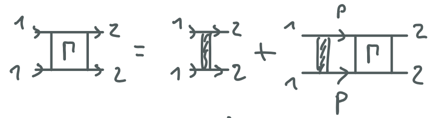
$$\Gamma_v^{0,ph} = -g_3 - \left(4g_1g_3 - 2g_2g_3 \right) \Pi_{ph}(M)$$

(2) Diagrams for Γ_u



$$\Gamma_u = \Gamma_u^{0,ph} + \Pi_{pp}(0) \left(\underbrace{\Gamma_u^{0,ph}\Gamma_u}_{p=1} + \underbrace{2\Gamma_v^{0,ph}\Gamma_v}_{p=2,3} \right)$$

Diagrams for Γ_v



$$\Gamma_v = \Gamma_v^{0,ph} + \Pi_{pp}(0) \left(\underbrace{\Gamma_u^{0,ph}\Gamma_v}_{p=1} + \underbrace{\Gamma_v^{0,ph}\Gamma_u}_{p=2} + \underbrace{\Gamma_v^{0,ph}\Gamma_v}_{p=3} \right)$$

$$\Rightarrow \quad \Gamma_u = \frac{1}{3}\left(\frac{\Gamma_u^{0,ph} + 2\Gamma_v^{0,ph}}{1-(\Gamma_u^{0,ph}+2\Gamma_v^{0,ph})\Pi_{pp}(0)} + 2\,\frac{\Gamma_u^{0,ph} - \Gamma_v^{0,ph}}{1-(\Gamma_u^{0,ph}-\Gamma_v^{0,ph})\Pi_{pp}(0)} \right)$$

$$\Gamma_v = \frac{1}{3}\left(\frac{\Gamma_u^{0,ph} + 2\Gamma_v^{0,ph}}{1-(\Gamma_u^{0,ph}+2\Gamma_v^{0,ph})\Pi_{pp}(0)} - \frac{\Gamma_u^{0,ph} - \Gamma_v^{0,ph}}{1-(\Gamma_u^{0,ph}-\Gamma_v^{0,ph})\Pi_{pp}(0)} \right)$$

$$\Rightarrow \quad \Gamma_u + 2\Gamma_v = \frac{\Gamma_u^{0,ph} + 2\Gamma_v^{0,ph}}{1-(\Gamma_u^{0,ph}+2\Gamma_v^{0,ph})\Pi_{pp}(0)}$$

is of the form $\quad \Gamma_A = \dfrac{\Gamma_A^0}{1-\Gamma_A^0\Pi_{pp}}$

$$\Gamma_u - \Gamma_v = \frac{\Gamma_u^{0,ph} - \Gamma_v^{0,ph}}{1 - (\Gamma_u^{0,ph} - \Gamma_v^{0,ph})\Pi_{pp}(0)} \qquad \Gamma_E = \frac{\Gamma_E^0}{1 - \Gamma_E^0 \Pi_{pp}}$$

▷ To get pairing, either $\Gamma_A^0 = \Gamma_u^{0,ph} + 2\Gamma_v^{0,ph} > 0$ or $\Gamma_E^0 = \Gamma_u^{0,ph} - \Gamma_v^{0,ph} > 0$

- To leading order in interaction:

$\Gamma_A^0 = -(g_4 + 2g_3)$ $\qquad$ $\Gamma_E^0 = -g_4 + g_3$

↪ "no chance" $\qquad$ ↪ "maybe"

↪ Estimate: if we started with onsite Coulomb repulsion $\frac{U}{2}\sum_{i\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma} c_{i\sigma'}^\dagger c_{i\sigma'}$

