Superconductivity and Low Temperature Physics I

Lecture Notes
Winter Semester 2021/2022

R. Gross

Chapter 4

Microscopic Theory

Superconductivity and Low Temperature Physics I

Lecture No. 7
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Chapter 4

➡ 4. Microscopic Theory

4. BCS Theory

- after discovery of superconductivity, initially **many phenomenological theories** have been developed
  - → London theory (1935)
  - → macroscopic quantum model of superconductivity (1948)
  - → Ginzburg-Landau-Abrikosov-Gorkov theory (early 1950s)

- **problem**:
  - → phenomenological theories do not provide insight into the microscopic processes responsible for superconductivity
  - → impossible to engineer materials to increase T_c, if mechanisms are not known

- superconductivity originates from **interactions among conduction electrons**
  - → theoretical models for the description of ***interacting electrons*** are required
    - - very complicated: kinetic energy of conduction electrons ~ 5 eV, while interaction energy $\sim$ meV
      - → find attractive interaction which causes ordering in electron system despite high kinetic energy
    - - go beyond single electron (quasiparticle) models
    - - not available at the time of discovery of superconductivity

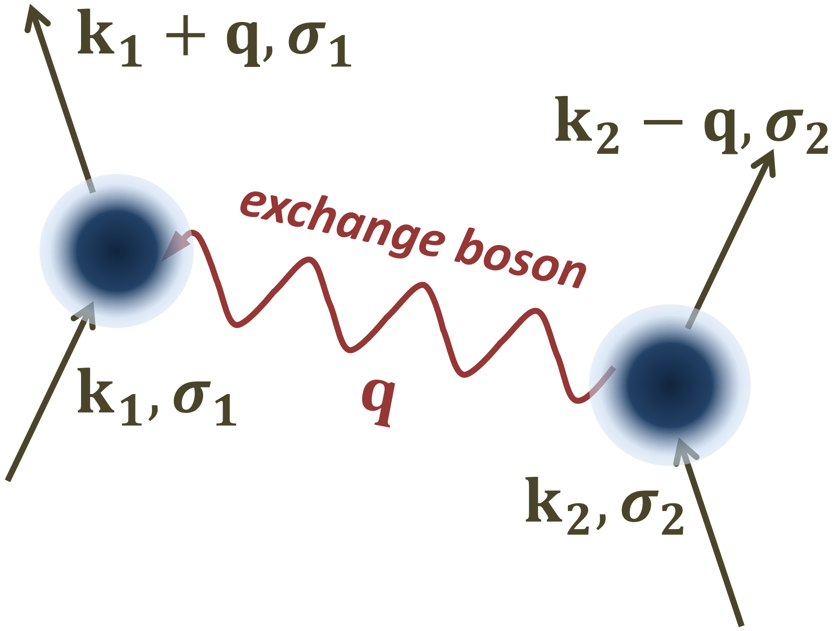
4. BCS Theory

- development of **BCS theory by J. Bardeen, L.N. Cooper and J.R. Schrieffer** in 1957
  - key element is ***attractive interaction*** among conduction electrons
  - 1956: Cooper shows that attractive interaction results in ***pair formation*** and in turn in an instability of the Fermi sea
  - 1957: Bardeen, Cooper and Schrieffer develop self-consistent formulation of the superconducting state: ***condensation of pairs in coherent ground state***
  - paired electrons are denoted as ***Cooper pairs***

- general description of interactions by exchange bosons
  - Bardeen, Cooper and Schrieffer identify ***phonons*** as the relevant exchange bosons
  - suggested by experimental observation

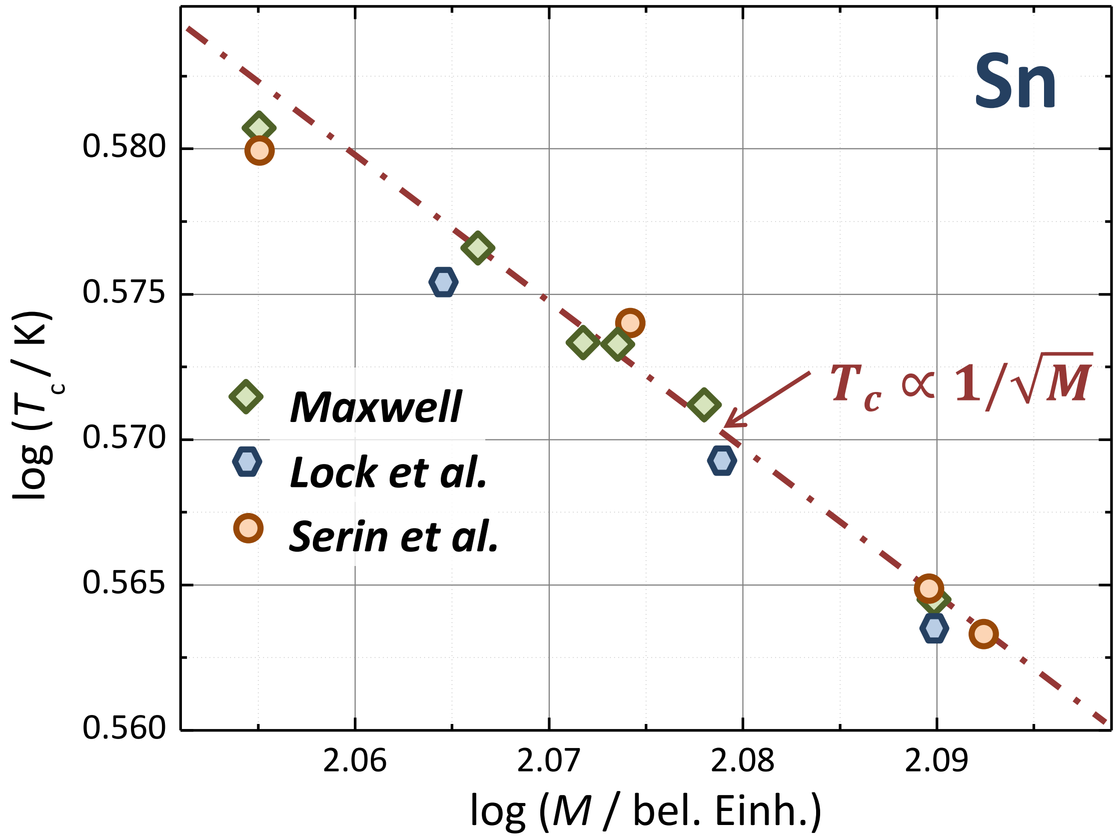
    $T_c \propto 1/\sqrt{M} \propto \omega_{ph}$ ***isotope effect***
  - in general, detailed nature of exchange boson does not play any role in BCS theory
  - many possible exchange bosons:

    magnons, polarons, plasmons, polaritons, spin fluctuations, …..



4. BCS Theory

isotop effect yields hint on type of exchange boson:

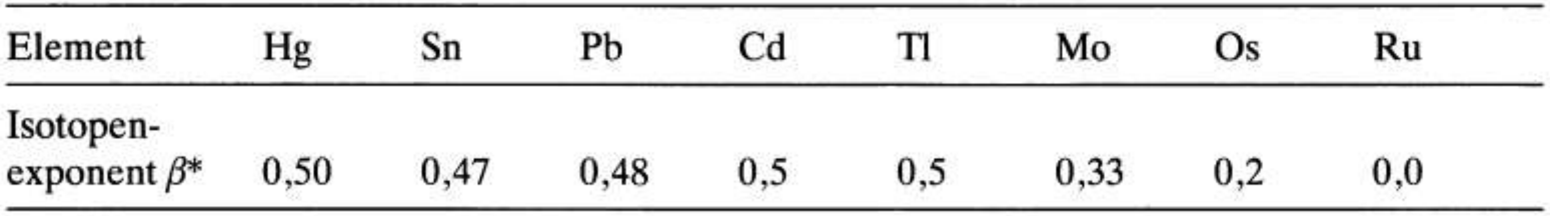


data from:
E. Maxwell, Phys. Rev. 86, 235 (1952)

B. Serin, C.A. Reynolds, C. Lohman,
Phys. Rev. 86, 162 (1952)

J.M. Lock, A.B. Pippard, D. Shoenberg,
Proc. Cambridge Phil. Soc. 47, 811 (1951)

in general: $T_c \propto 1/M^{\beta^\star}$



Element	Hg	Sn	Pb	Cd	Tl	Mo	Os	Ru
Isotopen-exponent β^*	0,50	0,47	0,48	0,5	0,5	0,33	0,2	0,0

4.1 Attractive Electron–Electron Interaction

- **intuitive assumption**:

  superconductivity results from ***ordering phenomenon of conduction electrons***

- **problem**:
  - conduction electrons have ***large (Fermi) velocity*** due to Pauli exclusion principle: $\approx 10^6$ m/s $\approx 0.01\ c$
  - corresponding (Fermi) temperature is above 10 000 K
  - in contrast: transition to superconductivity occurs at ≈ 1 – 10 K (≈ meV)

- **task**:
  - ➢ find ***interaction mechanism*** that results in ordering of conduction electrons despite their high kinetic energy
  - ➢ initial attempts fail:

    → Coulomb interaction (Heisenberg, 1947)
    → magnetic interaction (Welker, 1929)
    → …..

4.1.1 Phonon Mediated Interaction

- known fact since 1950:
  - T_c depends on isotope mass

- conclusion:
  - lattice plays an important role for superconductivity
  - initial proposals for phonon mediated e-e interaction (1950):

    H. Fröhlich, J. Bardeen

- ***static model of lattice mediated e-e interaction:***
  - one electron causes elastic distortion of lattice:
    attractive interaction with positive ions results in positive charge accumulation
  - second electron is attracted by this positive charge accumulation:
    effective binding energy

intuitive picture,
but has to be taken with care

http://www.max-wissen.de/

wrong suggestion:
- Cooper pairs are stable in time such as hydrogen molecule
- pairing in real space

4.1.1 Phonon Mediated Interaction

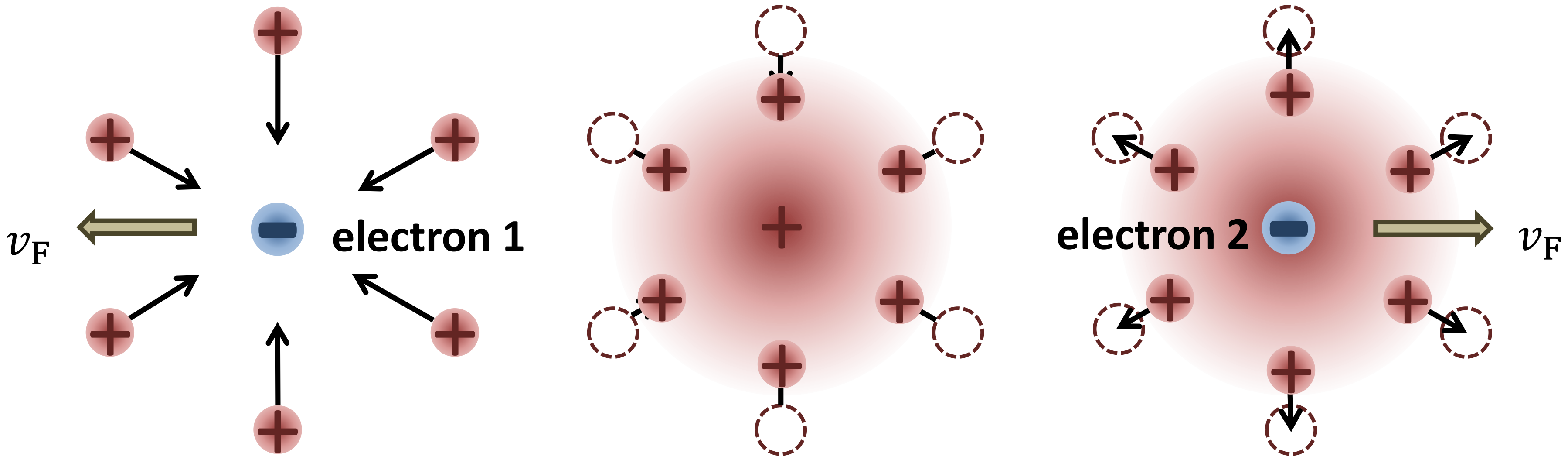
- ***dynamic model of lattice mediated e-e interaction:***

  - moving electrons distort lattice, causing temporary positive charge accumulation along their path

    → track of positive charge cloud

    → positive charge cloud can attract second electron

  - important: positive charge cloud rapidly relaxes again → ***dynamic model***



- important question: How fast relaxes positive charge cloud when electron moves through the lattice ?
- characteristic time scale τ:

  → frequency ω_q of lattice vibrations (phonons): $\tau = 1/\omega_q$

  → $\omega_{\mathrm{q}} \simeq 10^{12} - 10^{13}$ 1/s (maximum frequency: Debye frequency ω_{D})

4.1.1 Phonon Mediated Interaction

- resulting range of interaction (order of magnitude estimate)
  - how far can a second electron be, to attracted by the positive space charge before it relaxes
  - characteristic velocity of conduction electrons: $v_{\mathrm{F}} \simeq$ few 10^6 m/s

➔ ***interaction range***: $\boldsymbol{v_{\mathrm{F}} \cdot \tau \simeq 10^6 \frac{\mathrm{m}}{\mathrm{s}} \cdot 10^{-13}\ \mathrm{s} \simeq 0.1\ \mu\mathrm{m}}$ (is related to GL coherence length)

- important fact:
  - retarded reaction of slow ions results in large interaction range

    ➔ ***retarded interaction***
  - retarded interaction is essential for achieving attractive interaction

    ➔ without any retardation: - short interaction range

    - Coulomb repulsion between electrons dominates

- retarded interaction has been addressed during discussion of screening of phonons in metals

  ➔ ***retarded interaction potential:***

$$V(\mathbf{q}, \boldsymbol{\omega}) = \frac{e^2}{\epsilon(\mathbf{q}, \omega)\epsilon_0 q^2} = \underbrace{\left(\frac{e^2}{\epsilon_0(q^2 + k_s^2)}\right)}_{}\left(1 + \underbrace{\frac{\widetilde{\Omega}_p^2(\mathbf{q}))}{\omega^2 - \widetilde{\Omega}_p^2(\mathbf{q})}}_{}\right)$$

screened Coulomb potential

$1/k_s =$ Thomas-Fermi screening length

correction term is negative for

$\omega < \widetilde{\Omega}_p(\mathbf{q})$ → overscreening

$$\widetilde{\Omega}_p^2(\mathbf{q}) = \Omega_p^2(\mathbf{q}) / \left[1 + \frac{k_s^2}{q^2}\right]$$

q-dependent plasma frequency of the screened ions

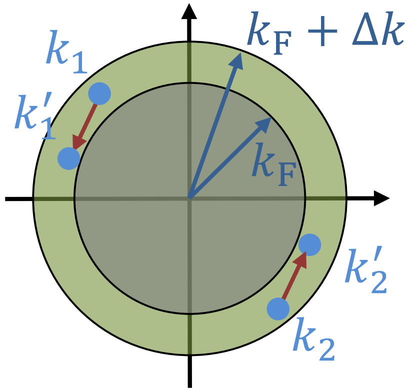
4.1.2 Cooper-Pairs

- ***Question***: How can we formally describe the pairing interaction?

- starting point: free electron gas at $T = 0$ (all states occupied up to $E_\mathrm{F} = \hbar^2 k_\mathrm{F}^2/2m$)

- ***Gedanken experiment***:
  - add two further electrons, which can interact via the lattice
  - describe the interaction by exchange of ***virtual phonon***

  virtual phonon: is generated and reabsorbed again within time $\Delta t \lesssim 1/\omega_q$



- wave vectors of electrons after exchange of virtual phonon with wave vector **q**:

$$\textbf{electron 1}:\ \mathbf{k}_1' = \mathbf{k}_1 + \mathbf{q} \qquad\qquad \textbf{electron 2}:\ \mathbf{k}_2' = \mathbf{k}_2 - \mathbf{q}$$

- total momentum is conserved: $\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_1' + \mathbf{k}_2' = \mathbf{K}'$

- note: - since at $T = 0$ all states are occupied below E_F, additional states have to be at $E > E_\mathrm{F}$

  - maximum phonon energy: $\hbar\omega_q = \hbar\omega_\mathrm{D}$ (Debye energy)

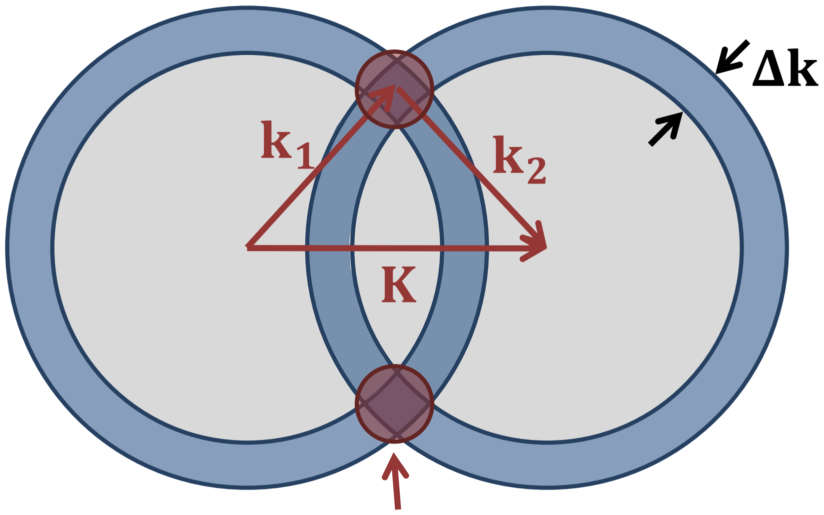
  ➔ accessible energy interval: $[E_\mathrm{F}, E_\mathrm{F} + \hbar\omega_\mathrm{D}]$

  ➔ interaction takes place in a spherical shell with radius k_F and thickness $\Delta k \simeq m\omega_\mathrm{D}/\hbar k_\mathrm{F}$

  ➔ for given $\mathbf{K}$ only specific wave vectors $\mathbf{k}_1, \mathbf{k}_2$ are allowed for interaction process

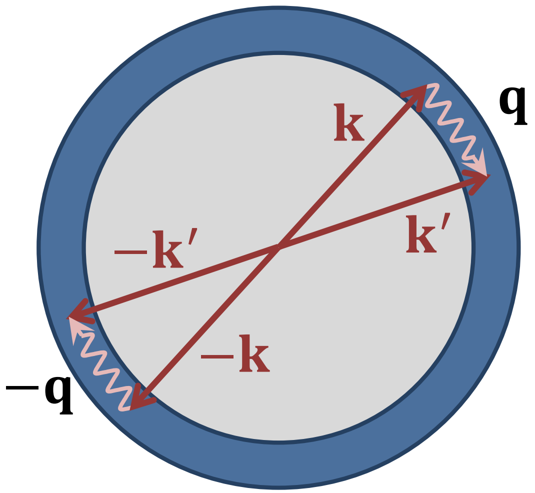
4.1.2 Cooper-Pairs

$\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2 > 0$



possible phase space for interaction

$\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2 = 0$



possible phase space is complete spherical shell

- ***important conclusion***: available phase space for interaction is maximum for $\mathbf{K} = \mathbf{0}$ or equivalently $\mathbf{k}_1 = -\mathbf{k}_2$

Cooper pairs with zero total momentum: $(\mathbf{k}\,, -\mathbf{k})$

$$\frac{\hbar^2 k_\mathrm{F}^2}{2m} + \hbar\omega_\mathrm{D} = \frac{\hbar^2 (k+\Delta k)^2}{2m} \simeq \frac{\hbar^2\left(k_\mathrm{F}^2 + 2k_\mathrm{F}\Delta k\right)}{2m} = \frac{\hbar^2 k_\mathrm{F}^2}{2m} + \frac{\hbar^2 k_\mathrm{F}\Delta k}{m} \quad \Rightarrow \quad \Delta k = \frac{m\omega_\mathrm{D}}{\hbar k_\mathrm{F}}$$

4.1.2 Cooper-Pairs

wave function of Cooper pairs and corresponding energy eigenvalues:

- ➢ two-particle wave function is chosen as product of two plane waves

$$\psi(\mathbf{r_1},\mathbf{r_2}) = a\ \exp(\imath\mathbf{k_1}\cdot\mathbf{r_1})\exp(\imath\mathbf{k_2}\cdot\mathbf{r_2}) = a\ \exp(\imath\mathbf{k}\cdot\mathbf{r})$$

with $\mathbf{k}=\mathbf{k}_1=-\mathbf{k}_2, \quad \mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$

- ➢ since pair-correlated electrons are permanently scattered into new states in interval $[k_\mathrm{F}, k_\mathrm{F}+\Delta k]$

  → pair wave function = superposition of product wave functions

$$\psi(\mathbf{r_1},\mathbf{r_2}) = \sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k\ \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}}$$

with $k_\mathrm{F} < k < k_\mathrm{F}+\Delta k$,
since restriction to energies $E_\mathrm{F} < E < E_\mathrm{F}+\hbar\omega_\mathrm{D}$

$|a_k|^2$: probability for realization of pair **$(\mathbf{k}\,, -\mathbf{k})$**

- note:
  - ➢ electron with $k < k_\mathrm{F}$ cannot participate in interaction since all states are occupied
  - ➢ we will see later that superconductor overcomes this problem by rounding-off $f(E)$ even at $T=0$
    - – superconductor first have to pay (kinetic) energy for rounding-off $f(E)$
    - – energy is obtained back by pairing interaction (potential energy)
    - – net energy gain

R. Gross and A. Marx , © Walther-Meißner-Institut (2004 - 2021)

4.1.2 Cooper-Pairs

wave function of Cooper pairs and corresponding energy eigenvalues:

- we assume that pairing interaction only depends on relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$
- Schrödinger equation: $$-\frac{\hbar^2}{2m}\left(\boldsymbol{\nabla}_1^2 + \boldsymbol{\nabla}_2^2\right)\psi(\mathbf{r_1},\mathbf{r_2}) + V(\mathbf{r})\psi(\mathbf{r_1},\mathbf{r_2}) = E\psi(\mathbf{r_1},\mathbf{r_2})$$
- insert $\psi(\mathbf{r_1},\mathbf{r_2}) = \sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k\, \mathrm{e}^{\imath\mathbf{k}\cdot\mathbf{r}}$, multiply by $\mathrm{e}^{-\imath\mathbf{k}'\cdot\mathbf{r}}$ and integrate over sample volume Ω

$$\int_\Omega \frac{\hbar^2k^2}{m}\sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k \exp(i\mathbf{k}\cdot\mathbf{r})\exp[-i(\mathbf{k}'\cdot\mathbf{r})]\,\mathrm{d}V + \int_\Omega V(\mathbf{r})\sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k \exp(i\mathbf{k}\cdot\mathbf{r})\exp[-i(\mathbf{k}'\cdot\mathbf{r})]\,\mathrm{d}V = \int_\Omega E\sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k \exp(i\mathbf{k}\cdot\mathbf{r})\exp[-i(\mathbf{k}'\cdot\mathbf{r})]\,\mathrm{d}V$$

- integration over sample volume Ω: $$\int_\Omega \exp[\imath(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]\;\mathrm{d}V = \begin{cases} 0 & \text{for } \mathbf{k}\neq\mathbf{k}' \\ \Omega & \text{for } \mathbf{k}=\mathbf{k}' \end{cases}$$

$$\underbrace{\int_\Omega \frac{\hbar^2k^2}{m}\sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k \exp(i\mathbf{k}\cdot\mathbf{r})\exp[-i(\mathbf{k}'\cdot\mathbf{r})]\,\mathrm{d}V}_{\frac{\hbar^2k^2}{m}a_k\Omega} + \underbrace{\int_\Omega V(\mathbf{r})\sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k \exp(i\mathbf{k}\cdot\mathbf{r})\exp[-i(\mathbf{k}'\cdot\mathbf{r})]\,\mathrm{d}V}_{\sum_{k'=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_{k'}\int V(\mathbf{r})\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}]\;dV} = \underbrace{\int_\Omega E\sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k \exp(i\mathbf{k}\cdot\mathbf{r})\exp[-i(\mathbf{k}'\cdot\mathbf{r})]\,\mathrm{d}V}_{E a_k\Omega}$$

scattering integral

4.1.2 Cooper-Pairs

- we use abbreviation

$$V_{\mathbf{k},\mathbf{k}'} = V_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} = V(\mathbf{k}-\mathbf{k}') = V(\mathbf{q}) = \frac{1}{\Omega}\int_{\Omega} V(\mathbf{r})\, \mathrm{e}^{\imath(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} \mathrm{d}V = \frac{1}{\Omega}\int_{\Omega} V(\mathbf{r})\, \mathrm{e}^{\imath\mathbf{q}\cdot\mathbf{r}} \mathrm{d}V$$

with $\mathbf{k}_1 = \mathbf{k}, \mathbf{k}_2 = -\mathbf{k}, \mathbf{q} = \mathbf{k}-\mathbf{k}'$

- result

$$\left(E - \frac{\hbar^2 k^2}{m}\right) a_k = \sum_{k'=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_{k'}\, V_{\mathbf{k},\mathbf{k}'}$$

problem:
we have to know all matrix elements$V_{\mathbf{k},\mathbf{k}'}$!!!