$g_4 = g_3 = U > 0$

so that $\Gamma_A^0 < 0$ and $\Gamma_E^0 = 0$ $\longrightarrow$ no pairing

- With Kohn-Luttinger corrections

$$\begin{aligned}
\Gamma_A^0 = \Gamma_u^{0,ph} + 2\Gamma_v^{0,ph} &= -(g_4 + 2g_3) - (g_4^2 + 2g_2^2 - 4g_1^2 + 4g_1g_2)\Pi_{ph}(0) - 2(4g_1g_3 - 2g_2g_3)\Pi_{ph}(M) \\
&= -3U - U^2\left[3\Pi_{ph}(0) + 4\Pi_{ph}(M)\right] \\
&< 0
\end{aligned}$$

$$\begin{aligned}
\Gamma_E^0 = \Gamma_u^{0,ph} - \Gamma_v^{0,ph} &= -g_4 + g_3 + (4g_1g_3 - 2g_2g_3)\Pi_{ph}(M) - (g_4^2 + 2g_2^2 - 4g_1^2 + 4g_1g_2)\Pi_{ph}(0) \\
&= 0 + U^2\left[2\Pi_{ph}(M) - 3\Pi_{ph}(0)\right] \\
&> 0 \quad \text{if} \quad \Pi_{ph}(M) > \tfrac{3}{2}\Pi_{ph}(0)
\end{aligned}$$

↪ pairing possible

note: bare interaction in "E-channel" being zero for onsite U makes it easier

↳ Is $\Pi_{ph}(M) > \frac{3}{2}\Pi_{ph}(0)$?

Yes! Due to nesting $\Pi_{ph}(M) \propto \ln^2 \frac{\varepsilon_c}{T}$ but $\Pi_{ph}(0) \propto \ln \frac{\varepsilon_c}{T}$

so that at small enough T, $\Pi_{ph}(M) \gg \Pi_{ph}(0)$

▷ Which pairing symmetry does this instability correspond to? → alternative next page

- Set up mean-field model for this instability:

↳ Pairing Hamiltonian (processes with fermion pairs with $\vec{k}, -\vec{k}$ & $\vec{q}, -\vec{q}$) with effective interaction for singlet pairing given by Γ_u and Γ_v

$$V_{pair} = \sum_{k,q}\left[\sum_{p=1}^{3} \Gamma_u\, c^\dagger_{p\uparrow}(k)\, c^\dagger_{p\downarrow}(-k)\, c_{p\downarrow}(-q)\, c_{p\uparrow}(q) + \sum_{\substack{p,p',\\ p\neq p'}} \Gamma_v\, c^\dagger_{p\uparrow}(k)\, c^\dagger_{p\downarrow}(-k)\, c_{p'\downarrow}(-q)\, c_{p'\uparrow}(q)\right]$$

↳ Kohn-Luttinger analysis: $\frac{\Gamma_u + 2\Gamma_v}{\Gamma_u - \Gamma_v} \ll 1 \Rightarrow \Gamma_v \approx -\frac{\Gamma_u}{2}$

$$\Rightarrow V_{pair} \approx \Gamma_u \left(b_1^\dagger, b_2^\dagger, b_3^\dagger\right) \underbrace{\begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix}}_{X} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \qquad \text{where} \quad b_p = \sum_q c_{p\downarrow}(-q)\, c_{p\uparrow}(q)$$

$$= \frac{3}{2}\Gamma_u \left[\left(\frac{b_2^\dagger - b_3^\dagger}{\sqrt{2}}, \frac{2b_1^\dagger - b_2^\dagger - b_3^\dagger}{\sqrt{6}}, 0 \right) \begin{pmatrix} 1 & & \\ & 1 & \\ & & 0 \end{pmatrix} \begin{pmatrix} \frac{b_2 - b_3}{\sqrt{2}} \\ \frac{2b_1 - b_2 - b_3}{\sqrt{6}} \\ 0 \end{pmatrix} \right.$$

eigenvalues of X are $\left(\frac{3}{2}, \frac{3}{2}, 0\right)$ and eigenvectors
$\frac{1}{\sqrt{2}}(0,1,-1)$
$\frac{1}{\sqrt{6}}(2,-1,-1)$
$\frac{1}{\sqrt{3}}(1,1,1)$

- Only two independent mean fields necessary $\quad \Delta_{xy} = \frac{1}{2}\langle b_2 - b_3 \rangle$

These two are degenerate $\quad \Delta_{x^2-y^2} = \frac{1}{6}\langle 2b_1 - b_2 - b_3 \rangle$

$$V_{pair} \approx \frac{3}{2}\Gamma_u \Big[\Delta^*_{xy} \sum_k \left(c_{2\downarrow}(-k)\, c_{2\uparrow}(k) - c_{3\downarrow}(-k)\, c_{3\uparrow}(k) \right) + \Delta_{xy} \sum_k \left(c^\dagger_{2\uparrow}(k)\, c^\dagger_{2\downarrow}(-k) - c^\dagger_{3\uparrow}(k)\, c^\dagger_{3\downarrow}(-k) \right)$$

$$+ \Delta^*_{x^2-y^2} \sum_k \left(2c_{1\downarrow}(-k)\, c_{1\uparrow}(k) - c_{2\downarrow}(-k)\, c_{2\uparrow}(k) - c_{3\downarrow}(-k)\, c_{3\uparrow}(k) \right) + \Delta_{x^2-y^2} \sum_k \left(2c^\dagger_{1\uparrow}(k)\, c^\dagger_{1\downarrow}(-k) - c^\dagger_{2\uparrow}(k)\, c^\dagger_{2\downarrow}(-k) - c^\dagger_{3\uparrow}(k)\, c^\dagger_{3\downarrow}(-k) \right) \Big]$$

▷ Which pairing symmetry does this instability correspond to?

- Mean-field gap equation: $\Delta_{ss'}(k) = -\int_{k'} \sum_{\sigma\sigma'} V_{ss'\sigma\sigma'}(k,k') \frac{\Delta_{\sigma'\sigma}(k')}{2E_{k'}} \tanh \frac{E_{k'}}{2T}$ (Eq. 3.2)

↪ Independent of spin (we considered singlet pairing)

↪ In patch model: $\int_{BZ} d^2k \to \sum_p \int_{\varepsilon<\varepsilon_c} d^2k$ and $V(k,k') = \begin{cases} \Gamma_u & k,k' \text{ at same patch } p \\ \Gamma_v & k,k' \text{ at different patches } p,p' \end{cases}$

$E(k) \to \sqrt{\varepsilon_p(k) + |\Delta_p|^2}$ (assume gap constant within each patch)

- Kohn-Luttinger analysis: $\frac{\Gamma_u + 2\Gamma_v}{\Gamma_u - \Gamma_v} \ll 1 \Rightarrow \Gamma_v \approx -\frac{\Gamma_u}{2}$

- Gap equation becomes:
$$\Delta_p = -\sum_{p'} \int \frac{d^2k}{(2\pi)^2} V_{pp'} \frac{\Delta_{p'}}{2E_{p'}(k)} \tanh \frac{E_{p'}(k)}{2T}$$
$$= -\int \frac{d^2k}{(2\pi)^2} \Gamma_u \left[\frac{\Delta_p}{2E_p(k)} \tanh \frac{E_p(k)}{2T} - \frac{1}{2} \sum_{p\neq p'} \frac{\Delta_{p'}}{2E_{p'}(k)} \tanh \frac{E_{p'}(k)}{2T} \right]$$

Sec. 3.4 and 4.2.2: $\int \frac{d^2k}{(2\pi)^2} \frac{1}{2E_k} \tanh \frac{E_k}{2T} \xrightarrow[T\to T_c]{} \int \frac{d^2k}{(2\pi)^2} \frac{1}{2\varepsilon_p(k)} \tanh \frac{\varepsilon_p(k)}{2T} = \rho_0 \ln^2 \frac{\varepsilon_c}{T_c}$ for $T \to T_c$, $\Delta \to 0$