- simplifying assumption to solve the problem:

$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -V_0 & \text{for } k' > k_\mathrm{F}, k < k_\mathrm{F} + \Delta k \\ 0 & \text{else} \end{cases}$$

with $\Delta k = \frac{m\omega_\mathrm{D}}{\hbar k_\mathrm{F}}$

$$\left(E - \frac{\hbar^2 k^2}{m}\right) a_k = \sum_{k'=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_{k'}\, V_{\mathbf{k},\mathbf{k}'} \quad \Rightarrow \quad a_k = \frac{-V_0}{E - (\hbar^2 k^2/m)} \sum_{k'=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_{k'}$$

4.1.2 Cooper-Pairs

- summing up over all k using $\sum_k a_k = \sum_{k'} a_{k'}$ yields:

$$\sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k = V_0 \sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} \frac{1}{\left(\frac{\hbar^2 k^2}{m} - E\right)} \sum_{k'=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_{k'} \quad \Rightarrow \quad \boxed{1 = V_0 \sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} \frac{1}{\left(\frac{\hbar^2 k^2}{m} - E\right)}}$$

- we introduce pair density of states $\widetilde{D}(E) = D(E)/2$: sum ⇒ integral ($D(E)$ = DOS for both spin directions)

$$\boxed{1 = V_0 \frac{D(E_\mathrm{F})}{2} \int_{E_\mathrm{F}}^{E_\mathrm{F}+\hbar\omega_\mathrm{D}} \frac{\mathrm{d}\epsilon}{2\epsilon - E}}$$

with $\epsilon = \dfrac{\hbar^2 k^2}{2m}$

4.1.2 Cooper-Pairs

– integration and resolving for E results in

$$1 = V_0 \frac{D(E_\mathrm{F})}{2} \int_{E_\mathrm{F}}^{E_\mathrm{F}+\hbar\omega_\mathrm{D}} \frac{d\varepsilon}{(2\varepsilon - E)} = V_0 \frac{D(E_\mathrm{F})}{2} \cdot \frac{1}{2} \ln|2\varepsilon - E| \Big|_{E_\mathrm{F}}^{E_\mathrm{F}+\hbar\omega_\mathrm{D}}$$

with $\int \frac{dx}{ax+b} = \frac{1}{a} \ln|ax+b|$

$$\frac{4}{V_0 D(E_\mathrm{F})} = \ln|2E_\mathrm{F} + 2\hbar\omega_\mathrm{D} - E| - \ln|2E_\mathrm{F} - E|$$

$$\Rightarrow -\frac{4}{V_0 D(E_\mathrm{F})} = \ln \frac{|2E_\mathrm{F} - E|}{|2E_\mathrm{F} + 2\hbar\omega_\mathrm{D} - E|}$$

$$\exp\left(-\frac{4}{V_0 D(E_\mathrm{F})}\right) = \frac{|2E_\mathrm{F} - E|}{|2E_\mathrm{F} + 2\hbar\omega_\mathrm{D} - E|}$$

$$\Rightarrow |2E_\mathrm{F} + 2\hbar\omega_\mathrm{D} - E| \ \exp\left(-\frac{4}{V_0 D(E_\mathrm{F})}\right) = |2E_\mathrm{F} - E|$$

$$|2E_\mathrm{F} - E| \left[1 - \exp\left(-\frac{1}{V_0 D(E_\mathrm{F})}\right)\right] = 2\hbar\omega_\mathrm{D} \exp\left(-\frac{1}{V_0 D(E_\mathrm{F})}\right)$$

$$E = 2E_\mathrm{F} - 2\hbar\omega_\mathrm{D} \frac{\exp\left(-\frac{4}{V_0 D(E_\mathrm{F})}\right)}{1 - \exp\left(-\frac{4}{V_0 D(E_\mathrm{F})}\right)}$$

– for weak interaction $V_0 D(E_\mathrm{F}) \ll 1$ we obtain:

$$E \simeq 2E_\mathrm{F} - 2\hbar\omega_\mathrm{D} \exp\left(-\frac{4}{V_0 D(E_\mathrm{F})}\right)$$

- ➢ binding energy of Cooper pairs is ∝ $\hbar\omega_\mathrm{D}$ (→ isotope effect as $\omega_D \propto M^{-1/2}$))
- ➢ as $\hbar\omega_\mathrm{D} \ll E_\mathrm{F}$ and $\exp\left(-\frac{4}{V_0 D(E_\mathrm{F})}\right) \ll 1$ → binding energy is very small

4.1.2 Cooper-Pairs

– binding energy of Cooper pairs:

$$E \simeq 2E_\mathrm{F} - 2\hbar\omega_\mathrm{D} \exp\left(-\frac{4}{V_0 D(E_\mathrm{F})}\right)$$

important result:

➔ energy of interacting electron pair is smaller than $2E_\mathrm{F}$
➔ bound pair state (Cooper pair)
➔ binding energy depends on V_0 and maximum phonon energy $\hbar\omega_\mathrm{D}$

Note 1:

- ➢ electrons with $k < k_\mathrm{F}$ cannot participate in interactions as all states for $E < E_\mathrm{F}$ are occupied (no free scattering state)
- ➢ superconductor solves this problem by smearing out Fermi distribution even at $T = 0$
  - ➢ superconductor first has to pay kinetic energy to occupy state above E_F
  - ➢ increase of kinetic energy is overcompensated by pairing energy (potential energy)
  - ➢ total energy I reduced ➔ condensation energy

Note 2:

- ➢ in Gedanken experiment we have considered only two additional electrons above E_F
- ➢ in real superconductor: interaction of all electrons in energy interval around E_F
- ➢ electron gas becomes instable against pairing
  - ➔ instability causes transition into new ground state: ***BCS ground state***

4.1.2 Cooper-Pairs

estimate of the interaction range from the uncertainty relation

$$\Delta k = \frac{m\omega_\mathrm{D}}{\hbar k_\mathrm{F}} = \frac{\omega_\mathrm{D}}{v_\mathrm{F}} \quad \Rightarrow \quad \Delta x = \frac{1}{\Delta k} = \frac{v_\mathrm{F}}{\omega_\mathrm{D}}$$

with $v_\mathrm{F} \sim 10^6$ m/s and $\omega_\mathrm{D} \sim 10^{13}\ \mathrm{s}^{-1}$ ➔ **interaction range $R \sim 100$ nm**

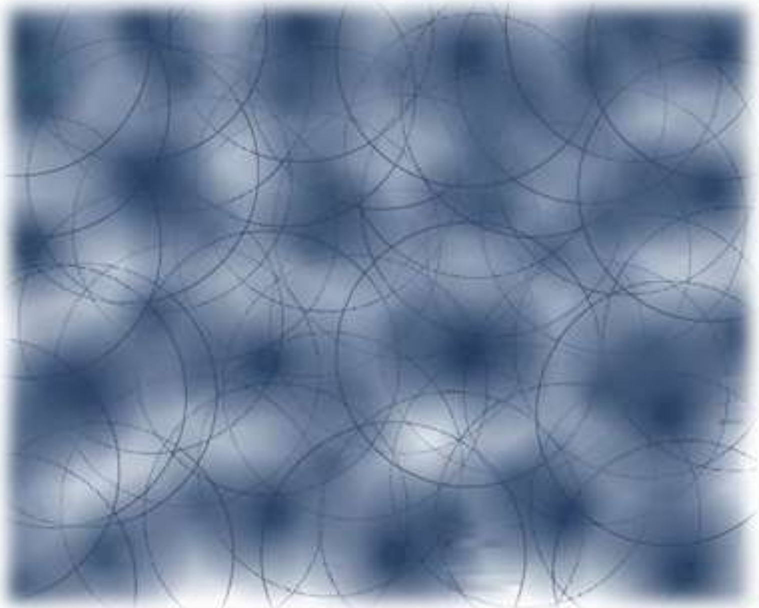
how many Cooper pairs do we find in volume $\frac{4}{3}\pi R^3$ defined by interaction range

- electron density in metal: $D(E_\mathrm{F})/V \sim 10^{28}\ \mathrm{eV}^{-1}\mathrm{m}^{-3}$
- relevant energy interval: $\hbar\omega_\mathrm{D} \sim 0.01\ - 0.1\ \mathrm{eV}$

$$N = 10^{28} \cdot 0.1 \cdot \frac{4}{3}\pi\,(10^{-7})^3 \sim \mathbf{10^6}$$

➔ strong overlap of pairs

➔ formation of ***coherent many body state***



4.1.2 Cooper-Pairs

attactive interaction via exchange of virtual phonons: how does the matrix element $V_{\mathbf{k},\mathbf{k}'} = V_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}}$ look like?

– **pure Coulomb interaction**

$$V(\mathbf{q}) = \frac{e^2}{\epsilon_0 q^2} = \int \left(\frac{e^2}{4\pi\epsilon_0 r}\right) \mathrm{e}^{-\imath\mathbf{q}\cdot\mathbf{r}}\, \mathrm{d}^3 r$$

positive matrix element ➔ repulsive interaction

– **screened Coulomb interaction**

$$V(\mathbf{q},\boldsymbol{\omega}) = \frac{e^2}{\epsilon_0 (q^2 + k_s^2)} = \int \left(\frac{e^2}{4\pi\epsilon_0 r}\mathrm{e}^{-\imath k_s r}\right) \mathrm{e}^{-\imath\mathbf{q}\cdot\mathbf{r}}\, \mathrm{d}^3 r$$

positive matrix element ➔ repulsive interaction
(k_s = Thomas-Fermi wave number, $k_s \sim \pi/a$)

– **screened Coulomb interaction in metals**:

$$V(\mathbf{q},\boldsymbol{\omega}) = \frac{e^2}{\epsilon(\mathbf{q},\omega)\epsilon_0 q^2} = \left(\frac{e^2}{\epsilon_0 (q^2 + k_s^2)}\right)\left(1 + \frac{\widetilde{\Omega}_p^2(\mathbf{q})}{\omega^2 - \widetilde{\Omega}_p^2(\mathbf{q})}\right)$$

Thomas-Fermi-
wave vector

q-dependent plasma frequency
of screened ions in metal

negative matrix element if $\epsilon(\mathbf{q},\omega) < 0$
➔ attractive interaction

$$\widetilde{\Omega}_p^2(\mathbf{q}) = \Omega_p^2 \Big/ \left[1 + \frac{k_s^2}{q^2}\right]$$

$$\Omega_p^2 = \frac{n(Ze)^2}{\epsilon_0 M}$$

for small energy differences $(E_k - E_{k'})/\hbar = \omega < \widetilde{\Omega}_p(\mathbf{q})$ of the participating electrons
→ demoninator gets negative ➔ attractive interaction
➔ cut-off frequency: $\omega = \widetilde{\Omega}_p \simeq \omega_\mathrm{D}$ (Debye-Frequenz)

4.1.3 Symmetry of Pair Wavefunction

What is the symmetry of the pair wavefunction?

- **important**: pair consistst of two fermions ➔ *total wavefunction must be antisymmetric: minus sign for particle exchange*

$$\Psi(\mathbf{r_1},\boldsymbol{\sigma_1},\mathbf{r_2},\boldsymbol{\sigma_2}) = \underbrace{\frac{1}{\sqrt{V}}\, \mathrm{e}^{i\,\mathbf{K_s}\cdot\mathbf{R_s}}}_{\substack{\text{center of mass motion}\\ \text{we assume } \mathbf{K}_s = 0}} \underbrace{f(\mathbf{k},\mathbf{r})}_{\substack{\text{orbital}\\ \text{part}}} \underbrace{\chi(\boldsymbol{\sigma_1},\boldsymbol{\sigma_2})}_{\substack{\text{spin}\\ \text{part}}} = -\Psi(\mathbf{r_2},\boldsymbol{\sigma_2},\mathbf{r_1},\boldsymbol{\sigma_1})$$

$$\mathbf{R_s} = (\mathbf{r_1} + \mathbf{r_2})/2$$

$$\mathbf{r} = (\mathbf{r_1} - \mathbf{r_2})$$

$$\mathbf{K_s} = (\mathbf{k_1} + \mathbf{k_2})/2$$

$$\mathbf{k} = (\mathbf{k_1} - \mathbf{k_2})$$

- possible ***spin wavefunctions*** $\chi(\boldsymbol{\sigma_1},\boldsymbol{\sigma_2})$ for electron pairs

$$S = \begin{cases} 0 \quad m_s = 0 \qquad \chi^a = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) \\ 1 \quad m_s = \begin{cases} -1 & \chi^s = \downarrow\downarrow \\ 0 & \chi^s = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ +1 & \chi^s = \uparrow\uparrow \end{cases} \end{cases}$$

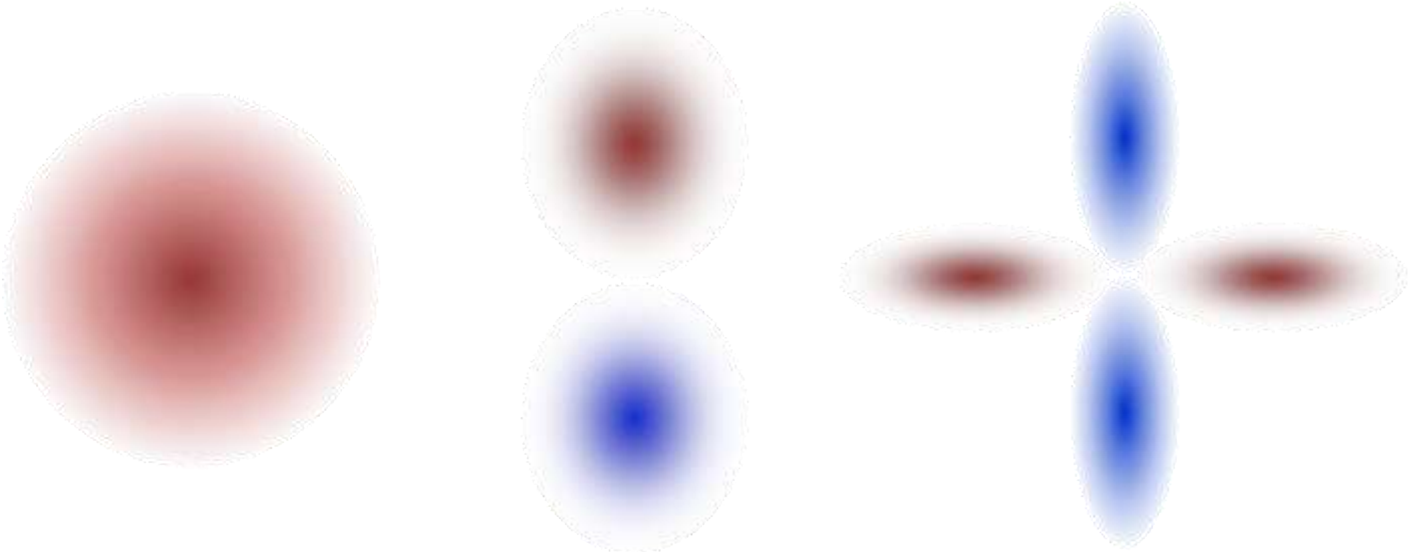
→**singlet pairing**, antisymmetric spin wavefunction
symmetric orbital function:
L = 0, 2, … (s, d, ….)

→**triplet pairing**, symmetric spin wavefunction
antisymmetric orbital function:
L = 1, 3, … (p, f, ….)

4.1.3 Symmetry of Pair Wavefunction

What is the symmetry of the pair wavefunction?

Singlet-Pairing	$S = 0$	$L = 0, 2, 4, \ldots$	symmetric orbital wavefunction
Triplet-Pairing	$S = 1$	$L = 1, 3, 5, \ldots$	antisymmetric orbital wavefunction



$L = 0$ **s-wave superconductor**

$L = 1$ **p-wave superconductor**

$L = 2$: **d-wave superconductor**

- **metallic superconductors:**
  $S = 0, L = 0$
- **high temperature (cuprate) superconductors:**
  $S = 0, L = 2$
- **suprafluid ^{3}He:**
  $S = 1, L = 1$

4.1.3 Symmetry of Pair Wavefunction

- isotropic interaction: $V_{\mathbf{k},\mathbf{k}'} = -V_0$

  → interaction only depends on $|\mathbf{k}|$
  → in agreement with angular momentum $L = 0$ (s – wave superconductor)

  – corresponding spin wavefunction must by antisymmetric

    → **spin singlet Cooper pairs ($S = 0$)**

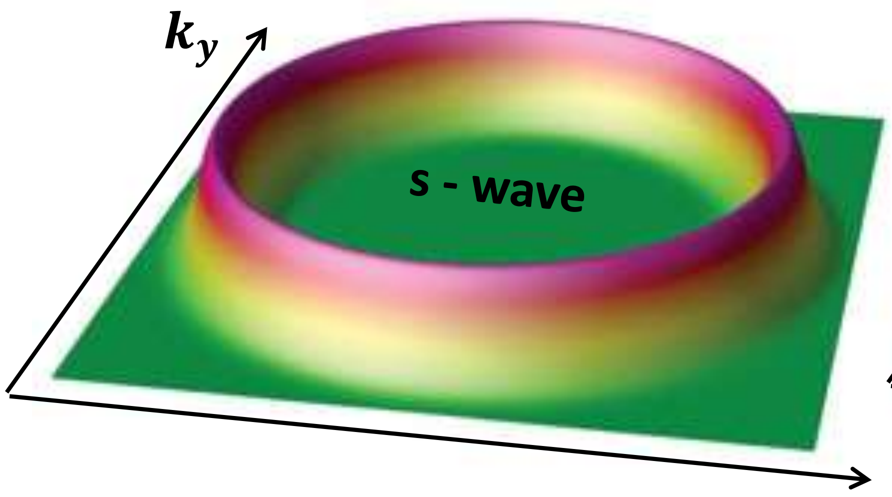
  – resulting Cooper pair: $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ spin singlet Cooper pair ($L = 0, S = 0$)

    - $L = 0, S = 0$ is realized in metallic superconductors (*s* – wave superconductor)
    - higher orbital momentum wavefunction in cuprate superconductors (HTS): $L = 2, S = 0$ (*d* – wave superconductor)

- **spin triplet Cooper pairs ($S = 1$):**
  - realized in superfluid ^{3}He: $L = 1, S = 1$ (*p* – wave pairing)
  - evidence for $L = 1, S = 1$ also for some heavy Fermion superconductors (e.g. UPt$_3$)

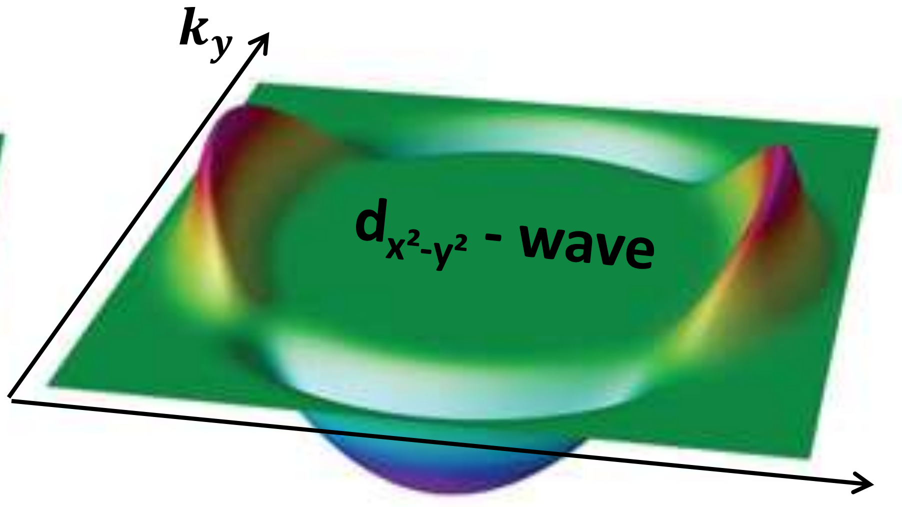
4.1.3 Symmetry of Pair Wavefunction

L = 0, *S* = 0



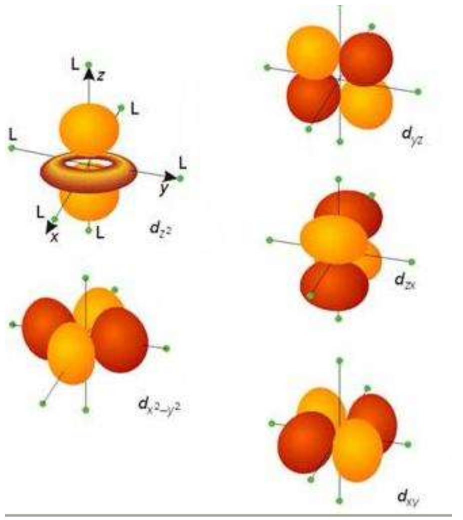
$$\Delta(\mathbf{k}) = \Delta_m$$

L = 2, *S* = 0



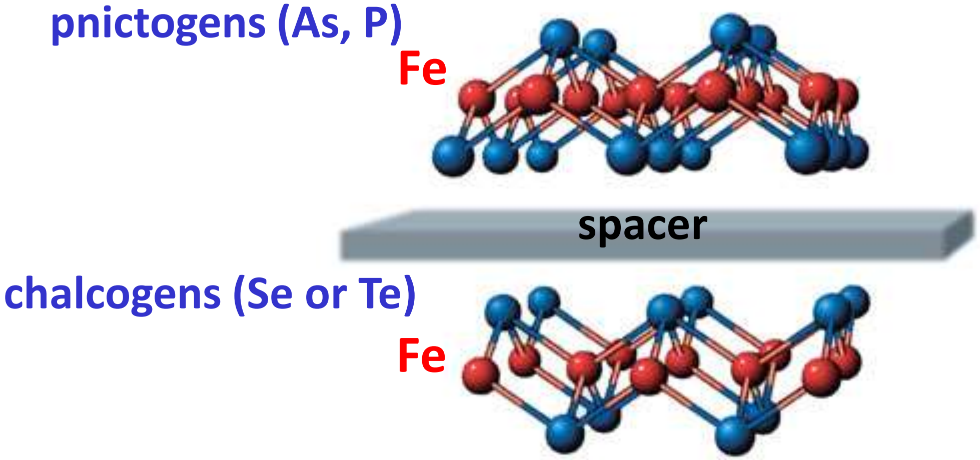
$$\Delta(\mathbf{k}) = \frac{\Delta_m}{2}\left(\cos k_y a - \cos k_x a\right)$$

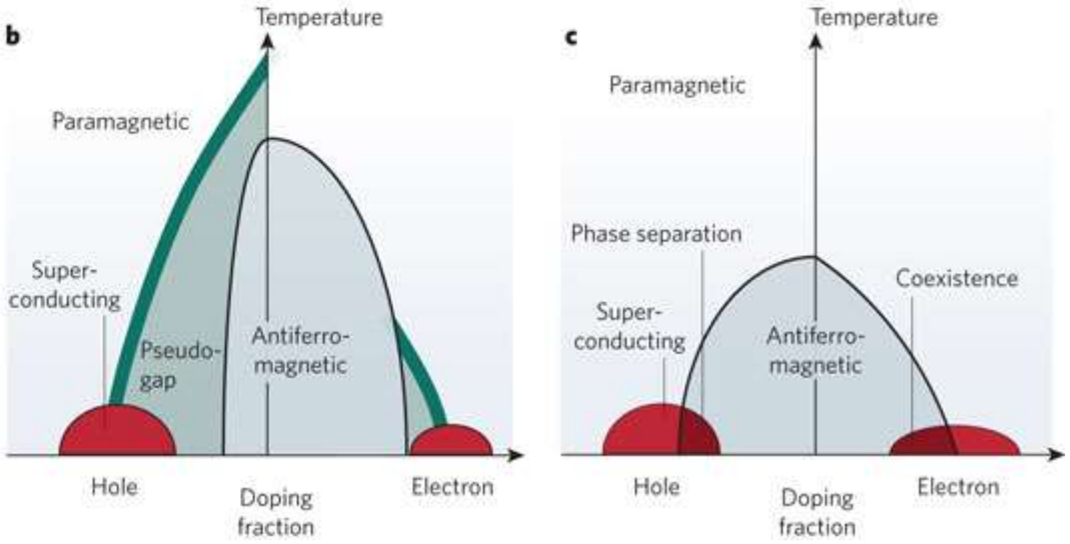
[Superconductivity gets an iron boost](#)
Igor I. Mazin
Nature **464**, 183-186(11 March 2010)

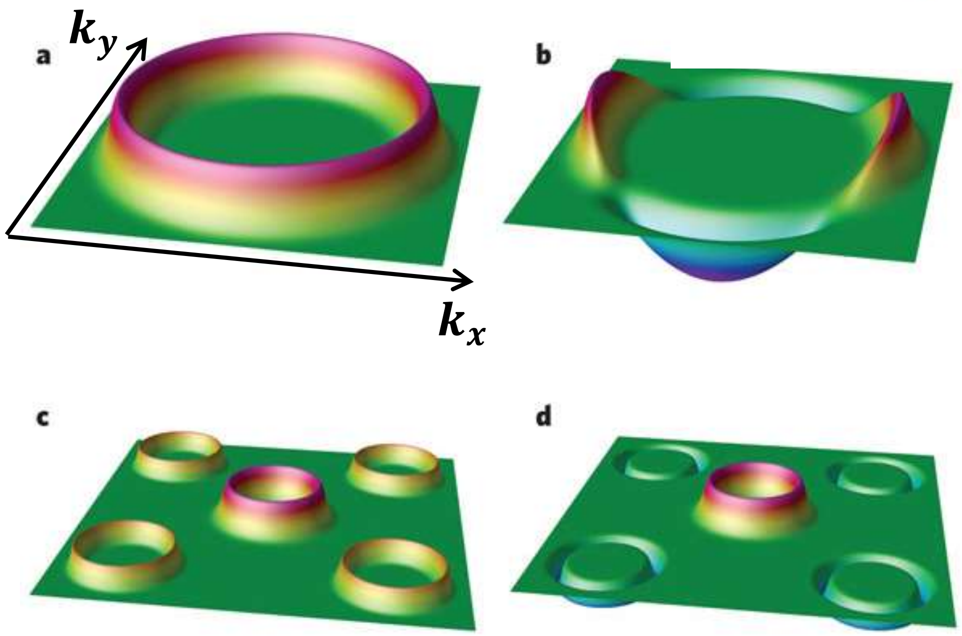


4.1.3 Symmetry of Pair Wavefunction

Example: iron-based superconductors – iron pnictides





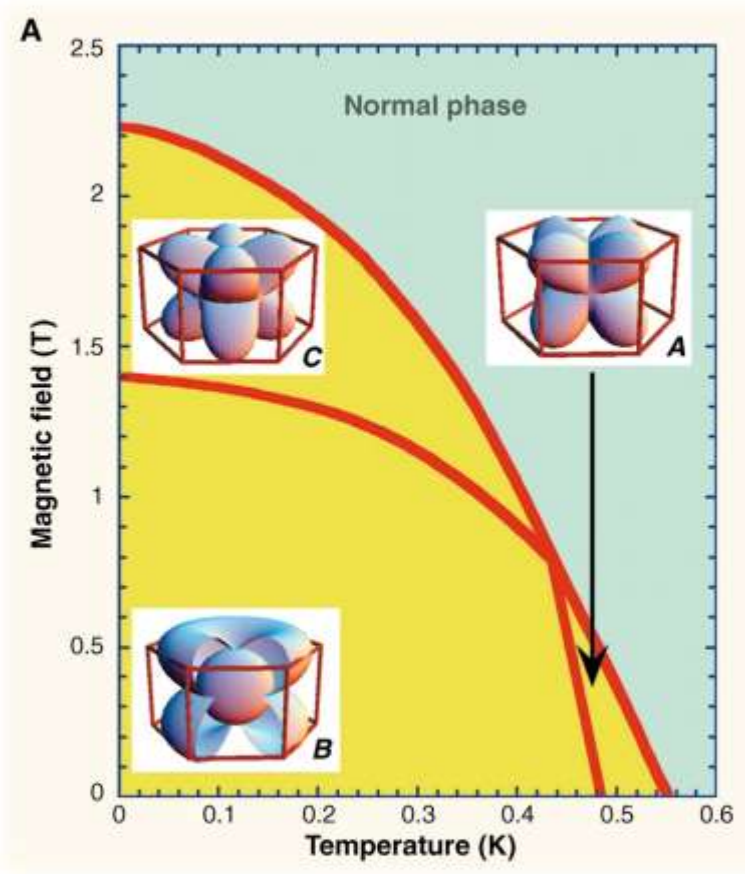


1. *a.* *s*-wave, e.g. in aluminium
2. *b.* *d*-wave, e.g. in copper oxides
3. c. two-band *s*-wave with the same sign, e.g. in MgB_2
4. d. an $s_\pm$-wave, e.g. in iron-based SC