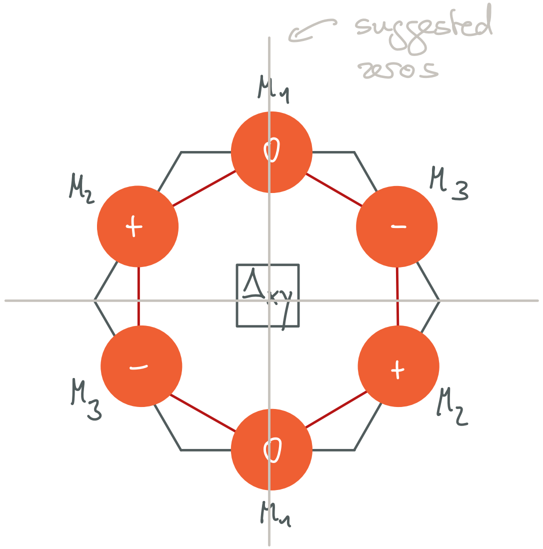
↪ same for all patches

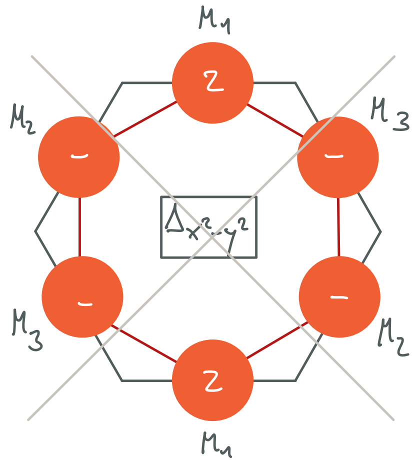
$$\Rightarrow \begin{pmatrix} \Delta_1 \\ \Delta_2 \\ \Delta_3 \end{pmatrix} = -\frac{1}{3} \Pi_{pp}(0,T_c) \Gamma_u \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} \Delta_1 \\ \Delta_2 \\ \Delta_3 \end{pmatrix}$$

- This eigenvalue equation has one solution with eigenvalue 0 → no pairing and two degenerate pairing solutions with eigenvalue $\frac{3}{6} \Pi_{pp} |\Gamma_u|$ and eigenvectors

$$\vec{\Delta}_{xy} = \begin{pmatrix} \Delta_1 \\ \Delta_2 \\ \Delta_3 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, \quad \Delta_{x^2-y^2} = \begin{pmatrix} \Delta_1 \\ \Delta_2 \\ \Delta_3 \end{pmatrix} = \frac{1}{\sqrt{6}} \begin{pmatrix} 2 \\ -1 \\ -1 \end{pmatrix}$$

- Suggested sign structure of pairing:



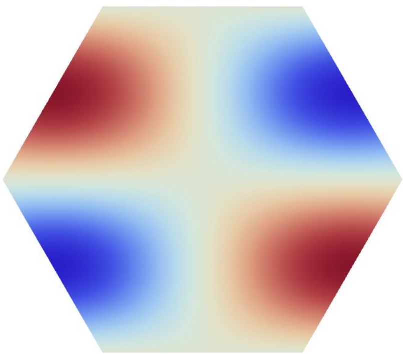


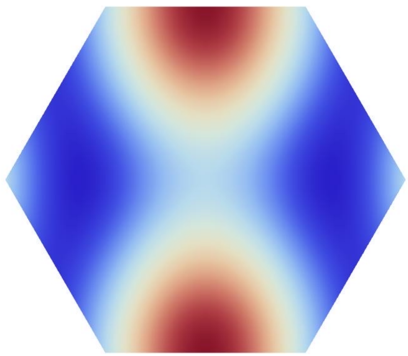
↳ discrete version of d-wave lattice harmonics ($\ell = 2$)

patches are blind to higher ℓ

$d_{xy} = 2\sqrt{3} \sin\frac{k_x}{2} \sin\frac{\sqrt{3} k_y}{2}$

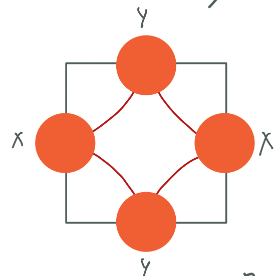
$d_{x^2-y^2} = 2\left(\cos k_x - \cos\frac{k_x}{2} \cos\frac{\sqrt{3} k_y}{2}\right)$





↳ Belong to 2D E_2 representation
(i.e. they must be degenerate due to symmetry)

- ▷ Kohn-Luttinger analysis:
  - Pairing possible with increased T_c due to Van Hove singularity
  - Electronic pairing mechanism from particle-hole corrections with momentum transfer M_p, (approximate) nesting important for inducing attraction
  - Two degenerate pairing solutions with symmetry of E_2 representation (d-wave)