4.1.3 Symmetry of Pair Wavefunction

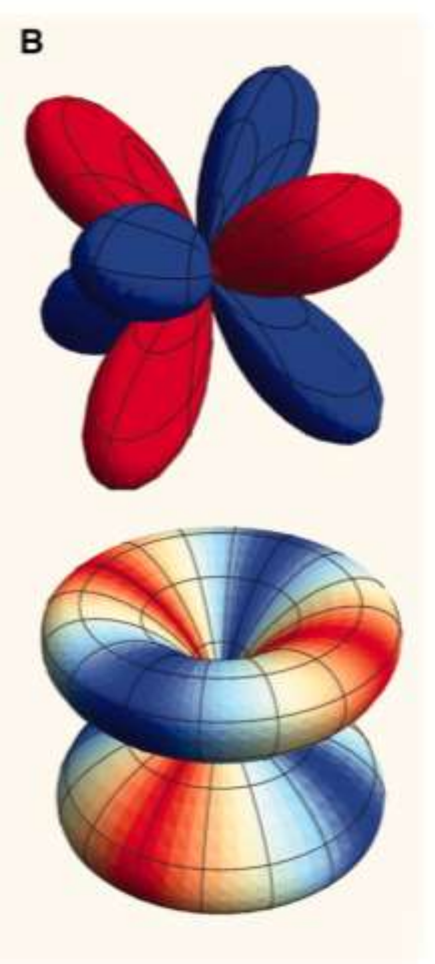
Example: UPt$_3$

phase diagram



Michael R. Norman, *Science 332, 196-200 (2011)*

f-wave (E_{2u}) Cooper pair wavefunction in three-dimensional momentum space



phase *A*

phase *B*

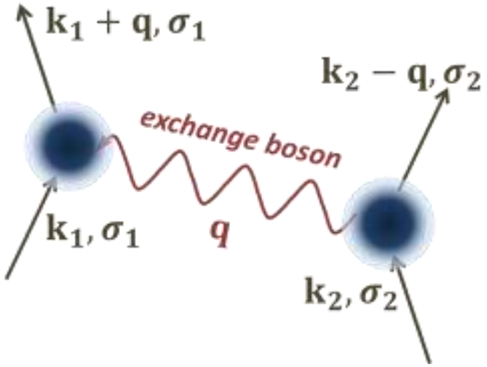
Superconductivity and Low Temperature Physics I

Lecture No. 8
09 December 2021

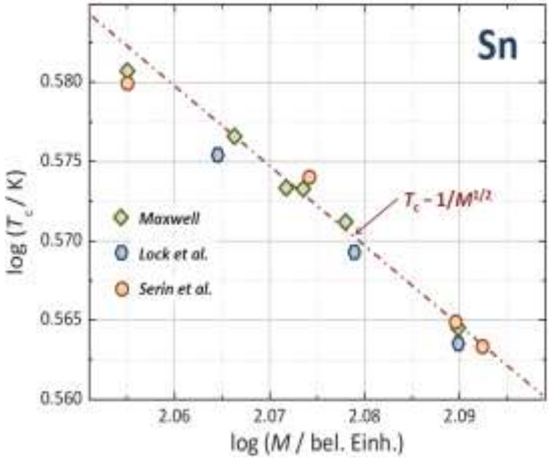
R. Gross

Summary of Lecture No. 7 (1)

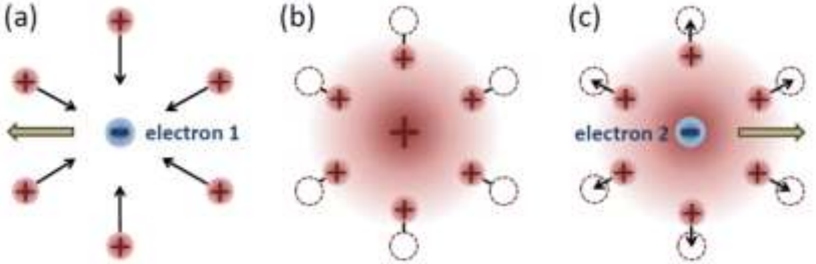
- ***microscopic theory of superconductivity***
  - problem: (i) high kinetic energy of conduction electrons: $E_{\mathrm{kin}} \sim$ eV (corresponding to $T \sim 10\,000$ K)
    (ii) small interaction strength: $E_{\mathrm{int}} \sim$ meV (corresponding to $T \sim 10$ K)
    ➔ find interaction resulting in ordering of conduction electrons despite high E_{kin}
  - Cooper (1956): even weak attractive interaction results in instability of free electron gas
    → ***pair formation: Cooper pairs***
  - general description of interaction by Feynman diagram:
    → which ***exchange boson*** results in atractive interaction of conduction electrons?
    → many candidates: ***phonon, magnon, polariton, plasmon, polaron, bipolaron***, ….



- ***isotope effect as „smoking gun" experiment (1951/1952)***
  - transition temperature of different isotopes: $\boldsymbol{T_c \propto 1/\sqrt{M}}$
    → as phonon frequency $\omega_{\mathrm{ph}} \propto 1/\sqrt{M}$ ➔ $\boldsymbol{T_c \propto \omega_{\mathrm{ph}}}$
    strong evidence for attractive interaction by exchange of virtuell phonons



- ***BCS-Theorie (1957)***
  - qualitative discussion of attractive interaction: slow reaction of positive ions
    → ***retarded interaction***
  - estimate of interaction range $R \simeq v_{\mathrm{F}}\tau \simeq v_{\mathrm{F}}/\omega_{\mathrm{D}}$ (ω_{D} = Debye frequency)
    $v_{\mathrm{F}} \simeq 10^6$m/s, $\omega_{\mathrm{D}} \simeq 10^{13}\mathrm{s}^{-1}$ → $R \simeq 100$ nm
  - $R \gg$ interaction range of screened Coulomb interaction of conduction electrons



Summary of Lecture No. 7 (2)

- ***attractive electron-electron interaction***
  - attractive interaction via lattice vibrations (exchange of virtual phonons: Fröhlich, Bardeen)
  - scattering matrix element (i) pure Coulomb interaction: $V(\mathbf{q}) = \frac{e^2}{\epsilon_0 q^2}$ (always positive → repulsive interaction)

    (ii) screened Coulomb interaction: $V(\mathbf{q},\boldsymbol{\omega}) = \frac{e^2}{\epsilon(\mathbf{q},\omega)\epsilon_0 q^2} = \left(\frac{e^2}{k_s^2+q^2}\right)\left(1+\frac{\widetilde{\Omega}_p^2(\mathbf{q})}{\omega^2-\widetilde{\Omega}_p^2(\mathbf{q})}\right)$

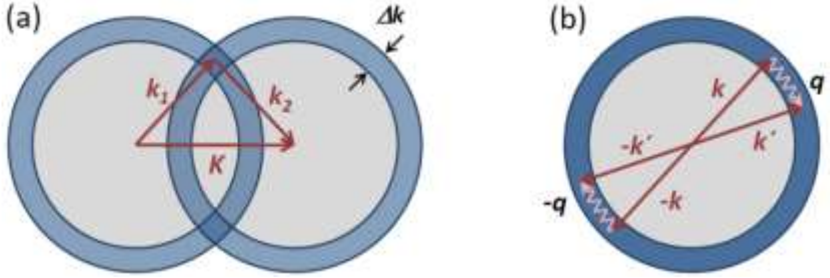
    Thomas-Fermi-
    wave vector

    q-dep. plasma frequency of
    screened ions in metal

  ➢ for $E_k - E_{k'} = \hbar\omega < \hbar\widetilde{\Omega}_p(\mathbf{q})$ of involved electrons: denominator becomes negative → negative matrix element → **attractive interaction**

  ➢ **cut-off frequency**: $\omega = \widetilde{\Omega}_p \simeq \omega_\mathrm{D}$ (Debye frequency)

- ***Cooper pairs***



  - ***„Gedanken" experiment***:
    we add 2 additional electrons to Fermi sea at $T=0$ and let them interact via exchange of phonons with wave number q
  - scattering process:

    electron 1: $\mathbf{k_1} \rightarrow \mathbf{k}_1' = \mathbf{k_1} + \mathbf{q}$

    electron 2: $\mathbf{k_2} \rightarrow \mathbf{k}_2' = \mathbf{k_2} - \mathbf{q}$

    total momentum: $\mathbf{K} = \mathbf{k_1} + \mathbf{k_2} = \mathbf{k}_1' + \mathbf{k}_2' = \mathbf{K}'$
  - only states with $E > E_\mathrm{F}$ are accessible due to full Fermi sea
  - as $\omega_\mathrm{ph} < \omega_\mathrm{D}$, interaction takes place in energy interval $[E_\mathrm{F}, E_\mathrm{F} + \hbar\omega_\mathrm{D}]$ corresponding to $k_\mathrm{F} \leq k \leq k_\mathrm{F} + \frac{m\omega_\mathrm{D}}{\hbar k_\mathrm{F}} = k_\mathrm{F} + \Delta k$
  - conservation of total momentum → wave vectors of scattering electron must be within cut surface of two intersecting circular rings of thickness Δk

    → **maximum cut surface (phase space) is obtained for $\mathbf{K} = \mathbf{0}$ or $\mathbf{k_1} = -\mathbf{k_2}$** → ***Cooper pairs*** $(\mathbf{k}, -\mathbf{k})$

Summary of Lecture No. 7 (3)

- ***Cooper pair interaction***
  - Ansatz: pair wave function = superposition of product wave functions: $\Psi(\mathbf{r}_1,\mathbf{r}_2) = \sum_{k=k_\mathrm{F}}^{k_\mathrm{F}+\Delta k} a_k \exp(i\mathbf{k}\cdot\mathbf{r})$ $\mathbf{r} = \mathbf{r_2} - \mathbf{r_1}$
  - Schrödinger equation: $-\frac{\hbar^2}{2m}\left(\nabla_1^2+\nabla_2^2\right)\Psi(\mathbf{r}_1,\mathbf{r}_2) + V(\mathbf{r})\,\Psi(\mathbf{r}_1,\mathbf{r}_2) = E\,\Psi(\mathbf{r}_1,\mathbf{r}_2)$
  - Vereinfachung: $V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -V_0 & \text{for } k' > k_\mathrm{F}, k < k_\mathrm{F}+\Delta k \\ 0 & \text{else} \end{cases}$ with $\Delta k = \frac{m\omega_\mathrm{D}}{\hbar k_\mathrm{F}}$
  - total energy: $\boxed{E \simeq 2E_\mathrm{F} - 2\hbar\omega_\mathrm{D}\exp\left(-\frac{1}{V_0 D(E_\mathrm{F})}\right)}$ for weak interaction: $V_0 D(E_\mathrm{F}) \ll 1)$ binding energy: $E - 2E_\mathrm{F} \propto \hbar\omega_\mathrm{D}$ (phonon energy)
  - uncertainty relation: $\Delta k\, \Delta x \geq 1$ ➔ $\Delta x \leq \frac{1}{\Delta k} = \frac{v_\mathrm{F}}{\omega_\mathrm{D}} \simeq 100\ \mathrm{nm}$

- ***symmetry of the pair wave function***
  - two fermions → **total wave function must be antisymmetric**

Singlet Pairing	$S = 0$	$L = 0, 2, 4, \ldots$
Triplet Pairing	$S = 1$	$L = 1, 3, 5, \ldots$

$$S = \begin{cases} 0 \quad m_s = 0 \qquad \chi^a = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) & \text{singlet pairing} \\ 1 \quad m_s = \begin{cases} -1 & \chi^s = \downarrow\downarrow \\ 0 & \chi^s = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ +1 & \chi^s = \uparrow\uparrow \end{cases} & \text{triplet pairing} \end{cases}$$

  - **examples**: metalic superconductors: $S = 0,\ L = 0$, high-temperature cuprate superconductors: $S = 0,\ L = 2$, superfluid ^{3}He: $S = 1,\ L = 1$

Chapter 4

4. Microscopic Theory

4.2 The BCS Ground State

- **discussed so far**:
  - nature of the attractive interaction
  - attractive interaction of conduction electrons by exchange of virtual phonons (only two electrons added to Fermi sea)
    ➔ pair formation: **Cooper pair**
  - symmetry of the pair wave function

- **not yet discussed**:
  - ***How does the ground state of the total electron system look like?***
  - ***What is the ground state energy?***

- **we expect**:
  - pairing mechanism goes on until the Fermi sea has changed significantly
  - if pairing energy goes to zero, pairing process will stop
  - detailed theoretical description is complicated ➔ we discuss only basics

4.2 The BCS Ground State

formalism of second quantization is used (>1927, Dirac, Fock, Jordan et al.)

- 2nd quantization formalism is useful to describe quantum many-body systems
- quantum many-body states are represented in the so-called Fock (number) state basis
  → Fock states are constructed by filling up each single-particle state with a certain number of identical particles
- 2nd quantization formalism introduces the creation and annihilation operators to construct and handle the Fock states
- 2nd quantization formalism is also known as the canonical quantization in quantum field theory, in which the fields are upgraded to field operators
  → analogous to 1st quantization, where the physical quantities are upgraded to operators

conduction electrons can be described by wave pakets

introduction of field operators (2nd quantization of a wave function)

$$\hat{\Psi}_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma} \; \mathrm{e}^{\imath \mathbf{k}\cdot\mathbf{r}} \quad \Longleftrightarrow \quad \hat{\mathrm{c}}_\sigma(\mathbf{k}) = \hat{\mathrm{c}}_{\mathbf{k}\sigma} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{\Psi}_\sigma \; \mathrm{e}^{-\imath \mathbf{k}\cdot\mathbf{r}}$$

annihilation operator
(destroys state with wave number **k**)

$$\hat{\Psi}_\sigma^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \; \mathrm{e}^{-\imath \mathbf{k}\cdot\mathbf{r}} \quad \Longleftrightarrow \quad \hat{\mathrm{c}}_\sigma^\dagger(\mathbf{k}) = \hat{\mathrm{c}}_{\mathbf{k}\sigma}^\dagger = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{\Psi}_\sigma^\dagger \; \mathrm{e}^{\imath \mathbf{k}\cdot\mathbf{r}}$$

creation operator
(ceates state with wave number **k**)

4.2 The BCS Ground State

formalism of second quantization is used (>1927, Dirac, Fock, Jordan et al.)

basic relations (fermionic operators):

$$\hat{c}^\dagger_{\mathbf{k}\sigma}\,|0\rangle = |1\rangle \qquad \hat{c}_{\mathbf{k}\sigma}|0\rangle = 0 \qquad \hat{c}^\dagger_{\mathbf{k}\sigma}\,|1\rangle = 0 \qquad \hat{c}_{\mathbf{k}\sigma}|1\rangle = |0\rangle$$

$$\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma} \qquad \hat{c}_{\mathbf{k}\sigma}\hat{c}^\dagger_{\mathbf{k}\sigma} = 1 - n_{\mathbf{k}\sigma} \qquad \langle 0|n_{\mathbf{k}\sigma}|0\rangle = 0; \quad \langle 1|n_{\mathbf{k}\sigma}|1\rangle = 1$$

particle number operator

$$\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}^\dagger_{\mathbf{k}\sigma} = 0 \qquad \hat{c}_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} = 0$$

Pauli exclusion principle

anti-commutation relations (fermions):

$$\left\{\hat{c}_{\mathbf{k}\sigma}\,,\hat{c}^\dagger_{\mathbf{k}'\sigma'}\right\} \equiv \hat{c}_{\mathbf{k}\sigma}\hat{c}^\dagger_{\mathbf{k}'\sigma'} + \hat{c}^\dagger_{\mathbf{k}'\sigma'}\hat{c}_{\mathbf{k}\sigma'} = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\boldsymbol{\sigma}\boldsymbol{\sigma}'}$$

$$\left\{\hat{c}_{\mathbf{k}\sigma}\,,\hat{c}_{\mathbf{k}'\sigma'}\right\} = \left\{\hat{c}^\dagger_{\mathbf{k}\sigma}\,,\hat{c}^\dagger_{\mathbf{k}'\sigma'}\right\} = 0$$

4.2 The BCS Ground State

formalism of second quantization is used (>1927, Dirac, Fock, Jordan et al.)

pair creation and annihilation operators:

$P_{\mathbf{k}}^{\dagger} = \hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger}$ **pair creation operator** $\qquad P_{\mathbf{k}} = \hat{c}_{-\mathbf{k}\downarrow}\,\hat{c}_{\mathbf{k}\uparrow}$ **pair annihilation operator**

$$[P_{\mathbf{k}}, P_{\mathbf{k}'}] = \hat{c}_{-\mathbf{k}\downarrow}\,\hat{c}_{\mathbf{k}\uparrow}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow} - \hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}\hat{c}_{-\mathbf{k}\downarrow}\,\hat{c}_{\mathbf{k}\uparrow} = 0$$

the last two operators of the first term on the r.h.s. can be moved to the front by an even number of permutations ➔ **sign is preserved**

$$\left[P_{\mathbf{k}}^{\dagger}, P_{\mathbf{k}'}^{\dagger}\right] = \hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger}\hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}'\downarrow}^{\dagger} - \hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}'\downarrow}^{\dagger}\hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger} = 0$$

$$\left[P_{\mathbf{k}}, P_{\mathbf{k}'}^{\dagger}\right] = \delta_{\mathbf{k}\mathbf{k}'}(1 - n_{\mathbf{k}\uparrow} - n_{-\mathbf{k}'\downarrow})$$ (see next slide)

- some of the commutator relations of the pair operators are similar to those of bosons, although the pair operators consist only of electron (fermionic) operators
- $\left[P_{\mathbf{k}}, P_{\mathbf{k}}^{\dagger}\right] \neq 0$ but not equal to $\delta_{\mathbf{k}\mathbf{k}'}$ as expected for bosons, depends on **k** and T

➔ **pair operators do commute but are no bosonic operators**

powers of pair operators

$$P_{\mathbf{k}}^{\dagger}P_{\mathbf{k}}^{\dagger} = \left(P_{\mathbf{k}}^{\dagger}\right)^{2} = \hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger}\hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger} = -\underbrace{\hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{\mathbf{k}\uparrow}^{\dagger}}_{=0}\underbrace{\hat{c}_{-\mathbf{k}\downarrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger}}_{=0} = 0$$

antisymmetry of fermionic wavefunction requires that powers of the pair operators disappear

4.2 The BCS Ground State

formalism of second quantization is used (>1927, Dirac, Fock, Jordan et al.)

pair creation and annihilation operators:

$$\left[P_{\mathbf{k}}, P_{\mathbf{k}}^{\dagger}\right] = \hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}'\downarrow}^{\dagger} - \hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}'\downarrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}$$

$$= \hat{c}_{-\mathbf{k}\downarrow}\left(1 - \hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{\mathbf{k}\uparrow}\right)\hat{c}_{-\mathbf{k}'\downarrow}^{\dagger} - \hat{c}_{-\mathbf{k}'\downarrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{\mathbf{k}\uparrow}$$

$$= \left(1 - \hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{\mathbf{k}\uparrow}\right)\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}'\downarrow}^{\dagger} - \hat{c}_{-\mathbf{k}'\downarrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{\mathbf{k}\uparrow}$$

$$= \left(1 - \hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{\mathbf{k}\uparrow}\right)\left(1 - \hat{c}_{-\mathbf{k}'\downarrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}\right) - \hat{c}_{-\mathbf{k}'\downarrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}'\uparrow}^{\dagger}\hat{c}_{\mathbf{k}\uparrow}$$

$$= \delta_{\mathbf{k}\mathbf{k}'}(1 - n_{\mathbf{k}\uparrow})(1 - n_{-\mathbf{k}\downarrow}) - n_{-\mathbf{k}\downarrow}n_{\mathbf{k}\uparrow}$$

$$\left[P_{\mathbf{k}}, P_{\mathbf{k}}^{\dagger}\right] = \delta_{\mathbf{k}\mathbf{k}'}(1 - n_{\mathbf{k}\uparrow} - n_{-\mathbf{k}\downarrow})$$

4.2 The BCS Ground State

formalism of second quantization is used (>1927, Dirac, Fock, Jordan et al.)

BCS Hamiltonian for N interacting electrons

$$\mathcal{H}_{\mathrm{BCS}} = \underset{\text{spin}}{\sum_{\sigma}} \sum_{i=1}^{N} \Bigg(\underbrace{-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2}_{\text{kinetic energy}} + \underbrace{V_{\mathrm{ext}}(\mathbf{r})}_{\text{potential energy}} \Bigg) + \frac{1}{2} \sum_{\sigma} \sum_{i,j=1}^{N} \underbrace{V_{\mathrm{int}}(\mathbf{r}_i - \mathbf{r}_j)}_{\text{interaction energy}}$$

insertion of field operators and intergation over volume ➔ FT of $\mathcal{H}_{\mathrm{BCS}}$ into k-space
(see R. Gross, A. Marx, „Festkörperphysik“, 3. Auflage, appendix H.2)

$$\mathcal{H}_{\mathrm{BCS}} = \underbrace{\sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma}}_{\text{energy of non-interacting free electron gas}} + \underbrace{\frac{1}{2} \sum_{\sigma_1,\sigma_2} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}}^{N} V_{\mathbf{q}}\, \hat{c}^{\dagger}_{\mathbf{k_1+q},\sigma_1} \hat{c}^{\dagger}_{\mathbf{k_2-q},\sigma_2} \hat{c}_{\mathbf{k_2},\sigma_2} \hat{c}_{\mathbf{k_1},\sigma_1}}_{\text{interaction energy}}$$

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}, V_{\mathrm{ext}}(\mathbf{r}) = 0$$

$$V_{\mathbf{q}} = \frac{1}{\Omega} \int_{\Omega} V(\mathbf{r})\, \mathrm{e}^{\imath \mathbf{q}\cdot\mathbf{r}} \mathrm{d}V$$

factor $\frac{1}{2}$ avoids double counting

operator describes scattering from state
$(\mathbf{k}_1, \sigma_1\, ; \mathbf{k}_2, \sigma_2)$ into $(\mathbf{k}_1 + \mathbf{q}\, , \sigma_1\, ;\ \mathbf{k}_2 - \mathbf{q}, \sigma_2)$ by exchange of phonon with wave vector $\boldsymbol{q}$

4.2 The BCS Ground State

formalism of second quantization is used (>1927, Dirac, Fock, Jordan et al.)

BCS Hamiltonian for N interacting electrons

simplification of interaction term for pairs with $\mathbf{k}_1 = \mathbf{k},\ \mathbf{k}_2 = -\mathbf{k},\ \ \sigma_1 = \uparrow,\ \sigma_2 = \downarrow$ and $V_\mathbf{q} = V_{\mathbf{k},\mathbf{k}'}$ with $\mathbf{q} = \mathbf{k} - \mathbf{k}'$

$$\frac{1}{2}\sum_{\sigma_1,\sigma_2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}}^{N} V_\mathbf{q}\, \hat{c}^\dagger_{\mathbf{k}_1+\mathbf{q},\sigma_1}\hat{c}^\dagger_{\mathbf{k}_2-\mathbf{q},\sigma_2}\hat{c}_{\mathbf{k}_2,\sigma_2}\hat{c}_{\mathbf{k}_1,\sigma_1} \Rightarrow \sum_{\mathbf{k},\mathbf{k}'}^{N} V_{\mathbf{k},\mathbf{k}'}\, \underbrace{\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}}_{P^\dagger_\mathbf{k}}\underbrace{\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}}_{P_{\mathbf{k}'}}$$

summation over spin yields factor 2

two particle interaction potential

pair **creation** and **annihilation** operators

$$\mathcal{H}_\mathrm{BCS} = \sum_\sigma\sum_\mathbf{k} \varepsilon_\mathbf{k}\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'}^{N} V_{\mathbf{k},\mathbf{k}'}\, \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}$$

often the energy is given with respect to chemical potential μ

➔ $\varepsilon_\mathbf{k} = \frac{\hbar^2\mathbf{k}^2}{2m}$ is replaced by $\xi_\mathbf{k} = \varepsilon_\mathbf{k} - \mu$

4.2 The BCS Ground State

R. Gross and A. Marx , © Walther-Meißner-Institut (2004 - 2021)

basic definitions, abreviations, assumptions, ….

1. weak isotropic interaction: $V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -V_0 & \text{for } |\xi_\mathbf{k}|, |\xi_{\mathbf{k}'}| < \hbar\omega_\mathrm{D} \\ 0 & \text{else} \end{cases}$ $\qquad V_0 D(E_\mathrm{F}) \ll 1$

2. pairing (Gorkov) amplitude: $g_{\mathbf{k}\sigma_1\sigma_2} \equiv \langle c_{-\mathbf{k}\sigma_1} c_{\mathbf{k}\sigma_2} \rangle \neq 0$

$$g^*_{\mathbf{k}\sigma_1\sigma_2} \equiv \left\langle c^\dagger_{-\mathbf{k}\sigma_1} c^\dagger_{\mathbf{k}\sigma_2} \right\rangle \neq 0$$

$\langle\cdots\rangle$ = statistical average

3. Pauli principle: pairing amplitude is antisymmetric for interchanging spins and wave vector:

$$g_{\mathbf{k}\sigma_1\sigma_2} = -g_{-\mathbf{k}\sigma_2\sigma_1}$$

4. spin part allows to distinguish between singlet and triplet pairing:

$$S = \begin{cases} 0 & m_s = 0 & \text{singlet pairing} \\ 1 & m_s = -1,0,+1 & \text{triplet pairing} \end{cases}$$

5. pairing potential:

$$\Delta_{\mathbf{k}\sigma_1\sigma_2} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}'\sigma_1\sigma_2}$$

$$\Delta^*_{\mathbf{k}'\sigma_1\sigma_2} \equiv -\sum_{\mathbf{k}} V_{\mathbf{k},\mathbf{k}'} g^*_{\mathbf{k}\sigma_1\sigma_2}$$

statistical average of pairing interaction

4.2 The BCS Ground State

calculation of the ground state energy

- ***Hamilton operator***:

$$\mathcal{H}_{\text{BCS}} = \sum_{\sigma}\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \underbrace{\hat{c}^{\dagger}_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma}}_{n_{\mathbf{k}\sigma} \,=\, \text{particle number operator}} + \sum_{\mathbf{k},\mathbf{k}'}^{N} V_{\mathbf{k},\mathbf{k}'}\, \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}$$

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} = \xi_{\mathbf{k}} + \mu$$

- how to solve the ***Schrödinger equation*** ?