- ▷ Completely analogous analysis for graphene at $3/8$ or $5/8$ filling & cuprates
  - Same Van Hove singularity in DOS & $\ln^2$-behavior in $\Pi_{pp}(0)$
  - Same effective patch model with couplings $g_1, \dots, g_4$ (Eq(4.1)), but 2 instead of 3 patches for cuprates
    ↳ other multiplicities in some Kohn-Luttinger diagrams: $\Gamma_u^{0,ph} = -g-[g_4^2+(N-1)g_2^2-2(N-1)g_1(g_1-g_2)]\Pi_{ph}(0)$
    $\Gamma_v^{0,ph} = -g_3-(4g_1g_3-2g_2g_3)\Pi_{ph}(M)$
    $N=3$: graphene, triangular lattice
    $N=2$: cuprates
  - Same pairing symmetry in graphene (d_{xy} & $d_{x^2-y^2}$), only non-degenerate $d_{x^2-y^2}$ in cuprates (→ different lattice symmetry group C_{4v})

5. Phenomenological theory

5.1. Landau free energy

- ▷ Landau: form of free energy dictated by symmetries
- ▷ Restrict here to uniform case: no spatial variations, no magnetic field
- ▷ Symmetries of order parameter for conventional superconductivity
  - $\Delta \sim \sum_k \langle c_{k\uparrow} c_{-k\downarrow} \rangle$ is a complex order parameter
  - Time-reversal : $\Delta \to \Delta^*$
    U(1) phase : $\Delta \to e^{i\phi}\Delta$

▷ Free energy must be invariant under symmetry transformations

→ It is a function of $|\Delta|^2 = \Delta^* \Delta$

- Most general form up to quartic order $\quad \mathcal{F} = a(T)\,|\Delta|^2 + b(T)\,|\Delta|^4$

- Parameters $a(T)$, $b(T)$ temperature dependent

↳ can be calculated from microscopic theory by integrating out fermions after Hubbard-Stratonovich transformation with pairing field

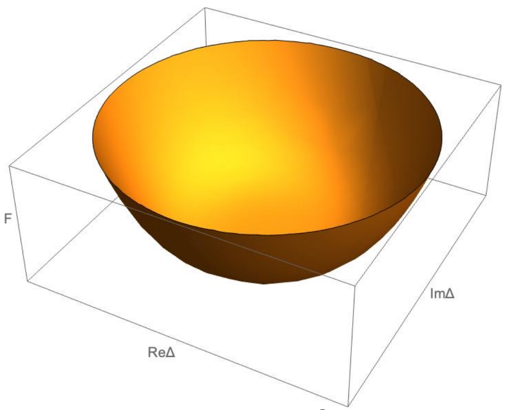
$a =$

$b =$

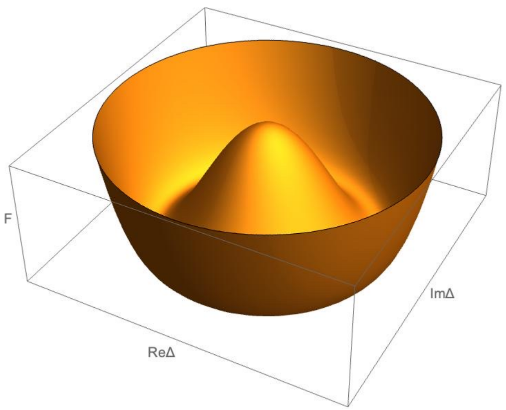
↳ can be fixed phenomenologically via experimental quantities e.g. specific heat $C = -T\frac{d^2S}{dT^2}$

↳ $a(T) \approx a'(T - T_c)$, $a' > 0$

$b(T) \approx b(T_c) = b > 0$



$T > T_c$, $a > 0$



$T < T_c$, $a < 0$

- Ground state determined by minimum of F

↳ For $T > T_c$: $|\Delta|_{min} = 0$

↳ For $T < T_c$ $|\Delta|_{min} = \sqrt{-\frac{a(T)}{2b}}$

▹ Generalisation for unconventional order parameters

- Gap $\Delta(k) = \psi(k)\, i\sigma_y + \vec{d}(k)\cdot\vec{\sigma}\, i\sigma_y$ depends on k

  ↪ need to include more symmetry operations

  e.g. rotation $\Delta(k) \to g\,\Delta(k) = \Delta(R_g \vec{k})$ R_g: rotation matrix

  ↪ Can be classified according to irreducible representations of lattice symmetry group (see Sec. 4.1):