→ most general form of N-electron wave function:

$$|\Psi_N\rangle = \sum g(\mathbf{k}_i, \dots, \mathbf{k}_l)\, \hat{c}^{\dagger}_{\mathbf{k}_i\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}_i\downarrow} \;\dots\; \hat{c}^{\dagger}_{\mathbf{k}_l\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}_l\downarrow}\, |0\rangle$$

\# of possibilities to place $N/2$ particles on M sites:

$$\frac{M!}{[M-(N/2)]!\,(N/2)!}$$

problem: huge number of possible realizations, typically $10^{10^{20}}$

➔ ***mean field approach***: occupation probability of state **k** only depends only on ***average occupation probability*** of other states

→ ***Bardeen, Cooper*** and ***Schrieffer*** used the following Ansatz (mean-field approach):

$$|\Psi_{\text{BCS}}\rangle = \prod_{\mathbf{k}=\mathbf{k}_1,\dots,\mathbf{k}_M} \left(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\right)|0\rangle$$

$|u_{\mathbf{k}}|^2$: probability that pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is empty

$|v_{\mathbf{k}}|^2$: probability that pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is occupied

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

4.2 The BCS Ground State

How to guess the BCS many particle wavefunction?

$$|\Psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}=\mathbf{k}_1,\ldots,\mathbf{k}_M} \left(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\right)|0\rangle$$

wave function assumed by Bardeen, Cooper and Schrieffer

➔ assume that the macroscopic wave function $\psi(\mathbf{r},t) = \psi_0(\mathbf{r},t)\mathrm{e}^{i\theta(\mathbf{r},t)}$ can be described by a ***coherent many particle state of fermions*** (motivated by strong overlap of Cooper pairs)

- ***coherent state of bosons***

discussed first by ***Erwin Schrödinger*** in 1926 when searching for a state of the quantum mechanical harmonic oscillator approximating best the behavior of a classical harmonic oscillator

E. Schrödinger, Der stetige Übergang von der Mikro- zur Makromechanik, Die Naturwissenschaften 14, 664-666 (1926).

transferred later by ***Roy J. Glauber*** to Fock state

R. J. Glauber, Coherent and Incoherent States of the Radiation Field, Phys. Rev. 131, 2766-2788 (1963).

Nobel Prize in Physics 2005 "***for his contribution to the quantum theory of optical coherence***", with the other half shared by John L. Hall and Theodor W. Hänsch.

4.2 The BCS Ground State

- ***Fock state representation of coherent state of bosons***

coherent state $|\alpha\rangle$ is expressed as an infinite linear combination of number (Fock) states

$$|\phi_n\rangle = \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n|0\rangle$$

boson creation operator

vacuum state

$$|\alpha\rangle = \mathrm{e}^{-|\alpha|^2/2}\underbrace{\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}}_{\text{normalization}}|\phi_n\rangle = \mathrm{e}^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\left(\alpha a^\dagger\right)^n}{n!}|0\rangle = \mathrm{e}^{-|\alpha|^2/2}\mathrm{e}^{\left(\alpha a^\dagger\right)}|0\rangle$$

Schrödinger (1926)

$\alpha = |\alpha|e^{i\varphi}$ is complex number

probability for occupation of n particles is given by Poisson distribution

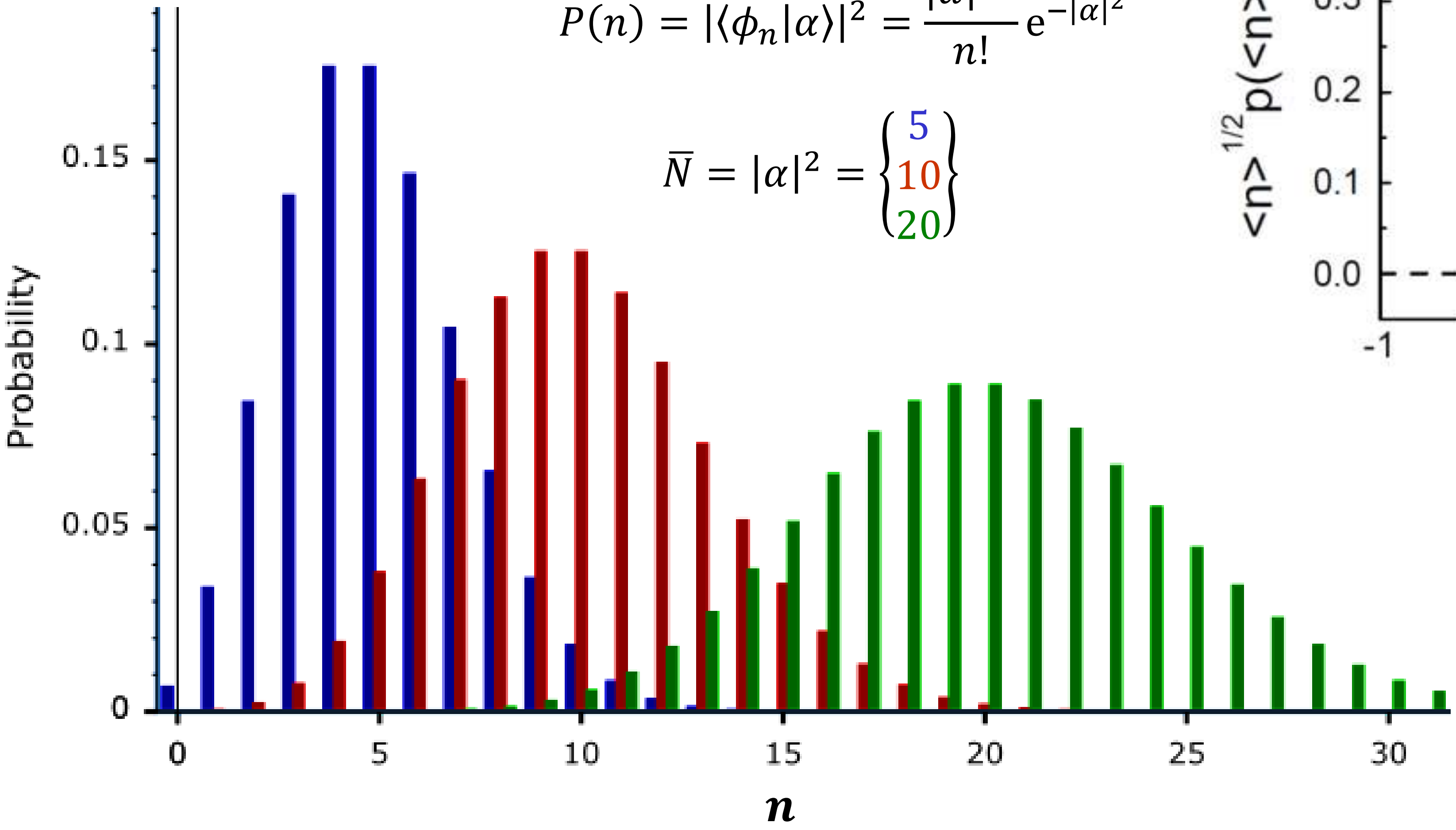
$$P(n) = |\langle\phi_n|\alpha\rangle|^2 = \frac{|\alpha|^{2n}}{n!}\mathrm{e}^{-|\alpha|^2}$$

- expectation value of number operator: $N = |\alpha|^2, \quad \Delta N = |\alpha| = \sqrt{N} \gg 1$
- relative standard deviation: $\frac{\Delta N}{N} = \frac{1}{\sqrt{N}} \ll 1$ (as $N \gg 1$)
- uncertainty relation $\Delta N\,\Delta\varphi \geq \frac{1}{2}, \quad \Delta\varphi \ll 1$

application: **coherent photonic state generated by laser**

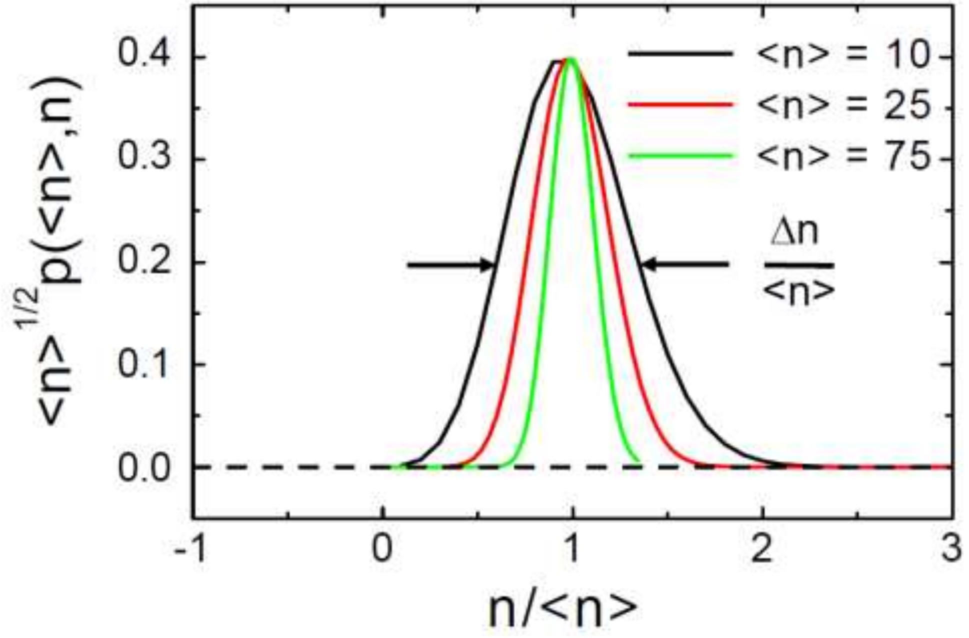
4.2 The BCS Ground State

- ***Poisson distribution***



$$P(n) = |\langle\phi_n|\alpha\rangle|^2 = \frac{|\alpha|^{2n}}{n!}\mathrm{e}^{-|\alpha|^2}$$

$$\bar{N} = |\alpha|^2 = \begin{Bmatrix} 5 \\ 10 \\ 20 \end{Bmatrix}$$



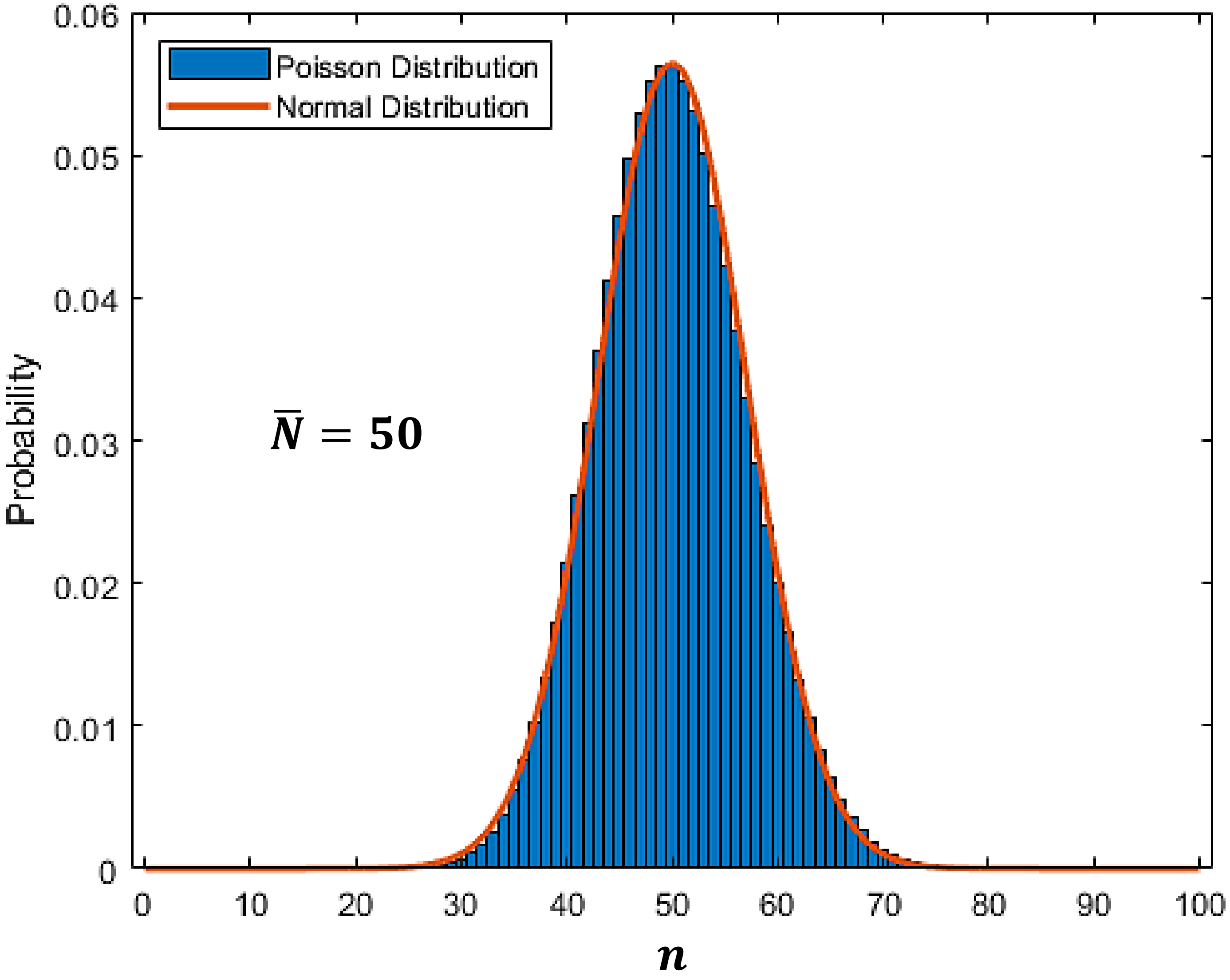
4.2 The BCS Ground State

- ***Poisson and normal distribution***

$$\boldsymbol{P(n)} = |\langle \phi_n | \alpha \rangle|^2 = \frac{|\alpha|^{2n}}{n!} \mathrm{e}^{-|\alpha|^2}$$

for large $\overline{N} = |\alpha|^2$ the Poisson distribution apporaches the normal (Gaussian) distribution:

$$\boldsymbol{P_{\overline{N}}(n)} = \frac{1}{\sqrt{2\pi \overline{N}}} \exp\left(-\frac{(n-\overline{N})^2}{2\overline{N}}\right)$$



4.2 The BCS Ground State

- ***Fock state representation of coherent state of fermions***

starting point: coherent bosonic state $|\alpha\rangle = \mathrm{e}^{-|\alpha|^2/2}\,\exp\left(\alpha a^\dagger\right)|0\rangle$

in analogy: **coherent fermionic state**

$$\boxed{|\Psi_{\mathrm{BCS}}\rangle = c_1 \exp\left(\sum_{\mathbf{k}} \alpha_{\mathbf{k}}\, P_{\mathbf{k}}^\dagger\right)|0\rangle}$$

summation over $\mathbf{k}$ since we have many fermionic modes

➢ we make use of the fact that higher powers of fermionic creation operators disappear due to ***Pauli principle*** (*key difference to bosonic system*):

$$P_{\mathbf{k}}^\dagger P_{\mathbf{k}}^\dagger = \left(P_{\mathbf{k}}^\dagger\right)^2 = \hat{\mathrm{c}}_{\mathbf{k}\uparrow}^\dagger \hat{\mathrm{c}}_{-\mathbf{k}\downarrow}^\dagger \hat{\mathrm{c}}_{\mathbf{k}\uparrow}^\dagger \hat{\mathrm{c}}_{-\mathbf{k}\downarrow}^\dagger = -\hat{\mathrm{c}}_{\mathbf{k}\uparrow}^\dagger \hat{\mathrm{c}}_{\mathbf{k}\uparrow}^\dagger \hat{\mathrm{c}}_{-\mathbf{k}\downarrow}^\dagger \hat{\mathrm{c}}_{-\mathbf{k}\downarrow}^\dagger = 0$$

⇒ $$|\Psi_{\mathrm{BCS}}\rangle = c_1 \exp\left(\sum_{\mathbf{k}} \alpha_{\mathbf{k}}\, P_{\mathbf{k}}^\dagger\right)|0\rangle = c_1 \prod_{\mathbf{k}} \exp\left(\alpha_{\mathbf{k}}\, P_{\mathbf{k}}^\dagger\right)|0\rangle = c_1 \prod_{\mathbf{k}} \left(1 + \alpha_{\mathbf{k}}\, P_{\mathbf{k}}^\dagger\right)|0\rangle$$

normalization: $\langle\Psi_{\mathrm{BCS}}^\star|\Psi_{\mathrm{BCS}}\rangle = c_1^2\left\langle 0\middle|\prod_{\mathbf{k}}\left(1+\alpha_{\mathbf{k}}^*\,P_{\mathbf{k}}\ \right)\left(1+\alpha_{\mathbf{k}}\,P_{\mathbf{k}}^\dagger\right)\middle|0\right\rangle = 1$ satisfied if all factors = 1

$$1 = c_1^2\left\langle 0\middle|\left(1+\alpha_{\mathbf{k}}^*\,P_{\mathbf{k}}\ \right)\left(1+\alpha_{\mathbf{k}}\,P_{\mathbf{k}}^\dagger\right)\middle|0\right\rangle = c_1^2\left(1+|\alpha_{\mathbf{k}}|^2\right)$$ ⇒ $$\boxed{c_1 = \frac{1}{\sqrt{\left(1+|\alpha_{\mathbf{k}}|^2\right)}}}$$

4.2 The BCS Ground State

- ***BCS ground state as coherent state of fermions***

$$|\Psi_{\mathrm{BCS}}\rangle = c_1 \prod_{\mathbf{k}} \left(1 + \alpha_{\mathbf{k}}\, P_{\mathbf{k}}^{\dagger}\right)|0\rangle = \frac{1}{\sqrt{(1+|\alpha_{\mathbf{k}}|^2)}} \prod_{\mathbf{k}} \left(1 + \alpha_{\mathbf{k}}\, P_{\mathbf{k}}^{\dagger}\right)|0\rangle$$

$$\Rightarrow \quad \boxed{|\Psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}^{\dagger} \hat{c}_{-\mathbf{k}\downarrow}^{\dagger}\right)|0\rangle}$$

$$\left.\begin{aligned} u_{\mathbf{k}} &= \frac{1}{\sqrt{(1+|\alpha_{\mathbf{k}}|^2)}} \\ v_{\mathbf{k}} &= \frac{\alpha_{\mathbf{k}}}{\sqrt{(1+|\alpha_{\mathbf{k}}|^2)}} \end{aligned}\right\} \quad \text{coherence factors}$$

coherent superposition of pair states → only average pair number is fixed

$$\Delta N = \sqrt{N} \gg 1 \qquad \frac{\Delta N}{N} = \frac{1}{\sqrt{N}} \ll 1 \qquad \Delta N\, \Delta\varphi \geq \tfrac{1}{2} \;\; \Rightarrow \;\; \Delta\varphi \ll 1$$

➔ uncertainties $\Delta N/N$ and $\Delta\varphi/2\pi$ are very small for large average pair numer $\overline{N}$

$u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are complex probability amplitudes:

$|u_{\mathbf{k}}|^2$: probability that pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is empty

$|v_{\mathbf{k}}|^2$: probability that pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is occupied

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

4.2 The BCS Ground State

- *some expectation values (1)*:

$$|\Psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}=\mathbf{k}_1,\dots,\mathbf{k}_M} \left(u_{\mathbf{k}} + v_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow}\right)|0\rangle$$

we use the identities:

- $\langle \mathcal{O}\phi|\Psi\rangle = \langle \phi|\mathcal{O}^\dagger\Psi\rangle$
- $\langle \phi|(\mathcal{AB})^\dagger|\Psi\rangle = \langle \phi|\mathcal{B}^\dagger\mathcal{A}^\dagger|\Psi\rangle$

(see exercise sheets for detailed derivation)

single spin particle number

$$\langle n_{\mathbf{k}\uparrow}\rangle = \left\langle \Psi_{\mathrm{BCS}}\middle|\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\middle|\Psi_{\mathrm{BCS}}\right\rangle$$

$$= \left\langle 0\middle|\left(u^\star_{\mathbf{k}} + v^\star_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}\right)\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\left(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\right) \times \prod\nolimits_{\mathbf{l}\neq\mathbf{k}} \underbrace{\left(u^\star_{\mathbf{l}} + v^\star_{\mathbf{l}}\hat{c}_{-\mathbf{l}\downarrow}\hat{c}_{\mathbf{l}\uparrow}\right)\left(u_{\mathbf{l}} + v_{\mathbf{l}}\hat{c}^\dagger_{\mathbf{l}\uparrow}\hat{c}^\dagger_{-\mathbf{l}\downarrow}\right)}_{|u_{\mathbf{l}}|^2 + |v_{\mathbf{l}}|^2 = 1}\middle|0\right\rangle$$

$$\langle n_{\mathbf{k}\uparrow}\rangle = |u_{\mathbf{k}}|^2 \underbrace{\left\langle 0\middle|\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\middle|0\right\rangle}_{=0} + u^\star_{\mathbf{k}}v_{\mathbf{k}}\underbrace{\left\langle 0\middle|\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\middle|0\right\rangle}_{=0} + v^\star_{\mathbf{k}}u_{\mathbf{k}}\underbrace{\left\langle 0\middle|\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\middle|0\right\rangle}_{=0} + |v_{\mathbf{k}}|^2\underbrace{\left\langle 0\middle|\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\middle|0\right\rangle}_{=1}$$

since $n_{\mathbf{k}\uparrow}|0\rangle = 0|0\rangle$

use even number of permutations to transform into terms $n_{\mathbf{k}\uparrow}|0\rangle = 0|0\rangle$

use anti-commutator $\left\{\hat{c}_{\mathbf{k}\sigma}\, , \hat{c}^\dagger_{\mathbf{k}'\sigma'}\right\} = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}$

$$\langle n_{\mathbf{k}\uparrow}\rangle = |v_{\mathbf{k}}|^2$$

average total pair number

$$\bar{N} = \langle\mathcal{N}\rangle = \sum_{\mathbf{k}\sigma}\langle n_{\mathbf{k}\sigma}\rangle = \sum_{\mathbf{k}\sigma}|v_{\mathbf{k}}|^2 = 2\sum_{\mathbf{k}}|v_{\mathbf{k}}|^2 = \sum_{\mathbf{k}}|v_{\mathbf{k}}|^2 - |u_{\mathbf{k}}|^2 + 1$$

4.2 The BCS Ground State

- *some expectation values (2)*:

(see exercise sheets for detailed derivation)

statistical fluctuation of averge particle number

$$\Delta N = \left\langle \mathcal{N} - \langle \mathcal{N} \rangle \right\rangle^2 = \langle \mathcal{N}^2 \rangle - \langle \mathcal{N} \rangle^2$$

$$\bar{N} = \langle \mathcal{N} \rangle = \sum_{\mathbf{k}\sigma} \langle n_{\mathbf{k}\sigma} \rangle = \sum_{\mathbf{k}\sigma} |v_{\mathbf{k}}|^2 = 2 \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2$$

$$\Delta N = \sqrt{4 \sum_{\mathbf{k}} |u_{\mathbf{k}}|^2 |v_{\mathbf{k}}|^2} \propto \bar{N}$$

note that $\sum_{\mathbf{k}} \propto$ volume $\propto \bar{N}$, as sum over $\mathbf{k}$ values in specific energy interval scales with volume at constant particle density

ΔN gets very large for large $\bar{N}$, but **relative fluctuation $\Delta N / \bar{N}$ becomes vanishingly small**

4.2 The BCS Ground State

- *some expectation values (3)*:

(see exercise sheets for detailed derivation)

pairing or Gorkov amplitude

$$g_{\mathbf{k}\sigma_1\sigma_2} \equiv \langle \Psi_{\mathrm{BCS}} | c_{-\mathbf{k}\sigma_1} c_{\mathbf{k}\sigma_2} | \Psi_{\mathrm{BCS}} \rangle = u_{\mathbf{k}} v_{\mathbf{k}}^\star$$

$$g^\dagger_{\mathbf{k}\sigma_1\sigma_2} \equiv \left\langle \Psi_{\mathrm{BCS}} \middle| c^\dagger_{-\mathbf{k}\sigma_1} c^\dagger_{\mathbf{k}\sigma_2} \middle| \Psi_{\mathrm{BCS}} \right\rangle = u^\star_{\mathbf{k}} v_{\mathbf{k}}$$

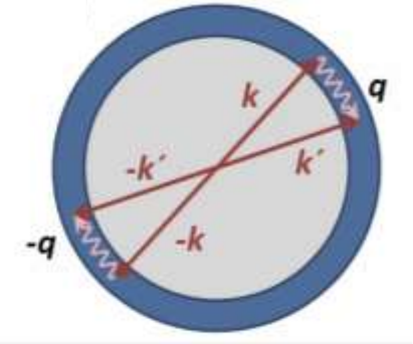
BCS Hamiltonian

$$\mathcal{H}_{\mathrm{BCS}} = \sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \, \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \, \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow}$$

$$\left\langle \Psi_{\mathrm{BCS}} \middle| \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} \middle| \Psi_{\mathrm{BCS}} \right\rangle = |v_{\mathbf{k}}|^2$$

$$\left\langle \Psi_{\mathrm{BCS}} \middle| \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} \middle| \Psi_{\mathrm{BCS}} \right\rangle = v_{\mathbf{k}} \, v^\star_{\mathbf{k}'} u_{\mathbf{k}'} u^\star_{\mathbf{k}}$$

$$\langle \Psi_{\mathrm{BCS}} | \mathcal{H}_{\mathrm{BCS}} | \Psi_{\mathrm{BCS}} \rangle = \underbrace{2 \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} |v_{\mathbf{k}}|^2}_{\substack{= \bar{N}\,\varepsilon_{\mathbf{k}} \\ \text{(kinetic energy)}}} + \underbrace{\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \, v_{\mathbf{k}} \, v^\star_{\mathbf{k}'} u_{\mathbf{k}'} u^\star_{\mathbf{k}}}_{\text{interaction energy}}$$



4.2 The BCS Ground State

task: find the minimum of the expectation value $\langle \Psi_{\mathrm{BCS}} | \mathcal{H}_{\mathrm{BCS}} | \Psi_{\mathrm{BCS}} \rangle$ by variational method ($T = 0$)

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} = \xi_{\mathbf{k}} + \mu$$

$$\bar{N} = 2 \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2$$

we take the energy relative to the chemical potential μ

$$\langle E_{\mathrm{BCS}} - \bar{N}\,\mu \rangle = \langle \Psi_{\mathrm{BCS}} | \mathcal{H}_{\mathrm{BCS}} - \bar{N}\,\mu \, | \Psi_{\mathrm{BCS}} \rangle = 2 \sum_{\mathbf{k}} (\xi_{\mathbf{k}} + \mu)\, |v_{\mathbf{k}}|^2 - \bar{N}\,\mu + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, v_{\mathbf{k}}\, v_{\mathbf{k}'}^{\star} u_{\mathbf{k}'} u_{\mathbf{k}}^{\star}$$

$$\langle E_{\mathrm{BCS}} - \bar{N}\,\mu \rangle = \langle \Psi_{\mathrm{BCS}} | \mathcal{H}_{\mathrm{BCS}} - \bar{N}\,\mu \, | \Psi_{\mathrm{BCS}} \rangle = 2 \sum_{\mathbf{k}} \xi_{\mathbf{k}}\, |v_{\mathbf{k}}|^2 - \bar{N}\,\mu + \bar{N}\,\mu + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, v_{\mathbf{k}}\, v_{\mathbf{k}'}^{\star} u_{\mathbf{k}'} u_{\mathbf{k}}^{\star}$$

$$\delta \left\{ 2 \sum_{\mathbf{k}} \xi_{\mathbf{k}}\, |v_{\mathbf{k}}|^2 + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, v_{\mathbf{k}}\, v_{\mathbf{k}'}^{\star} u_{\mathbf{k}'} u_{\mathbf{k}}^{\star} \right\} = 0$$

minimization of expectation value by variation of the probability amplitudes yields expressions for $|u_{\mathbf{k}}|^2$ and $|v_{\mathbf{k}}|^2$