  Gap equation is eigenvalue equation: $\psi(k) = \int_{k'} V_s(k,k') \dfrac{\psi(k')}{\omega^2 + \xi_{k'}^2 + |\psi(k')|^2}$

  or $\vec{d}(k) = \int_{k'} V_t(k,k') \dfrac{\vec{d}(k')}{\omega^2 + \xi_{k'}^2 + |\vec{d}(k')|^2}$

  ↪ $\int_k = T \sum_\omega \int \frac{d^d k}{A_{BZ}}$

  Largest (most negative) eigenvalue yields largest T_c

  Eigenfunctions correspond to different irreducible representations whose dimensionality is given by degeneracy of eigenvalue (e.g. Sec. 4.2.3)

- Pick gap with largest T_c and write as sum over eigenfunctions

  $\psi(k) = \sum_m \eta_m \psi_m(\vec{k})$ or $\vec{d}(k) = \sum_m \eta_m \vec{d}_m(k)$

  $\psi_m, \vec{d}_m$: eigenfunctions = basis functions of irreducible representation

  ↪ e.g. in Sec. 4.2.3: $\psi(k) = \eta_1 d_{xy}(\vec{k}) + \eta_2 d_{x^2-y^2}(\vec{k})$

- Use η_m as order parameters in free energy

  ↪ They transform as coordinates under lattice symmetry transformations and as $\eta \to \eta^*$ & $\eta \to e^{i\phi}\eta$ under time-reversal & $U(1)$

↳ Landau free energy: $F = a(T) \sum_m |\eta_m|^2 + \sum_{m_1 \cdots m_4} b_{m_1 \cdots m_4} \eta^*_{m_1} \eta^*_{m_2} \eta_{m_3} \eta_{m_4}$

with $a(T) = a'(T - T_c)$ and $b_{m_1 \cdots m_4}$ satisfy special conditions so that the second term is invariant under time-reversal and lattice-symmetry operations

- Minimum depends on $b_{m_1 \cdots m_4}$ and determines which linear combination $\psi(k) = \sum_m \eta_m \psi_m(k)$ (or analogously for $\vec{d}(k)$) forms the ground state
- Additional symmetries can be spontaneously broken depending on linear combination

5.2 Topological (chiral) superconductivity

▷ Result of Sec. 4.2.3: Electronic mechanism for superconductivity of triangular lattice at Van Hove filling yields two degenerate, spin-singlet pairing solutions that belong to 2D irreducible representation E_2

$$\psi(k) = \eta_1 d_{xy}(k) + \eta_2 d_{x^2-y^2}(k)$$

Which linear combination is formed in ground state?

▷ Free energy is invariant under

- Time-reversal $\eta_i \to \eta_i^*$
- U(1) phase $\eta_i \to e^{i\phi} \eta_i$
- Rotations R and mirrors M of C_{6v} $\begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} \to R \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}$, $\begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} \to M \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}$

▷ Landau free energy has the form

$$F(\eta_1,\eta_2) = a\left(|\eta_1|^2+|\eta_2|^2\right) + b_1\left(|\eta_1|^2+|\eta_2|^2\right)^2 + b_2\left|\eta_1^2+\eta_2^2\right|^2$$

with $a = a'(T-T_c)$, $b_1 > 0$

▷ Minimum depends on sign of b_2 $(T<T_c)$:

- If $b_2 > 0$: $\eta_2 = \pm i\eta_1$ and $|\eta_1|^2 = \frac{|a|}{2b_1} =: \eta^2$

$$\Rightarrow \psi(k) = \eta\,(d_{xy} \pm i d_{x^2-y^2})$$

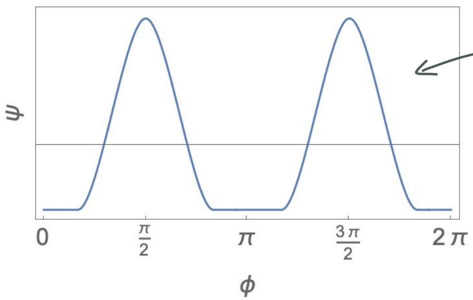
- If $b_2 < 0$: $\eta_1 = \eta\cos\theta$, $\eta_2 = \eta\sin\theta$
  - ↳ direction θ not fixed by quartic terms
  - ↳ sixth order term $F_\theta^{(6)} = \gamma\left[(\eta_1 - i\eta_2)^3(\eta_1^* - i\eta_2^*)^3 + c.c.\right] = 2\gamma|\eta|^6\cos 6\theta$

    note that this is only invariant under discrete rotations (contrary to terms up to 4th order)