4.2 The BCS Ground State

Method 1: we assume that $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are real and satisfy $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ (Bardeen, Cooper, Schrieffer: 1957)

$$u_{\mathbf{k}} = \sin\theta_{\mathbf{k}}\,, \qquad v_{\mathbf{k}} = \cos\theta_{\mathbf{k}}\,, \qquad \text{and} \qquad 2\sin\theta_{\mathbf{k}}\cos\theta_{\mathbf{k}} = \sin 2\theta_{\mathbf{k}}$$

$$\langle E_{\mathrm{BCS}} - \bar{N}\,\mu\rangle = 2\sum_{\mathbf{k}} \xi_{\mathbf{k}}\,|v_{\mathbf{k}}|^2 + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, v_{\mathbf{k}}\, v^{\star}_{\mathbf{k}'} u_{\mathbf{k}'} u^{\star}_{\mathbf{k}} = 2\sum_{\mathbf{k}} \xi_{\mathbf{k}} \cos^2\theta_{\mathbf{k}} + \frac{1}{4}\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \sin 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{k}'}$$

minimization $$\frac{\partial\langle E_{\mathrm{BCS}} - \bar{N}\,\mu\rangle}{\partial\theta_{\mathbf{l}}} = 0$$

$$\frac{\partial\langle E_{\mathrm{BCS}} - \bar{N}\,\mu\rangle}{\partial\theta_{\mathbf{l}}} = 0 = 2\xi_{\mathbf{l}}\underbrace{(-2\cos\theta_{\mathbf{l}}\sin\theta_{\mathbf{l}})}_{=-\sin 2\theta_{\mathbf{l}}} + \underbrace{\frac{1}{4}\frac{\partial}{\partial\theta_{\mathbf{l}}}\sum_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \sin 2\theta_{\mathbf{k}'}}_{\frac{1}{4}(2\cos 2\theta_{\mathbf{l}})\sum_{\mathbf{k}'} V_{\mathbf{l},\mathbf{k}'}\sin 2\theta_{\mathbf{k}'} + \sum_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} V_{\mathbf{k},\mathbf{l}} 2\cos 2\theta_{\mathbf{l}}}$$

$$2\xi_{\mathbf{l}}\sin 2\theta_{\mathbf{l}} = \frac{1}{2}\cos 2\theta_{\mathbf{l}}\left(\sum_{\mathbf{k}'} V_{\mathbf{l},\mathbf{k}'}\sin 2\theta_{\mathbf{k}'} + \sum_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} V_{\mathbf{k},\mathbf{l}}\right) \underbrace{=}_{V_{\mathbf{l},\mathbf{k}'} = V_{\mathbf{k},\mathbf{l}}} \cos 2\theta_{\mathbf{l}}\sum_{\mathbf{k}'} V_{\mathbf{l},\mathbf{k}'}\sin 2\theta_{\mathbf{k}'}$$

$$\tan 2\theta_{\mathbf{l}} = \frac{\sum_{\mathbf{k}'} V_{\mathbf{l},\mathbf{k}'}\sin\theta_{\mathbf{k}'}\cos\theta_{\mathbf{k}'}}{\xi_{\mathbf{k}}}$$

4.2 The BCS Ground State

- we switch back to old summation ($\mathbf{l} \rightarrow \mathbf{k}$) and restore $u_\mathbf{k} = \sin\theta_\mathbf{k}\,,\ v_\mathbf{k} = \cos\theta_\mathbf{k}$:

$$\Rightarrow \quad \tan 2\theta_\mathbf{k} = \frac{\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'}}{\xi_\mathbf{k}}$$

- we further use the pairing strength $\Delta_\mathbf{k} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'}$ $\quad\Rightarrow\quad \tan 2\theta_\mathbf{k} = -\frac{\Delta_\mathbf{k}}{\xi_\mathbf{k}}$

- with $\tan 2\theta_\mathbf{k} = \frac{\sin 2\theta_\mathbf{k}}{\cos 2\theta_\mathbf{k}} = \frac{2\sin\theta_\mathbf{k}\cos\theta_\mathbf{k}}{\underbrace{\cos^2\theta_\mathbf{k}}_{\frac{1}{2}+\frac{1}{2}\cos 2\theta_\mathbf{k}} - \underbrace{\sin^2\theta_\mathbf{k}}_{\frac{1}{2}-\frac{1}{2}\cos 2\theta_\mathbf{k}}} = \frac{2u_\mathbf{k}v_\mathbf{k}}{{u_\mathbf{k}}^2 - {v_\mathbf{k}}^2}$ we obtain $\quad\Rightarrow\quad \frac{2u_\mathbf{k}v_\mathbf{k}}{{u_\mathbf{k}}^2 - {v_\mathbf{k}}^2} = -\frac{\Delta_\mathbf{k}}{\xi_\mathbf{k}}$

- we define $E_\mathbf{k} \equiv \sqrt{\xi_\mathbf{k}^2 + \Delta_\mathbf{k}^2}$ and obtain the following expressions for $u_\mathbf{k}$ and $v_\mathbf{k}$ minimizing the energy

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

$$u_\mathbf{k}v_\mathbf{k} = g_\mathbf{k} = \frac{\Delta_\mathbf{k}}{2E_\mathbf{k}} \qquad \Delta_\mathbf{k} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}$$

pairing amplitude **self-consistent gap equation**

for k-independent $\Delta_\mathbf{k}$: minimum energy is $E_\mathbf{k} = \Delta$

we will see later that $E_\mathbf{k}$ is the energy required to add a single excitation to the ground state

➔ **minimum excitation energy is required, therefore Δ represents an energy gap in the excitation spectrum**

4.2 The BCS Ground State

$$|u_{\mathbf{k}}|^2 = \frac{1}{2}\left[1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right]$$

$$|v_{\mathbf{k}}|^2 = \frac{1}{2}\left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right]$$

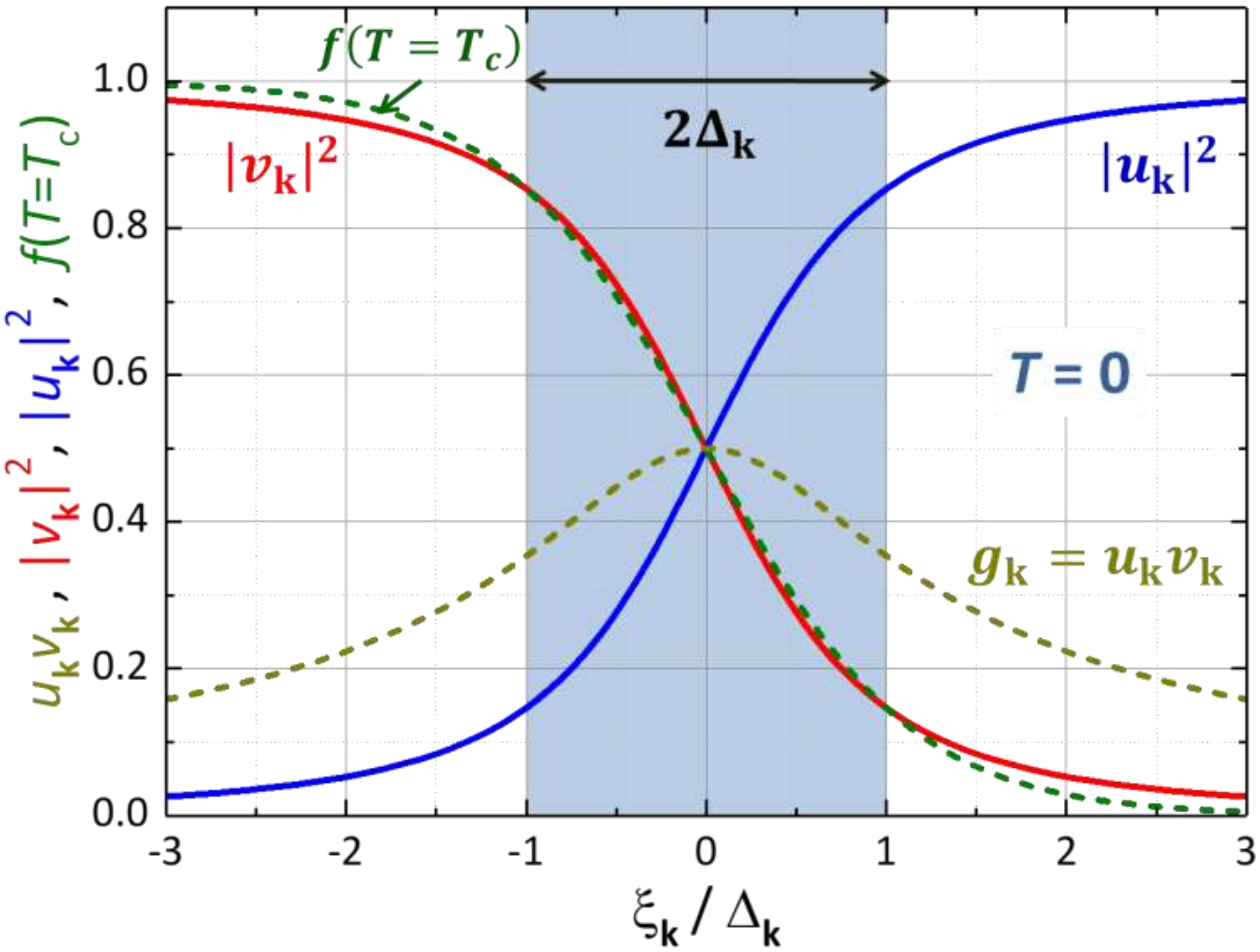
$$u_{\mathbf{k}}v_{\mathbf{k}} = g_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$$

$|v_{\mathbf{k}}|^2$: probability that $\mathbf{k}$ is occupied

→ probability $|v_{\mathbf{k}}|^2$ is smeared out around Fermi level even at $T = 0$:
increase of kinetic energy

→ smearing is required to allow for pairing interaction:
reduction of potential energy > increase of kinetic energy

→ $|v_{\mathbf{k}}|^2 \simeq f(T = T_c)$



4.2 The BCS Ground State

Method 2: we use the method of **Lagrangian multipliers**

- we use the following two constraints:

$$\phi_1 = 0 = \langle \mathcal{N} \rangle - 2\sum_{\mathbf{k}} |v_{\mathbf{k}}|^2 = \langle \mathcal{N} \rangle - \sum_{\mathbf{k}} |v_{\mathbf{k}}|^2 - |u_{\mathbf{k}}|^2 + 1$$

$$\phi_2 = 0 = |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 - 1 = u_{\mathbf{k}} u_{\mathbf{k}}^\star + v_{\mathbf{k}} v_{\mathbf{k}}^\star - 1$$

$$\mathcal{L}(u_{\mathbf{k}}^\star, v_{\mathbf{k}}^\star, \lambda_1, \lambda_2) = \langle E_{\mathrm{BCS}} \rangle - \lambda_1 \phi_1 - \lambda_2 \phi_2$$

λ_1, λ_2: Lagrangian multipliers

with $\langle E_{\mathrm{BCS}} \rangle = 2\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} |v_{\mathbf{k}}|^2 + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, v_{\mathbf{k}}\, v_{\mathbf{k}'}^\star u_{\mathbf{k}'} u_{\mathbf{k}}^\star = 2\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} (|v_{\mathbf{k}}|^2 - |u_{\mathbf{k}}|^2 + 1) + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, v_{\mathbf{k}}\, v_{\mathbf{k}'}^\star u_{\mathbf{k}'} u_{\mathbf{k}}^\star$

- by setting the partial derivative of the Lagrangian function $\mathcal{L}$ with respect to $u_{\mathbf{k}}^\star$ and$v_{\mathbf{k}}^\star$ to zero we obtain the eigenvalue eqns:

$$\begin{aligned} (\varepsilon_{\mathbf{k}} - \lambda_1) u_{\mathbf{k}} + \Delta_{\mathbf{k}} v_{\mathbf{k}} - \lambda_2 u_{\mathbf{k}} &= 0 \\ \Delta_{\mathbf{k}}^\dagger u_{\mathbf{k}} - (\varepsilon_{\mathbf{k}} - \lambda_1) v_{\mathbf{k}} - \lambda_2 v_{\mathbf{k}} &= 0 \end{aligned} \quad \Rightarrow \quad \begin{pmatrix} (\varepsilon_{\mathbf{k}} - \lambda_1) & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^\dagger & -(\varepsilon_{\mathbf{k}} - \lambda_1) \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \lambda_2 \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}$$

with $\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}'}$
$= -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'}^\star$

- physical meaning of the Lagrangian multipliers
  - i. λ_1 shifts the energy and corresponds the the chemical potential μ
  - ii. λ_2 corresponds to the eigenvalue of the the vector $(u_{\mathbf{k}}, v_{\mathbf{k}})$ and is given by the energy $\pm E_{\mathbf{k}}$ of the quasiparticles excited out of the condensate

- solving the eigenvalue eqns yields $E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$, $|u_{\mathbf{k}}|^2 = \frac{1}{2}\left[1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right]$, $|v_{\mathbf{k}}|^2 = \frac{1}{2}\left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right]$, $u_{\mathbf{k}} v_{\mathbf{k}}^\star = g_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$

4.2.1 The BCS Gap Equation

solution of the self-consistent gap equation ($T = 0$)

$$\Delta_{\mathbf{k}} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2\sqrt{\xi_{\mathbf{k}'}^{2} + \left|\Delta_{\mathbf{k}'}\right|^{2}}}$$

cannot be solved analytically in the general case

- simple solution only if the gap $\Delta_{\mathbf{k}}$ and the interaction potential $V_{\mathbf{k},\mathbf{k}'}$ are assumed $\mathbf{k}$-independent: $\Delta_{\mathbf{k}} = \Delta$, $V_{\mathbf{k},\mathbf{k}'} = -V_0$

$$1 = V_0 \sum_{\mathbf{k}'} \frac{1}{2\sqrt{\xi_{\mathbf{k}'}^{2} + |\Delta|^{2}}}$$

transforming sum into integration

with pair density $\widetilde{D}(E) \simeq D(E_\mathrm{F})/2$

$$1 = \frac{V_0 D(E_\mathrm{F})}{2} \int_{-\hbar\omega_\mathrm{D}}^{\hbar\omega_\mathrm{D}} \frac{\mathrm{d}\xi}{2\sqrt{\xi^{2} + |\Delta|^{2}}}$$

- with $\int \frac{dx}{\sqrt{x^2+a^2}} = \operatorname{arcsinh}\left(\frac{x}{a}\right)$ we obtain

$$1 = \frac{V_0 D(E_\mathrm{F})}{4} \int_{-\hbar\omega_\mathrm{D}}^{\hbar\omega_\mathrm{D}} \frac{\mathrm{d}\xi}{\sqrt{\xi^{2} + |\Delta|^{2}}} = \frac{V_0 D(E_\mathrm{F})}{4} \operatorname{arcsinh}\left(\frac{\hbar\omega_\mathrm{D}}{\Delta}\right)\Bigg|_{-\hbar\omega_\mathrm{D}}^{+\hbar\omega_\mathrm{D}} = \frac{V_0 D(E_\mathrm{F})}{2} \operatorname{arcsinh}\left(\frac{\hbar\omega_\mathrm{D}}{\Delta}\right)$$

$$\Rightarrow \quad \Delta = \frac{\hbar\omega_\mathrm{D}}{\sinh\left(2/V_0 D(E_\mathrm{F})\right)} \simeq 2\hbar\omega_\mathrm{D}\, \mathrm{e}^{-2/V_0 D(E_\mathrm{F})}$$

energy gap corresponds to binding energy estimated for single Cooper pair

factor 2 in argument of exp. function since we have assumed that the two additional electrons are in the $[E_\mathrm{F},\ E_\mathrm{F} + \hbar\omega_\mathrm{D}]$ and not between $[E_\mathrm{F} - \hbar\omega_\mathrm{D},\ E_\mathrm{F} + \hbar\omega_\mathrm{D}]$

$V_0 D(E_\mathrm{F}) \ll 1$: weak coupling approximation, $\sinh x \simeq \frac{1}{2}\exp x$

4.2.2 Ground State Energy

calculation of the BCS condensation energy

- calculate expectation value of BCS Hamiltonian for $T = 0$

$$E_{\mathrm{BCS}} = \langle \Psi_{\mathrm{BCS}} | \mathcal{H}_{\mathrm{BCS}} - \mu \mathcal{N} | \Psi_{\mathrm{BCS}} \rangle = 2 \sum_{\mathbf{k}} \xi_{\mathbf{k}} |v_{\mathbf{k}}|^2 + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \, v_{\mathbf{k}} \, v_{\mathbf{k}'}^{\star} u_{\mathbf{k}'} u_{\mathbf{k}}^{\star}$$

energy relative to chemical potential

$$\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \boldsymbol{\mu}$$

- we plug in the results for the coherence factors and the pair amplitude

$$|u_{\mathbf{k}}|^2 = \frac{1}{2}\left[1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right], \quad |v_{\mathbf{k}}|^2 = \frac{1}{2}\left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right], \quad u_{\mathbf{k}} v_{\mathbf{k}}^{\star} = g_{\mathbf{k}}^{*} = \frac{\Delta_{\mathbf{k}}^{*}}{2E_{\mathbf{k}}}, \quad u_{\mathbf{k}}^{\star} v_{\mathbf{k}} = g_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$$

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

$$E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^{2} + \Delta_{\mathbf{k}}^{2}},$$

$$E_{\mathrm{BCS}} = \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} - \frac{\xi_{\mathbf{k}}^{2}}{E_{\mathbf{k}}} \right) - \sum_{\mathbf{k}} g_{\mathbf{k}}^{*} \Delta_{\mathbf{k}} = \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} - \frac{\xi_{\mathbf{k}}^{2}}{E_{\mathbf{k}}} \right) \underbrace{- 2 \sum_{\mathbf{k}} g_{\mathbf{k}}^{*} \Delta_{\mathbf{k}}}_{- \sum_{\mathbf{k}} \Delta_{\mathbf{k}}^{2} / 2E_{\mathbf{k}}} + \sum_{\mathbf{k}} g_{\mathbf{k}}^{*} \Delta_{\mathbf{k}}$$

$$E_{\mathrm{BCS}} = \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - E_{\mathbf{k}}) + \sum_{\mathbf{k}} g_{\mathbf{k}}^{*} \Delta_{\mathbf{k}}$$

4.2.2 Ground State Energy

- for simplicity we assume for $V_{\mathbf{k},\mathbf{k}'} = -V_0$ and $\Delta_{\mathbf{k}} = \Delta$)

$$E_{\mathrm{BCS}} = \langle \Psi_{\mathrm{BCS}} | \mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu | \Psi_{\mathrm{BCS}} \rangle = \sum_{\mathbf{k}} \{\xi_{\mathbf{k}} - E_{\mathbf{k}} + \; g_{\mathbf{k}}^{*}\Delta\}$$

- subtract mean energy of normal state at $T = 0$ (making use of symmetry around μ)

$$\langle \Psi_{\mathrm{BCS}} | \mathcal{H}_{\mathrm{n}} - \mathcal{N}\mu | \Psi_{\mathrm{BCS}} \rangle = \lim_{\Delta \to 0} \langle \Psi_{\mathrm{BCS}} | \mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu | \Psi_{\mathrm{BCS}} \rangle = \sum_{\mathbf{k}} \xi_{\mathbf{k}} - |\xi_{\mathbf{k}}| = 2 \sum_{|\mathbf{k}| < \mathbf{k}_{\mathrm{F}}} \xi_{\mathbf{k}}$$

$$\Delta E \;= \sum_{|\mathbf{k}| < \mathbf{k}_{\mathrm{F}}} \xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta \, g_{\mathbf{k}}^{*} - 2\xi_{\mathbf{k}} + \sum_{|\mathbf{k}| \geq \mathbf{k}_{\mathrm{F}}} \xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta \, g_{\mathbf{k}}^{*}$$

- we use $-\xi_{\mathbf{k}} = |\xi_{\mathbf{k}}|$ for $|k| < k_{\mathrm{F}}$ and $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}$

$$\Delta E \;= 2 \sum_{|\mathbf{k}| \geq \mathbf{k}_{\mathrm{F}}} \left(\xi_{\mathbf{k}} - \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2} + \Delta \, g_{\mathbf{k}}^{*} \right) \underbrace{=}_{\Delta \, g_{\mathbf{k}}^{\dagger} = \frac{\Delta^2}{2\sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}}} 2 \sum_{|\mathbf{k}| \geq \mathbf{k}_{\mathrm{F}}} \left(\xi_{\mathbf{k}} - \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2} + \frac{\Delta^{2}}{2\sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}} \right)$$

4.2.2 Ground State Energy

$$\Delta E = 2 \sum_{|\mathbf{k}| \geq k_\mathrm{F}} \left(\xi_\mathbf{k} - \sqrt{\xi_\mathbf{k}^2 + |\Delta|^2} + \frac{\Delta^2}{2\sqrt{\xi_\mathbf{k}^2 + |\Delta|^2}} \right)$$

- replace summation by integration ……. after some algebra (see appendix H.3 in R. Gross, A. Marx, Festkörperphysik, 3. Auflage, de Gruyter (2018)):

$$\Delta E = E_\mathrm{cond}(0) = -\frac{1}{4} D(E_\mathrm{F})\, \Delta^2(0)$$

$D(E_\mathrm{F})$ = DOS for both spin directions

interpretation of the result:

- ➢ number of Cooper pairs: $\frac{D(E_\mathrm{F})}{2}\, \Delta(0)$
- ➢ average energy gain per Cooper pair: $-\frac{\Delta(0)}{2}$

- compare to $g_s - g_n = E_\mathrm{cond}(0) = -B_\mathrm{cth}^2(0)/2\mu_0$ (thermodynamics)

$$\Rightarrow \quad \mathrm{B_{cth}}(0) = \sqrt{\frac{\mu_0 D(E_\mathrm{F}) \Delta^2(0)}{2V}}$$

4.2.2 Ground State Energy

- condensation energy per volume:

$$\frac{E_{\mathrm{cond}}(0)}{V} = -\frac{1}{4}\,\frac{D(E_{\mathrm{F}})}{V}\,\Delta^2(0) = -\frac{1}{4}N(E_{\mathrm{F}})\,\Delta^2(0)$$

with $N(E_{\mathrm{F}}) = \frac{3n}{2E_{\mathrm{F}}}$ and $\frac{\Delta(0)}{k_{\mathrm{B}}T_c} = \frac{\pi}{\mathrm{e}^{\gamma}} = 1.7638\ldots$ we obtain

$$\frac{E_{\mathrm{cond}}(0)}{V} = -\frac{3}{8}\,n\,\frac{\Delta^2(0)}{E_{\mathrm{F}}} = \frac{3}{8}\left(\frac{\pi}{\mathrm{e}^{\gamma}}\right)^2\frac{(k_{\mathrm{B}}T_c)^2}{E_{\mathrm{F}}} = -1.167\;n\,\frac{(k_{\mathrm{B}}T_c)^2}{E_{\mathrm{F}}}$$

➔ **average condensation energy per electron is of the order of $(k_{\mathrm{B}}T_c)^2/E_{\mathrm{F}}$**

➔ **plausibility:**

only a small fraction $k_{\mathrm{B}}T_c/E_{\mathrm{F}}$ of the electrons is participating in pairing process and the average energy reduction per electron is about $k_{\mathrm{B}}T_c$

4.2.3 The Bogoliubov-Valatin Transformation

- so far we have found the BCS ground state wave function and the energy gap at zero temperature

- **next step**:
  - **determine the properties of the superconducting state at finite temperature**
  - **determine the energy of excitations out of the ground state**

- **how to proceed?**
  - **use BCS ground state as reference state**
  - **discuss effect of small deviations (e.g. by adding a small number of excitations to the ground state)**

- we use the identities (with $\delta g_{\mathbf{k}}$, $\delta g_{\mathbf{k}}^*$ being small)

$$\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} = \underbrace{\left\langle \hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} \right\rangle}_{g_{\mathbf{k}}} + \underbrace{\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} - \left\langle \hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} \right\rangle}_{\delta g_{\mathbf{k}}}$$

$$\hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger} = \underbrace{\left\langle \hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger} \right\rangle}_{g_{\mathbf{k}}^*} + \underbrace{\hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger} - \left\langle \hat{c}_{\mathbf{k}\uparrow}^{\dagger}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger} \right\rangle}_{\delta g_{\mathbf{k}}^*}$$

with pairing amplitude:

$$g_{\mathbf{k}\sigma_1\sigma_2} \equiv \left\langle c_{-\mathbf{k}\sigma_1} c_{\mathbf{k}\sigma_2} \right\rangle \neq 0$$

$$g_{\mathbf{k}\sigma_1\sigma_2}^{\dagger} \equiv \left\langle c_{-\mathbf{k}\sigma_1}^{\dagger} c_{\mathbf{k}\sigma_2}^{\dagger} \right\rangle \neq 0$$

as the particle number is usually very large, the fluctuations $\delta g_{\mathbf{k}}$, $\delta g_{\mathbf{k}}^*$ are very small and we can neglect quadratic terms in $\delta g_{\mathbf{k}}$, $\delta g_{\mathbf{k}}^*$

4.2.3 The Bogoliubov-Valatin Transformation

- rewriting of pair creation and annihilation operators in $\mathcal{H}_{\rm BCS} = \sum_{\sigma} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}\, \hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'}^{N} V_{\mathbf{k},\mathbf{k}'}\, \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}$

$$\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} = \underbrace{\left\langle \hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} \right\rangle}_{g_{\mathbf{k}}} + \underbrace{\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} - \left\langle \hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} \right\rangle}_{\delta g_{\mathbf{k}}}$$

$$\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} = \underbrace{\left\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} \right\rangle}_{g^*_{\mathbf{k}}} + \underbrace{\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} - \left\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} \right\rangle}_{\delta g^*_{\mathbf{k}}}$$

pairing amplitude:

$$g_{\mathbf{k}\sigma_1\sigma_2} \equiv \left\langle c_{-\mathbf{k}\sigma_1} c_{\mathbf{k}\sigma_2} \right\rangle \neq 0$$

$$g^*_{\mathbf{k}\sigma_1\sigma_2} \equiv \left\langle c^\dagger_{-\mathbf{k}\sigma_1} c^\dagger_{\mathbf{k}\sigma_2} \right\rangle \neq 0$$

- insert into Hamiltonian and consider only terms linear in $\delta g_{\mathbf{k}}^{(\dagger)}$

$$\mathcal{H}_{\rm BCS} - \mathcal{N}\mu = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}\, n_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \left[g^*_{\mathbf{k}}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow} + g_{\mathbf{k}'}\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} - g^*_{\mathbf{k}} g_{\mathbf{k}'} \right]$$

- make use of pair potential $\Delta_{\mathbf{k}\sigma_1\sigma_2} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, g_{\mathbf{k}'\sigma_1\sigma_2}$ $\qquad$ $\Delta^*_{\mathbf{k}\sigma_1\sigma_2} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, g^*_{\mathbf{k}'\sigma_1\sigma_2}$

⇨ $$\mathcal{H}_{\rm BCS} - \mathcal{N}\mu = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}\, n_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left[\Delta^*_{\mathbf{k}}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow} + \Delta_{\mathbf{k}}\, \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} - \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} \right]$$

4.2.3 The Bogoliubov-Valatin Transformation

- we use

$$\sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}\, n_{\mathbf{k}\sigma} = \sum_{\mathbf{k}} \xi_{\mathbf{k}}\, (\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} + \underbrace{\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow}}_{=1-\hat{c}_{-\mathbf{k}\downarrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}})$$

$$\sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}\, n_{\mathbf{k}\sigma} = \sum_{\mathbf{k}} \xi_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} - \xi_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow} + \xi_{\mathbf{k}}$$

$$\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}}\, n_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left[\Delta^{*}_{\mathbf{k}}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow} + \Delta_{\mathbf{k}}\, \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow} - \Delta_{\mathbf{k}}\, g^{*}_{\mathbf{k}}\right]$$

$$\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^{*}_{\mathbf{k}} + \left(\hat{c}^{\dagger}_{\mathbf{k}\uparrow}, \hat{c}_{-\mathbf{k}\downarrow}\right) \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta_{\mathbf{k}} \\ -\Delta^{*}_{\mathbf{k}} & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} \right\}$$

➔ due to finite $\Delta_{\mathbf{k}}, \Delta^{*}_{\mathbf{k}}$, the Hamiltonian describes interacting electron gas with new quasiparticles consisting of ***superposition of electron and hole states***

- derive excitation energies by diagonalization of Hamiltonian

→ ***Bogoliubov-Valatin transformation***

→ define new fermionic operators $\alpha_{\mathbf{k}}, \beta^{\dagger}_{\mathbf{k}}$ and $\alpha^{\dagger}_{\mathbf{k}}, \beta_{\mathbf{k}}$ by unitary transformation (rotation)

4.2.3 The Bogoliubov-Valatin Transformation

- use unitarian matrix to rotate the energy matrix into eigenbasis of Bogoliubov quasiparticles

$$\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} + \underbrace{\left(\hat{c}^\dagger_{\mathbf{k}\uparrow}\,,\hat{c}_{-\mathbf{k}\downarrow}\right)}_{\mathcal{C}^\dagger_{\mathbf{k}}} \underbrace{\begin{pmatrix} \xi_{\mathbf{k}} & -\Delta_{\mathbf{k}} \\ -\Delta^*_{\mathbf{k}} & -\xi_{\mathbf{k}} \end{pmatrix}}_{\mathcal{E}_{\mathbf{k}}} \underbrace{\begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix}}_{\mathcal{C}_{\mathbf{k}}} \right\}$$

spinors

energy matrix

$$\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} + \underbrace{\mathcal{C}^\dagger_{\mathbf{k}}\mathcal{U}_{\mathbf{k}}}_{\mathcal{B}^\dagger_{\mathbf{k}}} \underbrace{\mathcal{U}^\dagger_{\mathbf{k}}\,\mathcal{E}_{\mathbf{k}}\,\mathcal{U}_{\mathbf{k}}}_{\tilde{\mathcal{E}}_{\mathbf{k}}} \underbrace{\mathcal{U}^\dagger_{\mathbf{k}}\mathcal{C}^\dagger_{\mathbf{k}}}_{\mathcal{B}_{\mathbf{k}}} \right\} = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} + \mathcal{B}^\dagger_{\mathbf{k}}\tilde{\mathcal{E}}_{\mathbf{k}}\mathcal{B}_{\mathbf{k}} \right\}$$

$$\mathcal{U}_{\mathbf{k}}\mathcal{U}^\dagger_{\mathbf{k}} = 1$$

spinors of Bogoliubov quasiparticle operators: $\mathcal{B}^\dagger_{\mathbf{k}} = \left(\alpha^\dagger_{\mathbf{k}}, \beta_{-\mathbf{k}}\right) = \mathcal{C}^\dagger_{\mathbf{k}}\mathcal{U}_{\mathbf{k}}$ $\quad$ $\mathcal{B}_{\mathbf{k}} = \left(\alpha_{\mathbf{k}}\,, \beta^\dagger_{-\mathbf{k}}\right) = \mathcal{U}^\dagger_{\mathbf{k}}\mathcal{C}_{\mathbf{k}}$

appropriate unitary matrix to make transformed energy matrix $\tilde{\mathcal{E}}_{\mathbf{k}} = \mathcal{U}^\dagger_{\mathbf{k}}\,\mathcal{E}_{\mathbf{k}}\,\mathcal{U}_{\mathbf{k}}$ diagonal:

$$\mathcal{U}_{\mathbf{k}} = \begin{pmatrix} u_{\mathbf{k}} & v^\star_{\mathbf{k}} \\ -v_{\mathbf{k}} & u^\star_{\mathbf{k}} \end{pmatrix} \qquad \mathcal{U}^\dagger_{\mathbf{k}} = \begin{pmatrix} u^\star_{\mathbf{k}} & -v^\star_{\mathbf{k}} \\ v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \quad \Rightarrow \quad \mathcal{U}^\dagger_{\mathbf{k}}\,\mathcal{E}_{\mathbf{k}}\,\mathcal{U}_{\mathbf{k}} = \tilde{\mathcal{E}}_{\mathbf{k}} = \begin{pmatrix} E_{\mathbf{k}} & D_{\mathbf{k}} \\ -D_{\mathbf{k}} & -E_{\mathbf{k}} \end{pmatrix}$$

choose $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ such that off-diagonal terms vanish

$$\Rightarrow \quad \boxed{\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} + \left(\alpha^\dagger_{\mathbf{k}}, \beta_{-\mathbf{k}}\right) \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}} \\ \beta^\dagger_{-\mathbf{k}} \end{pmatrix} \right\}}$$

eigenenergies $\pm E_{\mathbf{k}}$

4.2.3 The Bogoliubov-Valatin Transformation

$$\mathcal{B}_\mathbf{k}^\dagger = \left(\alpha_\mathbf{k}^\dagger, \beta_{-\mathbf{k}}\right) = \mathcal{C}_\mathbf{k}^\dagger \mathcal{U}_\mathbf{k} = \mathcal{U}_\mathbf{k}^\mathrm{T} \mathcal{C}_\mathbf{k}^\dagger \quad \Rightarrow \quad \left(\alpha_\mathbf{k}^\dagger, \beta_{-\mathbf{k}}\right) = \begin{pmatrix} u_\mathbf{k} & -v_\mathbf{k} \\ v_\mathbf{k}^\star & u_\mathbf{k}^\star \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow}^\dagger \\ \hat{c}_{-\mathbf{k}\downarrow} \end{pmatrix}$$

$$\mathcal{B}_\mathbf{k} = \left(\alpha_\mathbf{k}\,, \beta_{-\mathbf{k}}^\dagger\right) = \mathcal{U}_\mathbf{k}^\dagger \mathcal{C}_\mathbf{k} \quad \Rightarrow \quad \left(\alpha_\mathbf{k}\,, \beta_{-\mathbf{k}}^\dagger\right) = \begin{pmatrix} u_\mathbf{k}^\star & -v_\mathbf{k}^\star \\ v_\mathbf{k} & u_\mathbf{k} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix}$$

$$\begin{aligned} \alpha_\mathbf{k} &= u_\mathbf{k}^\star \hat{c}_{\mathbf{k}\uparrow} - v_\mathbf{k}^\star \hat{c}_{-\mathbf{k}\downarrow}^\dagger \\ \beta_{-\mathbf{k}}^\dagger &= v_\mathbf{k} \hat{c}_{\mathbf{k}\uparrow} + u_\mathbf{k} \hat{c}_{-\mathbf{k}\downarrow}^\dagger \\ \alpha_\mathbf{k}^\dagger &= u_\mathbf{k} \hat{c}_{\mathbf{k}\uparrow}^\dagger - v_\mathbf{k} \hat{c}_{-\mathbf{k}\downarrow} \\ \beta_{-\mathbf{k}} &= v_\mathbf{k}^\star \hat{c}_{\mathbf{k}\uparrow}^\dagger + u_\mathbf{k}^\star \hat{c}_{-\mathbf{k}\downarrow} \end{aligned}$$

creation and annihilation operators for ***Bogoliubov quasiparticles***: ***symmetric and anti-symmetric superposition of electron and hole states with opposite momentum and spin***

- operators satisfy fermionic anti-commutation rules: $\left\{\alpha_\mathbf{k}\,, \beta_{-\mathbf{k}'}^\dagger\right\} = \delta_{\mathbf{k}\mathbf{k}'}$ and $\left\{\alpha_\mathbf{k}\,, \alpha_{\mathbf{k}'}\right\} = \left\{\alpha_\mathbf{k}^\dagger\,, \alpha_{\mathbf{k}'}^\dagger\right\} = 0$

- inverse transformation

$$\mathcal{B}_\mathbf{k}^\dagger \mathcal{U}_\mathbf{k}^\dagger = \mathcal{C}_\mathbf{k}^\dagger \mathcal{U}_\mathbf{k} \mathcal{U}_\mathbf{k}^\dagger = \mathcal{C}_\mathbf{k}^\dagger \;\Rightarrow\; \mathcal{C}_\mathbf{k}^\dagger = \left(\mathcal{U}_\mathbf{k}^\dagger\right)^\mathrm{T} \mathcal{B}_\mathbf{k}^\dagger \quad \Rightarrow \quad \left(\hat{c}_{\mathbf{k}\uparrow}^\dagger\,, \hat{c}_{-\mathbf{k}\downarrow}\right) = \begin{pmatrix} u_\mathbf{k}^\star & v_\mathbf{k} \\ -v_\mathbf{k}^\star & u_\mathbf{k} \end{pmatrix} \begin{pmatrix} \alpha_\mathbf{k}^\dagger \\ \beta_{-\mathbf{k}} \end{pmatrix}$$

$$\mathcal{U}_\mathbf{k} \mathcal{B}_\mathbf{k} = \mathcal{U}_\mathbf{k} \mathcal{U}_\mathbf{k}^\dagger \mathcal{C}_\mathbf{k} = \mathcal{C}_\mathbf{k} \;\Rightarrow\; \mathcal{C}_\mathbf{k} = \mathcal{U}_\mathbf{k} \mathcal{B}_\mathbf{k} \quad \Rightarrow \quad \left(\hat{c}_{\mathbf{k}\uparrow}, \hat{c}_{-\mathbf{k}\downarrow}^\dagger\right) = \begin{pmatrix} u_\mathbf{k} & v_\mathbf{k}^\star \\ -v_\mathbf{k} & u_\mathbf{k}^\star \end{pmatrix} \begin{pmatrix} \alpha_\mathbf{k} \\ \beta_{-\mathbf{k}}^\dagger \end{pmatrix}$$

$$\begin{aligned} \hat{c}_{\mathbf{k}\uparrow}^\dagger &= u_\mathbf{k}^\star \alpha_\mathbf{k}^\dagger + v_\mathbf{k}\, \beta_{-\mathbf{k}} \\ \hat{c}_{-\mathbf{k}\downarrow} &= -v_\mathbf{k}^\star \alpha_\mathbf{k}^\dagger + u_\mathbf{k} \beta_{-\mathbf{k}} \\ \hat{c}_{\mathbf{k}\uparrow} &= u_\mathbf{k} \alpha_\mathbf{k} + v_\mathbf{k}^\star \beta_{-\mathbf{k}}^\dagger \\ \hat{c}_{-\mathbf{k}\downarrow}^\dagger &= -v_\mathbf{k} \alpha_\mathbf{k} + u_\mathbf{k}^\star \beta_{-\mathbf{k}}^\dagger \end{aligned}$$

4.2.3 The Bogoliubov-Valatin Transformation

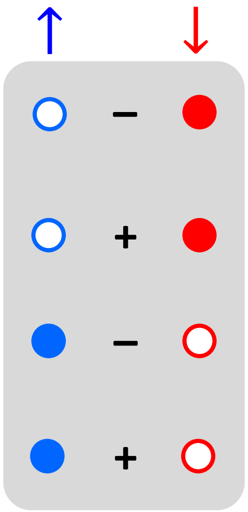
Bogoliubov quasiparticles

$$\begin{aligned} \alpha_{\mathbf{k}} &= u_{\mathbf{k}}^{\star}\hat{c}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}^{\star}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \\ \beta^{\dagger}_{-\mathbf{k}} &= v_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow} + u_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \\ \alpha^{\dagger}_{\mathbf{k}} &= u_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow} \\ \beta_{-\mathbf{k}} &= v_{\mathbf{k}}^{\star}\hat{c}^{\dagger}_{\mathbf{k}\uparrow} + u_{\mathbf{k}}^{\star}\hat{c}_{-\mathbf{k}\downarrow} \end{aligned}$$

$$\xi_{\mathbf{k}} = 0$$

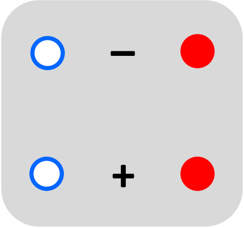
$$|u_{\mathbf{k}}|^2 = |v_{\mathbf{k}}|^2 = \frac{1}{2}$$

$$\begin{aligned} \alpha_{\mathbf{k}} &= 1/\sqrt{2}\left(\hat{c}_{\mathbf{k}\uparrow} - \hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\right) \\ \beta^{\dagger}_{-\mathbf{k}} &= 1/\sqrt{2}\left(\hat{c}_{\mathbf{k}\uparrow} + \hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\right) \\ \alpha^{\dagger}_{\mathbf{k}} &= 1/\sqrt{2}\left(\hat{c}^{\dagger}_{\mathbf{k}\uparrow} - \hat{c}_{-\mathbf{k}\downarrow}\right) \\ \beta_{-\mathbf{k}} &= 1/\sqrt{2}\left(\hat{c}^{\dagger}_{\mathbf{k}\uparrow} + \hat{c}_{-\mathbf{k}\downarrow}\right) \end{aligned}$$



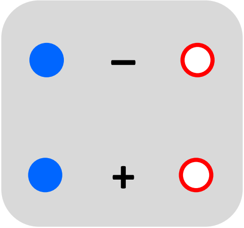
➔ symmetric and anti-symmetric superposition of electron and hole states with opposite spin direction

➔ $|u_{\mathbf{k}}|^2$ = hole fraction, $|v_{\mathbf{k}}|^2$ = electron fraction



→ *reduces* the total momentum by $\mathbf{k}$ and the total spin by $\hbar/2$

hole-like excitation

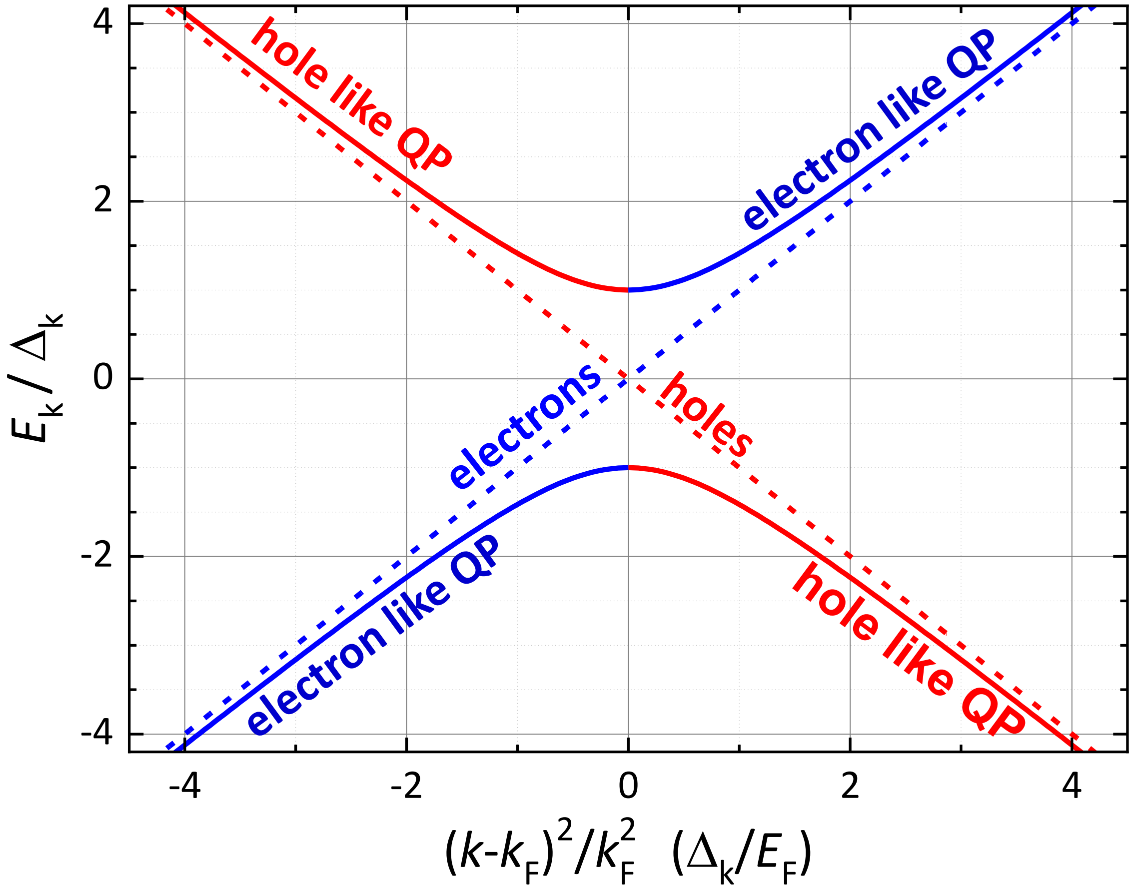


→ *increases* the total momentum by $\mathbf{k}$ and the total spin by $\hbar/2$

particle-like excitation

4.2.3 The Bogoliubov-Valatin Transformation

excitation spectrum of Bogoliubov quasiparticles and energy gap

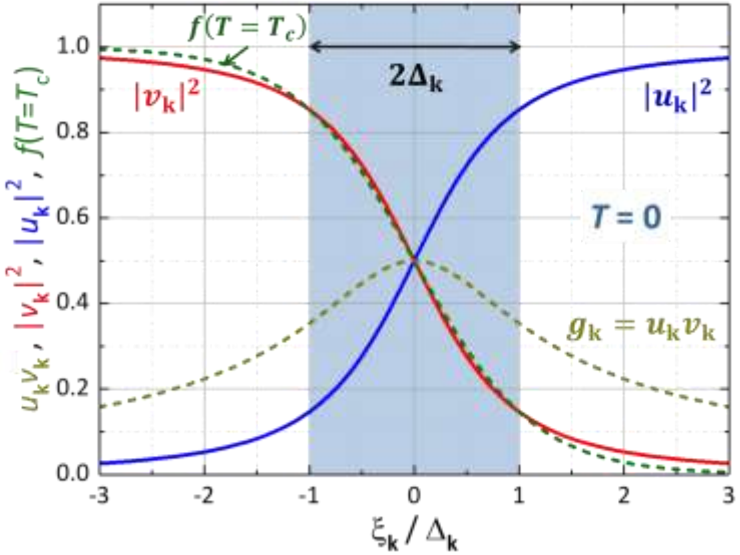


quasiparticle excitations: superposition of electron and hole states

reason: single particle excitation with wave vector $\mathbf{k}$ can only exist if at the same time there is a hole with wave vector $-\mathbf{k}$, *otherwise there would be a pair state*

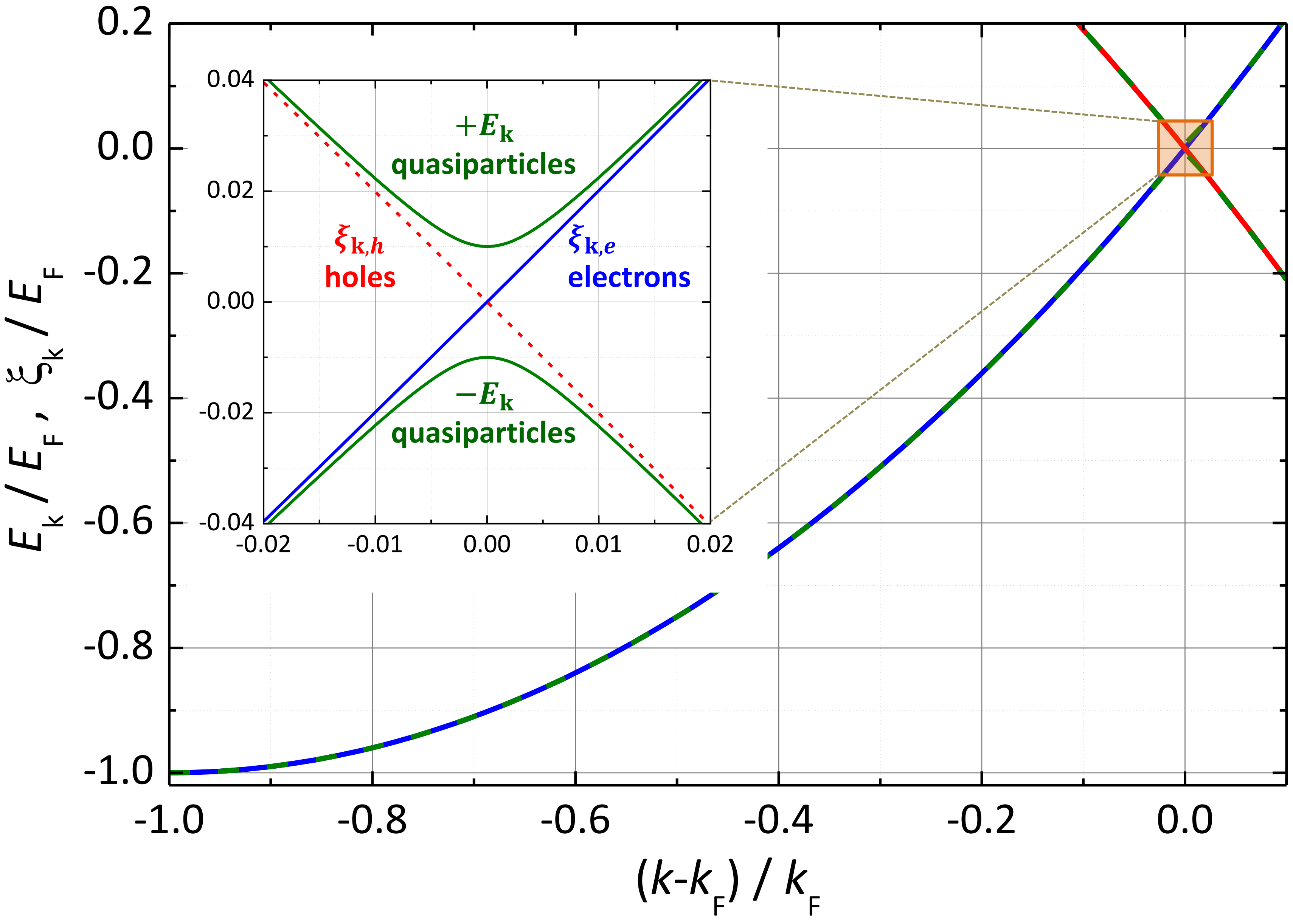
excitation energy

$$E_{\mathbf{k}} = \pm\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$$



$$\alpha_{\mathbf{k}} = u_{\mathbf{k}}^{\star}\hat{c}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}^{\star}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger}$$
$$\beta_{-\mathbf{k}}^{\dagger} = v_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow} + u_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow}^{\dagger}$$
$$\alpha_{\mathbf{k}}^{\dagger} = u_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow}^{\dagger} - v_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow}$$
$$\beta_{-\mathbf{k}} = v_{\mathbf{k}}^{\star}\hat{c}_{\mathbf{k}\uparrow}^{\dagger} + u_{\mathbf{k}}^{\star}\hat{c}_{-\mathbf{k}\downarrow}$$

4.2.3 The Bogoliubov-Valatin Transformation



R. Gross and A. Marx , © Walther-Meißner-Institut (2004 - 2021)

4.2.3 The Bogoliubov-Valatin Transformation

determine $|u_{\mathbf{k}}|^2$ and $|v_{\mathbf{k}}|^2$ by Bogoliubov-Valatin transformation

BCS Hamiltonian

$$\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g_{\mathbf{k}}^{*} + \left(\hat{c}_{\mathbf{k}\uparrow}^{\dagger}\,,\, \hat{c}_{-\mathbf{k}\downarrow} \right) \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta_{\mathbf{k}} \\ -\Delta_{\mathbf{k}}^{*} & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}_{-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix} \right\}$$

$$\begin{aligned} \hat{c}_{\mathbf{k}\uparrow}^{\dagger} &= u_{\mathbf{k}}^{\star}\alpha_{\mathbf{k}}^{\dagger} + v_{\mathbf{k}}\, \beta_{-\mathbf{k}} \\ \hat{c}_{-\mathbf{k}\downarrow} &= -v_{\mathbf{k}}^{\star}\alpha_{\mathbf{k}}^{\dagger} + u_{\mathbf{k}}\beta_{-\mathbf{k}} \\ \hat{c}_{\mathbf{k}\uparrow} &= u_{\mathbf{k}}\alpha_{\mathbf{k}} + v_{\mathbf{k}}^{\star}\beta_{-\mathbf{k}}^{\dagger} \\ \hat{c}_{-\mathbf{k}\downarrow}^{\dagger} &= -v_{\mathbf{k}}\alpha_{\mathbf{k}} + u_{\mathbf{k}}^{\star}\beta_{-\mathbf{k}}^{\dagger} \end{aligned}$$

- replace operators by Bogoliubov quasiparticle operators → resulting Hamiltonian:

$$\begin{aligned} \mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = & \sum_{\mathbf{k}} \left[2\xi_{\mathbf{k}} v_{\mathbf{k}}^{2} - \Delta_{\mathbf{k}}\, u_{\mathbf{k}} v_{\mathbf{k}}^{\star} - \Delta_{\mathbf{k}}^{\dagger} u_{\mathbf{k}}^{\star} v_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g_{\mathbf{k}}^{\dagger} \right] \\ & + \sum_{\mathbf{k}} \left[\xi_{\mathbf{k}} \left(u_{\mathbf{k}}^{2} - v_{\mathbf{k}}^{2} \right) + \Delta_{\mathbf{k}}\, u_{\mathbf{k}} v_{\mathbf{k}}^{\star} + \Delta_{\mathbf{k}}^{\dagger} u_{\mathbf{k}}^{\star} v_{\mathbf{k}} \right] \alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}} \\ & + \sum_{\mathbf{k}} \left[\xi_{\mathbf{k}} \left(u_{\mathbf{k}}^{2} - v_{\mathbf{k}}^{2} \right) + \Delta_{\mathbf{k}}\, u_{\mathbf{k}} v_{\mathbf{k}}^{\star} + \Delta_{\mathbf{k}}^{\dagger} u_{\mathbf{k}}^{\star} v_{\mathbf{k}} \right] \beta_{-\mathbf{k}}^{\dagger}\beta_{-\mathbf{k}} \\ & \left. \begin{aligned} & + \sum_{\mathbf{k}} \left[2\xi_{\mathbf{k}} u_{\mathbf{k}}^{\star} v_{\mathbf{k}}^{\star} + \Delta_{\mathbf{k}}\, v_{\mathbf{k}}^{\star 2} - \Delta_{\mathbf{k}}^{\dagger} u_{\mathbf{k}}^{\star 2} \right] \beta_{-\mathbf{k}}\alpha_{\mathbf{k}} \\ & + \sum_{\mathbf{k}} \left[2\xi_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} + \Delta_{\mathbf{k}}^{\dagger} v_{\mathbf{k}}^{2} - \Delta_{\mathbf{k}}\, u_{\mathbf{k}}^{2} \right] \alpha_{\mathbf{k}}^{\dagger}\beta_{-\mathbf{k}}^{\dagger} \end{aligned} \right\} \quad [\ldots] = \mathbf{0}\ ! \end{aligned}$$