    $\theta = n\frac{\pi}{3}$ if $\gamma < 0$ or $\theta = (n+\frac{1}{2})\frac{\pi}{3}$ for $\gamma > 0$

▷ State with $\psi(k) = \eta\left[\cos\theta\, d_{xy}(k) + \sin\theta\, d_{x^2-y^2}(k)\right]$ is a nematic superconductor

- Specific θ spontaneously chosen → breaks rotational symmetry
- Gap posseses nodes on Fermi surface
- E.g. $\theta = 0$:

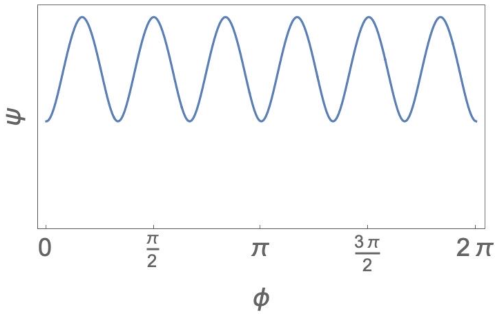


has 2-fold instead of 6-fold symmetry

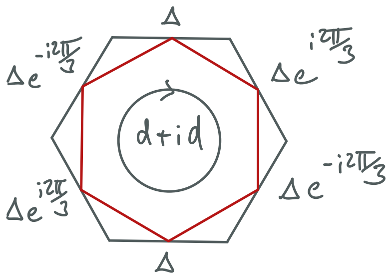
→ angle along FS

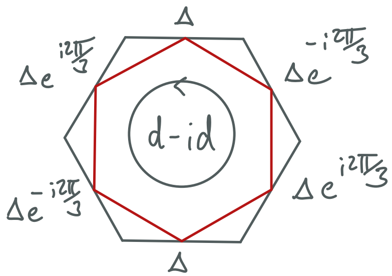
▷ State with $\psi(k) = \eta\left[d_{xy}(k) \pm i\, d_{x^2-y^2}(k)\right]$ is a chiral superconductor ($d \pm id$)

- Complex combination $\pm$ spontaneously chosen $\rightarrow$ breaks time-reversal symmetry
- Full gap on Fermi surface:



- Phase $\operatorname{Arg}\psi = \arctan \frac{\operatorname{Im}\psi}{\operatorname{Re}\psi}$ winds twice along Fermi surface





▷ Microscopic calculations often yield $b_2 > 0$ $\Rightarrow$ chiral superconductivity

- Intuitive argument: fully gapped state has larger condensation energy
  $\rightarrow$ energetically beneficial

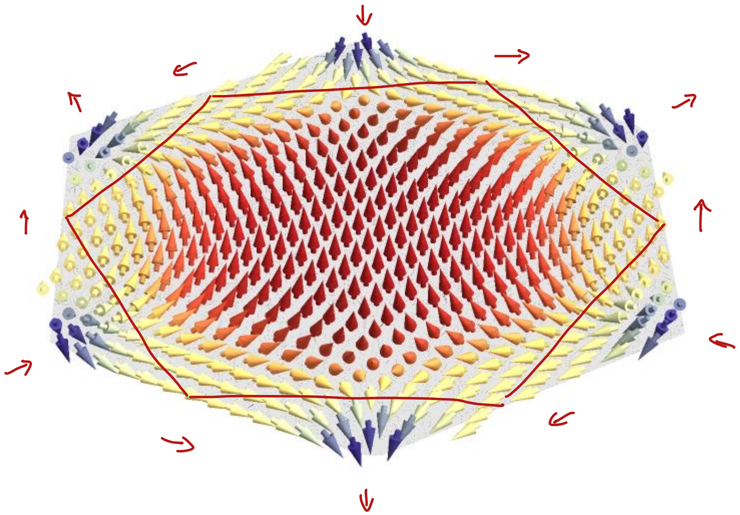
▷ Chiral superconductor is a (strong) topological superconductor