- ➢ we have to set expressions marked in red to zero to keep only diagonal terms
- ➢ $\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}$ and $\beta_{-\mathbf{k}}^{\dagger}\beta_{-\mathbf{k}}$ = quasiparticle number operators

4.2.3 The Bogoliubov-Valatin Transformation

$$2\xi_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} + \Delta_{\mathbf{k}}^{*} v_{\mathbf{k}}^{2} - \Delta_{\mathbf{k}}\, u_{\mathbf{k}}^{2} = 0 \quad \text{and} \quad 2\xi_{\mathbf{k}} u_{\mathbf{k}}^{\star} v_{\mathbf{k}}^{\star} + \Delta_{\mathbf{k}}\, v_{\mathbf{k}}^{\star 2} - \Delta_{\mathbf{k}}^{*} u_{\mathbf{k}}^{\star 2} = 0$$

- multiply by $\Delta_{\mathbf{k}}^{*}/u_{\mathbf{k}}^{2}$ ($\Delta_{\mathbf{k}}\,/u_{\mathbf{k}}^{*\,2}$), solve the resulting quadratic eqn. for $\Delta_{\mathbf{k}}^{*} v_{\mathbf{k}}/u_{\mathbf{k}}$ ($\Delta_{\mathbf{k}}\, v_{\mathbf{k}}^{*}/u_{\mathbf{k}}^{*}$)

$$2\xi_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}^{*}}{u_{\mathbf{k}}^{2}} + \Delta_{\mathbf{k}}^{*} v_{\mathbf{k}}^{2} \frac{\Delta_{\mathbf{k}}^{*}}{u_{\mathbf{k}}^{2}} - \Delta_{\mathbf{k}}\, u_{\mathbf{k}}^{2} \frac{\Delta_{\mathbf{k}}^{*}}{u_{\mathbf{k}}^{2}} = \left(\Delta_{\mathbf{k}}^{*} \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}\right)^{2} + 2\xi_{\mathbf{k}} \left(\Delta_{\mathbf{k}}^{*} \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}\right) + |\Delta_{\mathbf{k}}|^{2} = 0$$

$$\left(\Delta_{\mathbf{k}}^{*} \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}\right)_{1,2} = \left(\Delta_{\mathbf{k}} \frac{v_{\mathbf{k}}^{*}}{u_{\mathbf{k}}^{*}}\right)_{1,2} = -\xi_{\mathbf{k}} \pm \sqrt{\xi_{\mathbf{k}}^{2} + |\Delta_{\mathbf{k}}|^{2}} = -\xi_{\mathbf{k}} \pm E_{\mathbf{k}} \quad \text{with} \quad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^{2} + |\Delta_{\mathbf{k}}|^{2}}$$

negative sign is unphysical
→ corresponds to solution with maximum energy

note that the phases of $u_{\mathbf{k}}, v_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}^{*}$ ($u_{\mathbf{k}}^{*}$, $v_{\mathbf{k}}^{*}$ and $\Delta_{\mathbf{k}}$), although arbitrary, are related, since the quantity on the r.h.s. is real

➔ the relative phase of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ must be fixed and must be the phase of $\Delta_{\mathbf{k}}^{*}$

➔ we can choose $u_{\mathbf{k}}$ real and use $v_{\mathbf{k}} = |v_{\mathbf{k}}| e^{\imath\varphi}$, the phase of $v_{\mathbf{k}}$ corresponds to that of $\Delta_{\mathbf{k}}^{*}$

$$\left|\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}\right| = \frac{E_{\mathbf{k}} - \xi_{\mathbf{k}}}{|\Delta_{\mathbf{k}}|}$$

4.2.3 The Bogoliubov-Valatin Transformation

- with the condition $\left|\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}\right| = \frac{E_{\mathbf{k}}-\xi_{\mathbf{k}}}{|\Delta_{\mathbf{k}}|}$ and the normalization condition $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$ we obtain

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

probability that pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is empty/occupied

$$u_{\mathbf{k}} v_{\mathbf{k}}^{\star} = g_{\mathbf{k}}^{\star} = \frac{\Delta_{\mathbf{k}}^{*}}{2E_{\mathbf{k}}} \qquad u_{\mathbf{k}}^{\star} v_{\mathbf{k}} = g_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$$

pairing amplitude

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

$$\Delta_{\mathbf{k}}^{*} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, g_{\mathbf{k}'}^{*} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}^{*}}{2E_{\mathbf{k}'}}$$

self-consistent gap equation

4.2.3 The Bogoliubov-Valatin Transformation

reformulation of the BCS Hamilton operator

- we start from the Hamiltonian $\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} + (\alpha^\dagger_{\mathbf{k}}, \beta_{-\mathbf{k}}) \begin{pmatrix} E_{\mathbf{k}} & 0 \\ 0 & -E_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}} \\ \beta^\dagger_{-\mathbf{k}} \end{pmatrix} \right\}$

$$\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} \right\} + \sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} - E_{\mathbf{k}} \underbrace{\beta_{-\mathbf{k}} \beta^\dagger_{-\mathbf{k}}}_{=1-\beta^\dagger_{-\mathbf{k}}\beta_{-\mathbf{k}}} \right\}$$

$$= \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} \right\} + \sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} - E_{\mathbf{k}} + E_{\mathbf{k}} \beta^\dagger_{-\mathbf{k}} \beta_{-\mathbf{k}} \right\}$$

$$\Rightarrow \quad \mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \underbrace{\sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} \right\}} + \underbrace{\sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} + E_{\mathbf{k}} \beta^\dagger_{-\mathbf{k}} \beta_{-\mathbf{k}} \right\}}$$

mean-field contribution

differs from the normal state value by the condensation energy (see below)

contribution of **spinless Fermion system** with two kind of **quasiparticles** described by operators $\alpha^\dagger_{\mathbf{k}}, \alpha_{\mathbf{k}}$ and $\beta^\dagger_{-\mathbf{k}}, \beta_{-\mathbf{k}}$ and excitation energies $\pm E_{\mathbf{k}}$

spinless **quasiparticles** since they consist of superposition of spin-↑ and spin-↓ electrons

4.2.3 The Bogoliubov-Valatin Transformation

- note that the **Bogoliubov quasiparticles** are not part of the BCS ground state, as is evident from

$$\alpha_{\mathbf{k}}|\Psi_{\mathrm{BCS}}\rangle = 0$$

$$\beta_{-\mathbf{k}}|\Psi_{\mathrm{BCS}}\rangle = 0$$

- the occupation probability of the Bogoliubov particles is given by the Fermi-Dirac distribition

$$\left\langle \alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}} \right\rangle = \left\langle \beta_{-\mathbf{k}}^{\dagger}\beta_{-\mathbf{k}} \right\rangle = f(E_{\mathbf{k}}) = \frac{1}{\exp(E_{\mathbf{k}}/k_{\mathrm{B}}T) + 1}$$

Summary of Lecture No. 8 (1)

- ***BCS Hamilton operator***:

$$\mathcal{H}_{\mathrm{BCS}} = \sum_{\sigma}\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}\, \hat{c}^{\dagger}_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}$$

$\hat{c}^{\dagger}_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} = n_{\mathbf{k}\sigma} =$ particle number operator

$$\varepsilon_{\mathbf{k}} = \xi_{\mathbf{k}} + \mu = \frac{\hbar^2\mathbf{k}^2}{2m}$$

- ***Bardeen, Cooper*** and ***Schrieffer*** used the following Ansatz for the ground state wave function (mean-field approach):

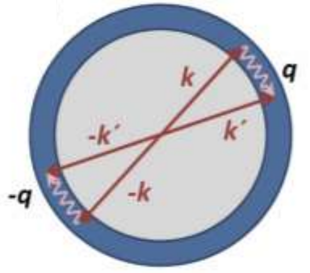
$$|\Psi_{\mathrm{BCS}}\rangle = \prod_{\mathbf{k}=\mathbf{k}_1,\ldots,\mathbf{k}_M} \left(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\right)|0\rangle$$

coherent fermionic state

$|u_{\mathbf{k}}|^2$: probability that pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is empty
$|v_{\mathbf{k}}|^2$: probability that pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is occupied
$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$

- ***expectation values:*** $\left\langle \Psi_{\mathrm{BCS}} \middle| \hat{c}^{\dagger}_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} \middle| \Psi_{\mathrm{BCS}} \right\rangle = |v_{\mathbf{k}}|^2$ $\quad$ $\left\langle \Psi_{\mathrm{BCS}} \middle| \hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow} \middle| \Psi_{\mathrm{BCS}} \right\rangle = v_{\mathbf{k}}\, v^{\star}_{\mathbf{k}'} u_{\mathbf{k}'} u^{\star}_{\mathbf{k}}$

$$\langle\Psi_{\mathrm{BCS}}|\mathcal{H}_{\mathrm{BCS}}|\Psi_{\mathrm{BCS}}\rangle = \underbrace{2\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}|v_{\mathbf{k}}|^2}_{\substack{=\overline{N}\,\varepsilon_{\mathbf{k}} \\ \text{(kinetic energy)}}} + \underbrace{\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, v_{\mathbf{k}}\, v^{\star}_{\mathbf{k}'} u_{\mathbf{k}'} u^{\star}_{\mathbf{k}}}_{\text{interaction energy}}$$



determination of $u_{\mathbf{k}}, v_{\mathbf{k}}$ by minimization of expectation value

Summary of Lecture No. 8 (2)

- *minimization of expectation value*

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

probability that pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is empty/occupied

$$u_{\mathbf{k}}v_{\mathbf{k}}^{\star} = g_{\mathbf{k}}^{\star} = \frac{\Delta_{\mathbf{k}}^{*}}{2E_{\mathbf{k}}} \qquad u_{\mathbf{k}}^{\star}v_{\mathbf{k}} = g_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$$

pairing amplitude

$$\Delta_{\mathbf{k}} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, g_{\mathbf{k}'} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \qquad \Delta_{\mathbf{k}}^{\dagger} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, g_{\mathbf{k}'}^{*} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}^{*}}{2E_{\mathbf{k}'}}$$

self-consistent gap equation

- *gap equation for $T = 0$*

$$\Delta = \frac{\hbar\omega_{\mathrm{D}}}{\sinh\big(2/V_0 D(E_{\mathrm{F}})\big)} \simeq 2\hbar\omega_{\mathrm{D}}\, \mathrm{e}^{-2/V_0 D(E_{\mathrm{F}})}$$

energy gap corresponds to binding energy estimated for single Cooper pair

$V_0 D(E_{\mathrm{F}}) \ll 1$: weak coupling approximation, $\sinh x \simeq \frac{1}{2}\exp x$

Summary of Lecture No. 8 (3)

- ***Bogoliubov-Valatin transformation → BCS Gap Equation and Excitation Spectrum***

$$\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} + \underbrace{\left(\hat{c}^\dagger_{\mathbf{k}\uparrow}, \hat{c}_{-\mathbf{k}\downarrow}\right) \mathcal{U}_{\mathbf{k}}}_{\mathcal{B}^\dagger_{\mathbf{k}}} \mathcal{U}^\dagger_{\mathbf{k}} \underbrace{\begin{pmatrix} \xi_{\mathbf{k}} & -\Delta_{\mathbf{k}} \\ -\Delta^*_{\mathbf{k}} & -\xi_{\mathbf{k}} \end{pmatrix}}_{\mathcal{E}_{\mathbf{k}}} \mathcal{U}_{\mathbf{k}} \underbrace{\mathcal{U}^\dagger_{\mathbf{k}} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix}}_{\mathcal{B}_{\mathbf{k}}} \right\} = \sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^\dagger_{\mathbf{k}} + \mathcal{B}^\dagger_{\mathbf{k}}\, \mathcal{U}^\dagger_{\mathbf{k}}\, \mathcal{E}_{\mathbf{k}}\, \mathcal{U}_{\mathbf{k}}\, \mathcal{B}_{\mathbf{k}} \right\}$$

$$\mathcal{B}^\dagger_{\mathbf{k}} = \left(\alpha^\dagger_{\mathbf{k}}, \beta_{-\mathbf{k}}\right) = \left(\hat{c}^\dagger_{\mathbf{k}\uparrow}, \hat{c}_{-\mathbf{k}\downarrow}\right) \mathcal{U}_{\mathbf{k}} \qquad \mathcal{B}_{\mathbf{k}} = \left(\alpha_{\mathbf{k}}, \beta^\dagger_{-\mathbf{k}}\right) = \mathcal{U}^\dagger_{\mathbf{k}} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix}$$

Bogoliubov quasiparticles: → superposition of electron and hole states with opposite momentum and spin

Task: find unitary matrix ($\mathcal{U}_{\mathbf{k}}\mathcal{U}^\dagger_{\mathbf{k}} = 1$) that makes the transformed energy matrix $\tilde{\mathcal{E}}_{\mathbf{k}} = \mathcal{U}^\dagger_{\mathbf{k}}\, \mathcal{E}_{\mathbf{k}}\, \mathcal{U}_{\mathbf{k}}$ diagonal:

$$\mathcal{U}_{\mathbf{k}} = \begin{pmatrix} u_{\mathbf{k}} & v^\star_{\mathbf{k}} \\ -v_{\mathbf{k}} & u^\star_{\mathbf{k}} \end{pmatrix} \qquad \mathcal{U}^\dagger_{\mathbf{k}} = \begin{pmatrix} u^\star_{\mathbf{k}} & -v^\star_{\mathbf{k}} \\ v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \Longrightarrow \mathcal{U}^\dagger_{\mathbf{k}}\, \mathcal{E}_{\mathbf{k}}\, \mathcal{U}_{\mathbf{k}} = \begin{pmatrix} E_{\mathbf{k}} & D_{\mathbf{k}} \\ -D_{\mathbf{k}} & -E_{\mathbf{k}} \end{pmatrix}$$

→ $D_{\mathbf{k}} = \mathbf{0}$

- ***reformulation of the BCS Hamilton operator***

$$\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \underbrace{\sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g^*_{\mathbf{k}} \right\}} + \underbrace{\sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} + E_{\mathbf{k}} \beta^\dagger_{-\mathbf{k}} \beta_{-\mathbf{k}} \right\}}$$

→ **minimization of free energy yields BCS gap equation for finite T**

mean-field contribution

differs from the normal state value by the condensation energy (see below)

contribution of **spinless Fermion system** with two kind of **quasiparticles** described by operators $\alpha^\dagger_{\mathbf{k}}, \alpha_{\mathbf{k}}$ and $\beta^\dagger_{-\mathbf{k}}, \beta_{-\mathbf{k}}$ and excitation energies $\pm E_{\mathbf{k}}$

spinless **quasiparticles** since they consist of superposition of spin-↑ and spin-↓ electrons

Superconductivity and Low Temperature Physics I

Lecture No. 9
16 December 2021

R. Gross

Chapter 4

4. Microscopic Theory

4.2.3 The BCS Gap Equation and QP Excitations

determination of temperature dependence of Δ by minimization of free energy

- Hamiltonian has two terms: $$\mathcal{H}_{\mathrm{BCS}} - \mathcal{N}\mu = \underbrace{\sum_{\mathbf{k}} \left\{ \xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta_{\mathbf{k}}\, g_{\mathbf{k}}^{*} \right\}}_{\text{constant term } \mathcal{H}_0} + \underbrace{\sum_{\mathbf{k}} \left\{ E_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + E_{\mathbf{k}} \beta_{-\mathbf{k}}^{\dagger} \beta_{-\mathbf{k}} \right\}}_{\text{term of free Fermi gas composed of two kind of fermions with energy } E_{\mathbf{k}}}$$

- grand canonical partition function:

$$Z = \mathrm{e}^{-\mathcal{H}_0/k_{\mathrm{B}}T} \prod_{\mathbf{k}} \left(1 + \mathrm{e}^{-E_{\mathbf{k}}/k_{\mathrm{B}}T}\right)\left(1 + \mathrm{e}^{E_{\mathbf{k}}/k_{\mathrm{B}}T}\right) = \mathrm{e}^{-\mathcal{F}/Nk_{\mathrm{B}}T}$$

(since $\mathcal{F} = -Nk_{\mathrm{B}}T \ln Z$)

partition function of an ideal Fermi gas:

$$\begin{aligned} Z &= \prod_{k} \sum_{n_k=0,1} \exp\left(-n_k(\epsilon_k - \mu)/k_{\mathrm{B}}T\right) \\ &= \prod_{k} \left[1 + \exp\left(-(\epsilon_k - \mu)/k_{\mathrm{B}}T\right)\right] \end{aligned}$$

- solve for free energy $\mathcal{F}$:

$$\frac{\mathcal{F}}{N} = \mathcal{H}_0 - k_{\mathrm{B}}T \sum_{\mathbf{k}} \left[\ln\left(1 + \mathrm{e}^{-E_{\mathbf{k}}/k_{\mathrm{B}}T}\right) + \ln\left(1 + \mathrm{e}^{E_{\mathbf{k}}/k_{\mathrm{B}}T}\right)\right]$$

- minimize free energy regarding variation of $\Delta_{\mathbf{k}}$: $$\frac{\partial \mathcal{F}}{\partial \Delta_{\mathbf{k}}} = 0, \qquad \frac{\partial \mathcal{F}}{\partial \Delta_{\mathbf{k}}^{\dagger}} = 0$$

4.2.3 The BCS Gap Equation and QP Excitations

$$\frac{\partial(\mathcal{F}/N)}{\partial\Delta_\mathbf{k}} = 0 = \frac{\partial}{\partial\Delta_\mathbf{k}}\left\{\mathcal{H}_0 - k_\mathrm{B}T\sum_\mathbf{k}\left[\ln\left(1+\mathrm{e}^{-E_\mathbf{k}/k_\mathrm{B}T}\right)+\ln\left(1+\mathrm{e}^{E_\mathbf{k}/k_\mathrm{B}T}\right)\right]\right\}$$

$$\mathcal{H}_0 = \xi_\mathbf{k} - E_\mathbf{k} + \Delta_\mathbf{k}\, g^*_\mathbf{k}$$

$$\Rightarrow \quad g^*_\mathbf{k} + \underbrace{\frac{\partial E_\mathbf{k}}{\partial\Delta_\mathbf{k}}}_{=\Delta^*_\mathbf{k}/2E_\mathbf{k}}\underbrace{\left[\frac{\mathrm{e}^{-E_\mathbf{k}/k_\mathrm{B}T}}{1+\mathrm{e}^{-E_\mathbf{k}/k_\mathrm{B}T}} - \frac{\mathrm{e}^{E_\mathbf{k}/k_\mathrm{B}T}}{1+\mathrm{e}^{E_\mathbf{k}/k_\mathrm{B}T}}\right]}_{=-\tanh\left(E_\mathbf{k}/2k_\mathrm{B}T\right)} = 0$$

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

$$g^*_\mathbf{k} = \frac{\Delta^*_\mathbf{k}}{2E_\mathbf{k}}\tanh\left(\frac{E_\mathbf{k}}{2k_\mathrm{B}T}\right) = u_\mathbf{k}v^\star_\mathbf{k}\;\tanh\left(\frac{E_\mathbf{k}}{2k_\mathrm{B}T}\right)$$

$$u_\mathbf{k}v^\star_\mathbf{k} = \frac{\Delta^*_\mathbf{k}}{2E_\mathbf{k}}$$

pairing susceptibility/amplitude: ability of the electron system to form pairs

- we use $\Delta^*_\mathbf{k} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\, g^*_{\mathbf{k}'}$ and obtain:

$$\Delta^*_\mathbf{k} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}\frac{\Delta^*_{\mathbf{k}'}}{2E_{\mathbf{k}'}}\tanh\left(\frac{E_{\mathbf{k}'}}{2k_\mathrm{B}T}\right)$$

BCS gap equation

- set of equations for variables $\Delta_\mathbf{k}$
- equations are nonlinear, since $E_\mathbf{k}$ depends on $\Delta_\mathbf{k}$
- solve numerically, analytical solutions in limiting cases

4.2.3 The BCS Gap Equation and QP Excitations

energy gap Δ and transition temperature T_c

- trivial solution: $\Delta_{\mathbf{k}} = 0$, results in $v_{\mathbf{k}} = 1$ for $\xi_{\mathbf{k}} < 0$ and $v_{\mathbf{k}} = 0$ for $\xi_{\mathbf{k}} > 0$

→ intuitive expectation for normal state

- non-trivial solution: we use approximations $V_{\mathbf{k},\mathbf{k}'} = -V_0$ and $\Delta_{\mathbf{k}} = \Delta$

$$\Delta^*_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta^*_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_{\mathrm{B}}T}\right) \Longrightarrow \boxed{1 = V_0 \sum_{\mathbf{k}'} \frac{1}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_{\mathrm{B}}T}\right)}$$

- we use pair density of states $\widetilde{D}(E) = D(E)/2$ and change from summation to integration

simple solutions for (i) $T \to 0$
(ii) $T \to T_c$

R. Gross and A. Marx , © Walther-Meißner-Institut (2004 - 2021)

4.2.3 The BCS Gap Equation and QP Excitations

i. solution for $T \to 0$:

(already discussed above for $V_{\mathbf{k},\mathbf{k}'} = -V_0$ and $\Delta_{\mathbf{k}} = \Delta$)

$$1 = V_0 \sum_{\mathbf{k}'} \frac{1}{2E_{\mathbf{k}'}} \underbrace{\tanh\left(\frac{E_{\mathbf{k}'}}{2k_{\mathrm{B}}T}\right)}_{=1 \text{ for } T \to 0}$$

transforming sum into integration

$$1 = \frac{V_0 D(E_{\mathrm{F}})}{2} \int_{-\hbar\omega_{\mathrm{D}}}^{\hbar\omega_{\mathrm{D}}} \frac{\mathrm{d}\xi}{2\sqrt{\xi_{\mathbf{k}}^2 + |\Delta(0)|^2}}$$

with $\widetilde{D}(E) \simeq D(E_{\mathrm{F}})/2$

$$1 = \frac{V_0 D(E_{\mathrm{F}})}{4} \int_{-\hbar\omega_{\mathrm{D}}}^{\hbar\omega_{\mathrm{D}}} \frac{\mathrm{d}\xi}{\sqrt{\xi_{\mathbf{k}}^2 + |\Delta(0)|^2}} = \frac{V_0 D(E_{\mathrm{F}})}{4} \operatorname{arcsinh}\left(\frac{\hbar\omega_{\mathrm{D}}}{\Delta(0)}\right)\Bigg|_{-\hbar\omega_{\mathrm{D}}}^{+\hbar\omega_{\mathrm{D}}} = \frac{V_0 D(E_{\mathrm{F}})}{2} \operatorname{arcsinh}\left(\frac{\hbar\omega_{\mathrm{D}}}{\Delta(0)}\right)$$

- solve for Δ:

$$\Delta(0) = \frac{\hbar\omega_{\mathrm{D}}}{\sinh\left(2/V_0 D(E_{\mathrm{F}})\right)} \simeq 2\hbar\omega_{\mathrm{D}}\, \mathrm{e}^{-2/V_0 D(E_{\mathrm{F}})}$$

$V_0 D(E_{\mathrm{F}}) \ll 1$: weak coupling approximation

- compare to expression derived for energy of two interacting electrons (“Gedanken” experiment):

$$E \simeq 2E_{\mathrm{F}} - 2\hbar\omega_{\mathrm{D}}\, \mathrm{e}^{-4/V_0 D(E_{\mathrm{F}})}$$

factor 2 in argument of exponential function since we have assumed that the two additional electrons are in interval between E_{F} and $E_{\mathrm{F}} + \hbar\omega_{\mathrm{D}}$ and not between $E_{\mathrm{F}} - \hbar\omega_{\mathrm{D}}$ and $E_{\mathrm{F}} + \hbar\omega_{\mathrm{D}}$

4.2.3 The BCS Gap Equation and QP Excitations

ii. solution for $T \to T_c$: $E_{\mathbf{k}} \to |\xi_{\mathbf{k}}|$ since $\Delta_{\mathbf{k}} \to 0$

$$1 = V_0 \sum_{\mathbf{k}'} \frac{1}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_\mathrm{B}T}\right) \quad \Rightarrow \quad 1 = V_0 \sum_{\mathbf{k}'} \frac{1}{2\xi_{\mathbf{k}'}} \tanh\left(\frac{\xi_{\mathbf{k}'}}{2k_\mathrm{B}T}\right)$$

$$1 = \frac{V_0 D(E_\mathrm{F})}{4} \int_{-\hbar\omega_\mathrm{D}}^{\hbar\omega_\mathrm{D}} \frac{1}{\xi_{\mathbf{k}'}} \tanh\left(\frac{\xi_{\mathbf{k}'}}{2k_\mathrm{B}T_c}\right) \mathrm{d}\xi = \frac{V_0 D(E_\mathrm{F})}{4} \int_{-\hbar\omega_\mathrm{D}/2k_\mathrm{B}T_c}^{\hbar\omega_\mathrm{D}/2k_\mathrm{B}T_c} \frac{\tanh x}{x} \mathrm{d}x \qquad \text{with } x = \xi_{\mathbf{k}}/2k_\mathrm{B}T_c$$

- integral gives $2\ln(p\,\hbar\omega_\mathrm{D}/2k_\mathrm{B}T_c)$ with $p = \frac{2\mathrm{e}^\gamma}{\pi} \simeq 1.13$ and $\gamma = 0.577\ldots$ (Euler constant)

⇨ $$\boxed{k_\mathrm{B}T_c = 1.13\,\hbar\omega_\mathrm{D}\,\mathrm{e}^{-2/V_0 D(E_\mathrm{F})}}$$

critical temperature is proportional to Debye frequency $\omega_\mathrm{D} \propto 1/\sqrt{M}$
➔ **explains isotope effect !!**