- Classify by integer invariant (→ winding number)
- Can be defined via "Skyrmion" number

$$C = \frac{1}{4\pi} \int_{BZ} d^2k \; \vec{m} \cdot \left(\frac{\partial \vec{m}}{\partial k_x} \times \frac{\partial \vec{m}}{\partial k_y} \right)$$

with pseudo-spin $\vec{m} = \frac{1}{\sqrt{\xi_k^2 + |\psi(k)|^2}} \begin{pmatrix} \mathrm{Re}\,\psi(k) \\ \mathrm{Im}\,\psi(k) \\ \xi_k \end{pmatrix}$

↪ $\vec{m}$ follows phase winding along Fermi surface



← Calculated with lattice harmonics

$d_{xy}(k) = 2\sqrt{3} \sin\frac{k_x}{2} \sin\frac{\sqrt{3}k_y}{2}$

$d_{x^2-y^2}(k) = 2\left(\cos k_x - \cos\frac{k_x}{2} \cos\frac{\sqrt{3}k_y}{2}\right)$

- For $d \pm id$ state : $C = \pm 2$

- Chern number also determines spin and thermal Hall response

$$\sigma^s_{xy} = C\,\frac{\hbar}{8\pi}$$

$$\varkappa = C\,\frac{\pi k_B^2}{6\hbar}$$

- Chern number determines number of chiral edge states
  - Chiral superconductor has fully gapped bulk, but gapless edge states
  - Possibility of Majorana modes for odd C

- Analogous for other chiral superconductors
  - E.g. "p+ip" has $C = \pm 1$

- Calculate C for simple example:
  - Consider circular Fermi surface from dispersion $\xi_k \approx \frac{k^2}{2m} - \mu$ ← e.g. triangular lattice at smaller fillings
  - Approximate gap components by angular harmonics

$$\psi(k) = \eta\left[\psi_1(k) + i\,\psi_2(k)\right]$$

with $\psi_1(k) = \cos(l\theta)$, $\psi_2(k) = \sin(l\theta)$, $\theta = \arctan\frac{k_y}{k_x}$ →

$l=1$: E_1 representation (p-wave)

$l=2$ E_2 representation (d-wave)

$l=3$ B_1 & B_2 → not degenerate

$l=4$ E_2 again (g-wave)

$$\hookrightarrow \quad \vec{m} = \frac{1}{\sqrt{\xi_k^2 + \eta^2}} \begin{pmatrix} \eta \cos l\theta \\ \eta \sin l\theta \\ \xi_k \end{pmatrix}$$

$$\frac{\partial m}{\partial k_x} = -\frac{1}{\sqrt{\xi_k^2+\eta^2}}\left[\frac{\xi_k \frac{\partial \xi_k}{\partial k_x}}{\xi_k^2+\eta^2}\begin{pmatrix}\eta\cos l\theta\\ \eta\sin l\theta\\ \xi_k\end{pmatrix} + \begin{pmatrix}-l\eta\frac{k_y}{k^2}\sin l\theta\\ l\eta\frac{k_y}{k^2}\cos l\theta\\ -\frac{\partial \xi_k}{\partial k_x}\end{pmatrix}\right]$$

$$\frac{\partial m}{\partial k_y} = -\frac{1}{\sqrt{\xi_k^2+\eta^2}}\left[\frac{\xi_k \frac{\partial \xi_k}{\partial k_y}}{\xi_k^2+\eta^2}\begin{pmatrix}\eta\cos l\theta\\ \eta\sin l\theta\\ \xi_k\end{pmatrix} + \begin{pmatrix}-l\eta\frac{k_x}{k^2}\sin l\theta\\ l\eta\frac{k_x}{k^2}\cos l\theta\\ -\frac{\partial \xi_k}{\partial k_y}\end{pmatrix}\right]$$

$$\hookrightarrow \quad C = -\frac{1}{4\pi}\int dk \int d\theta\, \frac{k}{m}\, \frac{l\eta^2}{\sqrt{\xi_k^2+\eta^2}^3}$$

$$= -\frac{l}{2}\eta^2 \int_{-\infty}^{\infty} du\, \frac{1}{\sqrt{u^2+\eta^2}^3}$$

$$= -l$$