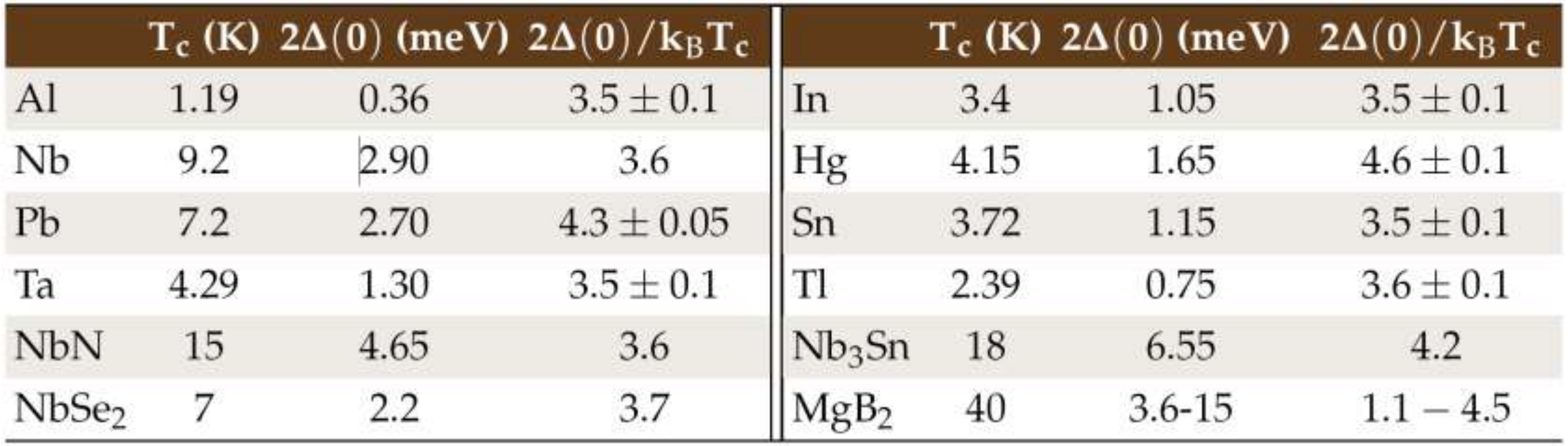
4.2.3 The BCS Gap Equation and QP Excitations

relation between energy gap at zero temperature and critical temperature

$$\underbrace{\Delta(0) \simeq 2\hbar\omega_\mathrm{D}\,\mathrm{e}^{-2/V_0 D(E_\mathrm{F})} \quad\Longleftrightarrow\quad k_\mathrm{B}T_c = \frac{2\mathrm{e}^{\gamma}}{\pi}\hbar\omega_\mathrm{D}\,\mathrm{e}^{-2/V_0 D(E_\mathrm{F})}}$$

$$\boxed{\frac{\Delta(0)}{k_\mathrm{B}T_c} = \frac{\pi}{\mathrm{e}^{\gamma}} = 1.764}$$

key prediction of BCS theory



	T_c (K)	$2\Delta(0)$ (meV)	$2\Delta(0)/k_BT_c$		T_c (K)	$2\Delta(0)$ (meV)	$2\Delta(0)/k_BT_c$
Al	1.19	0.36	3.5 ± 0.1	In	3.4	1.05	3.5 ± 0.1
Nb	9.2	2.90	3.6	Hg	4.15	1.65	4.6 ± 0.1
Pb	7.2	2.70	4.3 ± 0.05	Sn	3.72	1.15	3.5 ± 0.1
Ta	4.29	1.30	3.5 ± 0.1	Tl	2.39	0.75	3.6 ± 0.1
NbN	15	4.65	3.6	Nb_3Sn	18	6.55	4.2
$NbSe_2$	7	2.2	3.7	MgB_2	40	3.6-15	$1.1 - 4.5$

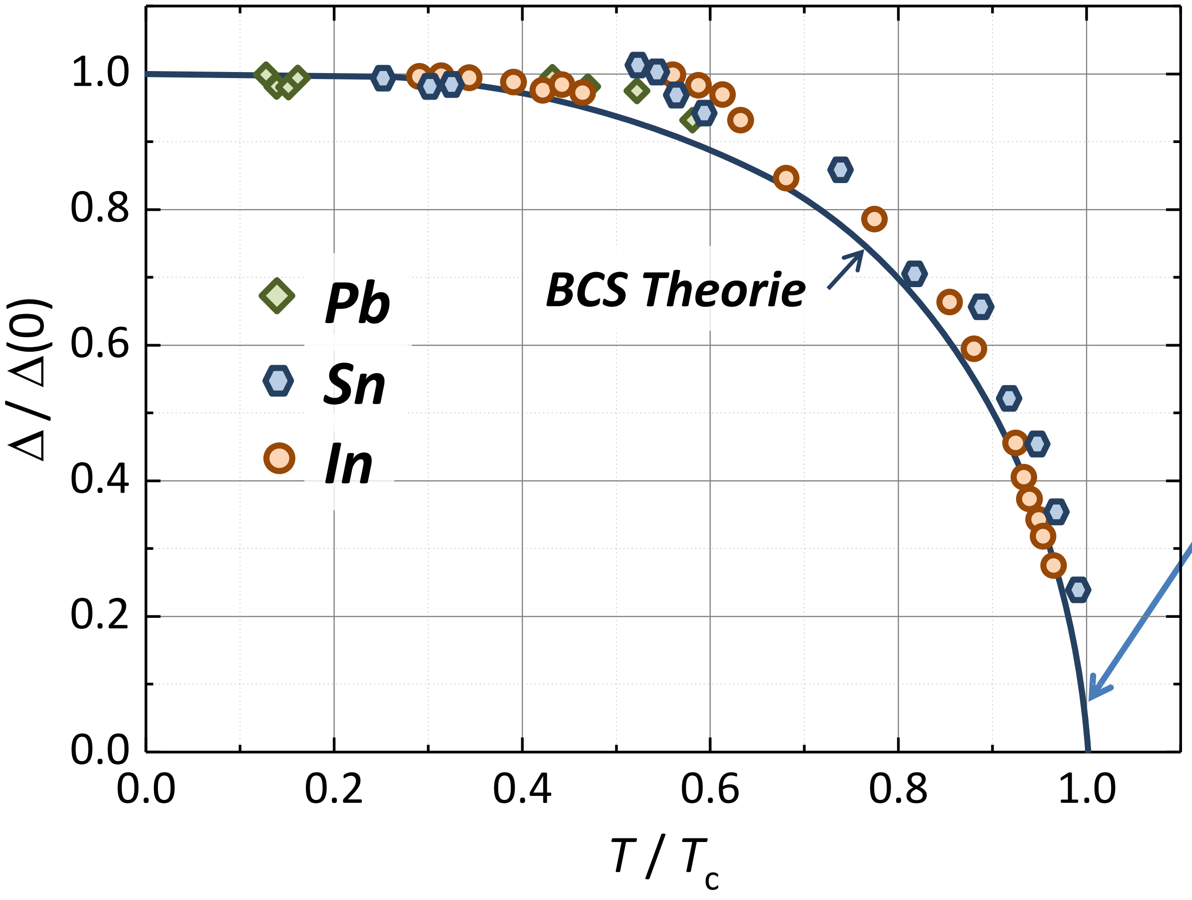
considerable deviations for „strong-coupling“ superconductors:

➔ $V_0 D(E_\mathrm{F}) \ll 1$ is no longer a good approximation

4.2.3 The BCS Gap Equation and QP Excitations

solution for $0 < T < T_c$ (numerical solution of integral)

$$1 = V_0 \sum_{\mathbf{k}'} \frac{1}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_\mathrm{B}T}\right) \quad \text{sum} \Rightarrow \text{integral} \quad 1 = \frac{V_0 D(E_\mathrm{F})}{2} \int_{-\hbar\omega_\mathrm{D}}^{\hbar\omega_\mathrm{D}} \frac{1}{2E_\mathbf{k}} \tanh\left(\frac{E_\mathbf{k}}{2k_\mathrm{B}T}\right) d\xi_\mathbf{k}$$



good approximation close to T_c:

$$\frac{\Delta(T)}{\Delta(0)} \simeq 1.74 \left(1 - \frac{T}{T_c}\right)^{1/2}$$

(characteristic result of mean-field theory)

B. Mühlschlegel, *Die thermodynamischen Funktionen des Supraleiters*, Z. Phys. 115, 313–327 (1959).

4.2.3 The BCS Gap Equation and QP Excitations

strong electron-phonon coupling

- BCS results are valid only for weak coupling: $V_0 D(E_\mathrm{F}) \ll 1$
- for $V_0 D(E_\mathrm{F}) \gtrsim 0.2$ a more elaborate treatment is required

phonons have influence on electrons but also electrons change e.g. phonon frequencies

- **Eliashberg theory**
  - replace couling constant $\lambda = V_0 D(E_\mathrm{F})$ by

$$\lambda(\omega) = 2 \int_0^\infty \frac{\alpha^2(\omega) F(\omega)}{\omega} \, \mathrm{d}\omega$$

$F(\omega)$: phonon density of states

$\alpha(\omega)$: matrix element of the electron-phonon interaction

G. M. Eliashberg, *Interactions Between Electrons and Lattice Vibrations in a Superconductor*, Zh. Éksp. Teor. Fiz. 38, 966 (1960) [Sov. Phys. JETP 11, 696-702 (1960)].

- **McMillan approximation**
  - several attempts have been made to improve predition for T_c using strong coupling theory, e.g. by McMillan:

$$T_c = \frac{\hbar\omega_\mathrm{D}}{1.45} \exp\left(\frac{1.04(1+\lambda)}{\lambda - \mu^\star(1 + 0.62\,\lambda)}\right)$$

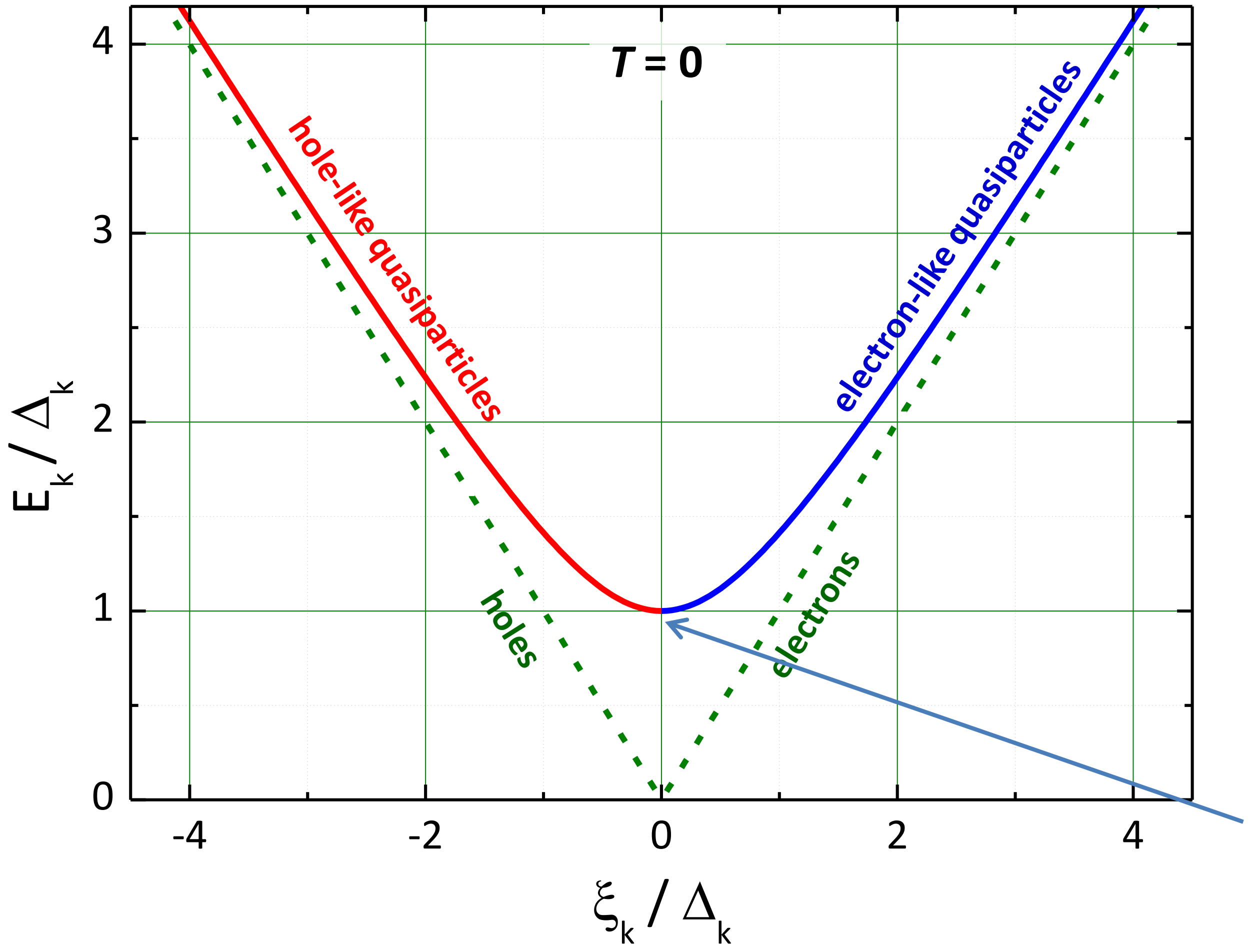
$\mu^\star$: matrix element of the short-range screened Coulomb repulsion

W. L. McMillan, *Transition Temperature of Strong-Coupled Superconductors*, Phys. Rev. 167, 331 (1968).

4.2.3 Energy Gap and Excitation Spectrum

dispersion of excitations (Bogoliubov quasiparticles) from the superconducting ground state

→ ***excitations represent superpositions of electron- and hole-type single particle states***
(reason: *single particle excitation with* $\mathbf{k}$ *can only exist if there is hole with* $-\mathbf{k}$, *if not, Cooper pair would form*)



excitation energy

$$E_{\mathbf{k}} = E_{-\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$$

- break up of Cooper pair requires energy $2E_{\mathbf{k}}$
- Δ represents energy gap for quasiparticle excitation from ground state
  ➔ minimum excitation energy

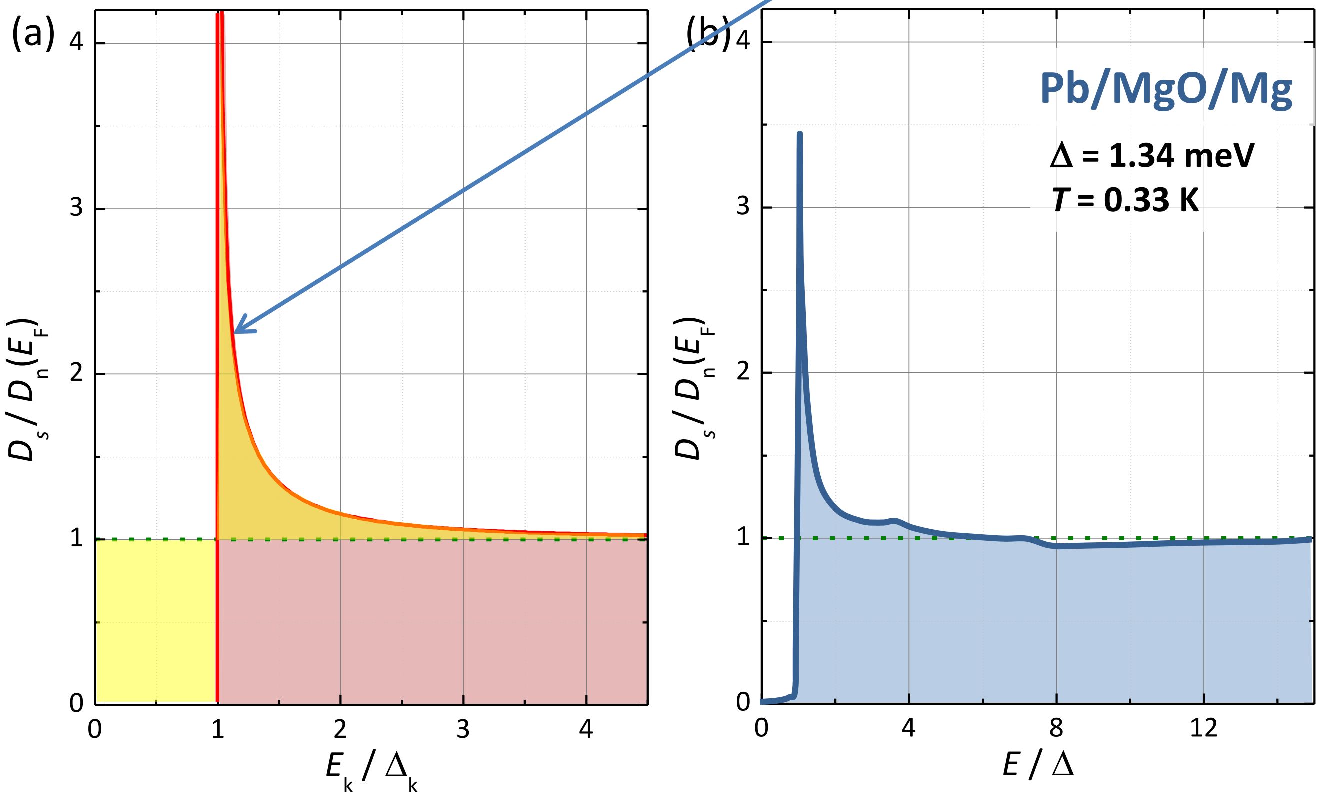
equal superposition of electron with wave vector $\mathbf{k}$ and hole with wave vector $-\mathbf{k}$

4.2.3 Energy Gap and Excitation Spectrum

density of states

- conservation of states on transition to sc state requires $D_s(E_\mathbf{k})\mathrm{d}E_\mathbf{k} = D_n(\xi_\mathbf{k})\mathrm{d}\xi_\mathbf{k}$
- close to E_F: $D_n(\xi_\mathbf{k}) \simeq D_n(E_\mathrm{F}) = const.$

$$D_s(E_\mathbf{k}) = D_n(\xi_\mathbf{k})\frac{\mathrm{d}\xi_\mathbf{k}}{\mathrm{d}E_\mathbf{k}} = \begin{cases} D_n(E_\mathrm{F})\dfrac{E_\mathbf{k}}{\sqrt{E_\mathbf{k}^2 - \Delta^2}} & \text{for} \quad E_\mathbf{k} > \Delta \\ 0 & \text{for} \quad E_\mathbf{k} < \Delta \end{cases}$$



I. Giaever,
Phys. Rev. **126**, 941 (1962)

4.3 Thermodynamic Quantities

- occupation probability of qp-excitations is given by $f(E_{\mathbf{k}}) = [\exp(E_{\mathbf{k}}/k_{\mathrm{B}}T) + 1]^{-1}$

  → i.e. by $\Delta_{\mathbf{k}}(T)$, which is contained in $\mathrm{E}_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2(T)}$

- ***entropy of electronic system*** (determined only by the occupation probability → is fixed by $\Delta_{\mathbf{k}}$)

$$S_s = -2k_{\mathrm{B}} \sum_{\mathbf{k}} \left\{ \underbrace{[1 - f(E_{\mathbf{k}})] \ln[1 - f(E_{\mathbf{k}})]}_{\text{hole like}} + \underbrace{f(E_{\mathbf{k}}) \ln[f(E_{\mathbf{k}})]}_{\text{electron like}} \right\}$$

$$S = -k_{\mathrm{B}} \sum_n p_n \ln p_n$$

- ***heat capacity***: $C_s = T \left(\frac{\partial S_s}{\partial T} \right)_{p.B}$ after some math:

$$C_s = \frac{2}{T} \sum_{\mathbf{k}} -\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}} \left(\underbrace{E_{\mathbf{k}}^2}_{\substack{\text{results from redistribution} \\ \text{of qp on available energy levels}}} - \underbrace{\frac{1}{2} T \frac{\mathrm{d}\Delta_{\mathbf{k}}^2(T)}{\mathrm{d}T}}_{\substack{\text{results from } T\text{-dependence} \\ \text{of energy gap}}} \right)$$

Yosida function:

$$Y(T) = \frac{1}{D(E_{\mathrm{F}})} \sum_{\mathbf{k}} -\frac{\partial f(E_{\mathbf{k}}, T)}{\partial E_{\mathbf{k}}} = \frac{1}{4k_{\mathrm{B}}T} \int_{-\mu}^{\infty} \frac{d\xi_{\mathbf{k}}}{\cosh^2(\xi_{\mathbf{k}}/2k_{\mathrm{B}}T)}$$

appears in many thermodynamic properties

$Y(T)$ describes the T-dependence of the qp excitations (normal fluid density): $n_n(T) = n\,Y(T)$

4.3 Thermodynamic Quantities

$$C_s = \frac{2}{T}\sum_{\mathbf{k}} -\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}\left(E_{\mathbf{k}}^2 - \frac{1}{2}T\frac{\mathrm{d}\Delta_{\mathbf{k}}^2(T)}{\mathrm{d}T}\right)$$

$$\mathrm{E}_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2(T)}$$

discussion of limiting cases

i. $T \ll T_c$:

- since $\Delta_{\mathbf{k}}(T) \simeq \Delta_{\mathbf{k}}(0) \gg k_{\mathrm{B}}T$, there are only a few thermally excited qp
- we use approximations $\mathrm{d}\Delta_{\mathbf{k}}^2(T)/\mathrm{d}T \simeq 0$ and $f(E_{\mathbf{k}}) = [\exp(E_{\mathbf{k}}/k_{\mathrm{B}}T) + 1]^{-1} \simeq \exp(-E_{\mathbf{k}}/k_{\mathrm{B}}T)$
- we assume $\Delta_{\mathbf{k}} = \Delta$ for simplicity and transfer sum into an integration

(we use $\Delta^2 + \xi_{\mathbf{k}}^2 = \Delta^2\left(1 + \xi_{\mathbf{k}}^2/\Delta^2\right) \simeq \Delta^2$ and $\sqrt{\Delta^2 + \xi_{\mathbf{k}}^2} = \Delta\sqrt{1 + \xi_{\mathbf{k}}^2/\Delta^2} \simeq \Delta + \xi_{\mathbf{k}}^2/2\Delta$, as $\partial f(E_{\mathbf{k}})/\partial E_{\mathbf{k}}$ has significant weight only for small values of $\xi_{\mathbf{k}}\,/\Delta$)

$$C_s = \frac{2}{T}\sum_{\mathbf{k}} -\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}\left(E_{\mathbf{k}}^2 - \frac{1}{2}T\frac{\mathrm{d}\Delta^2(T)}{\mathrm{d}T}\right) \simeq \frac{D(E_{\mathrm{F}})}{k_{\mathrm{B}}T^2}\,\Delta^2(0)\int_0^\infty \mathrm{e}^{-\sqrt{\Delta^2+\xi_{\mathbf{k}}^2}\,/k_{\mathrm{B}}T}\,\mathrm{d}\xi_{\mathbf{k}}$$

$$\frac{\Delta(0)}{k_{\mathrm{B}}T_c} = 1.76$$

$$C_s \simeq \frac{D(E_{\mathrm{F}})}{k_{\mathrm{B}}T^2}\,\Delta^2(0)\mathrm{e}^{-\Delta(0)/k_{\mathrm{B}}T}\underbrace{\int_0^\infty \mathrm{e}^{-\xi_{\mathbf{k}}^2/2\Delta(0)k_{\mathrm{B}}T}\,\mathrm{d}\xi_{\mathbf{k}}}_{\sqrt{\pi k_{\mathrm{B}}T\Delta(0)/2}}$$

$$\Rightarrow \quad \boxed{C_s \propto T^{-\frac{3}{2}}\mathrm{e}^{-\frac{\Delta(0)}{k_{\mathrm{B}}T}} \propto T^{-\frac{3}{2}}\mathrm{e}^{-1.76\frac{T}{T_c}} \ @\, T \ll T_c}$$

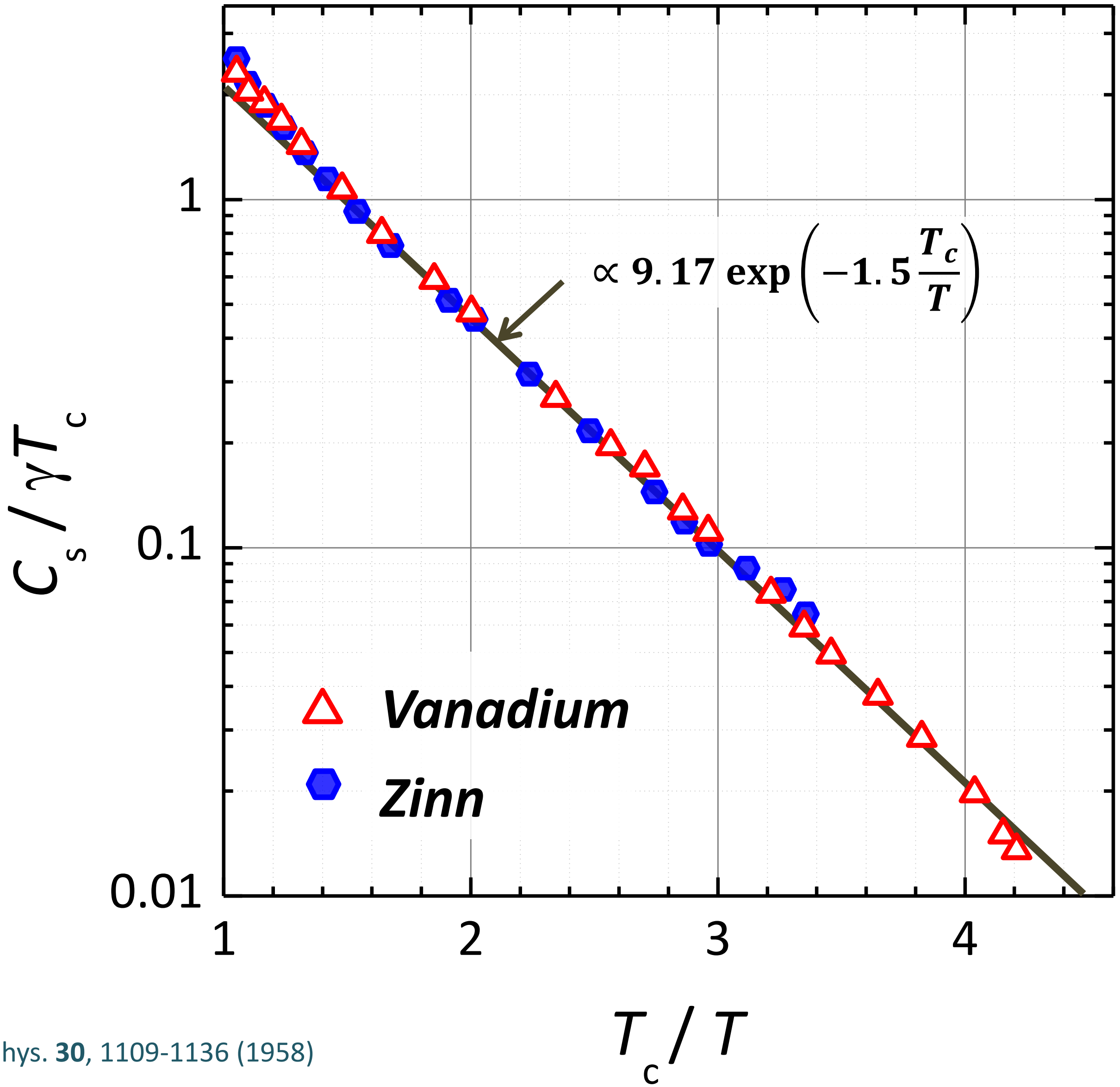
exponential decrease of heat capacity at low T

4.3 Thermodynamic Quantities

specific heat of superconductors at $T \ll T_c$:

exponential decrease of C_s with decreasing T:

$$C_s \propto T^{-\frac{3}{2}} \mathrm{e}^{-\frac{\Delta(0)}{k_\mathrm{B} T}} \propto T^{-\frac{3}{2}} \mathrm{e}^{-1.76\frac{T}{T_c}} \quad @\, T \ll T_c$$



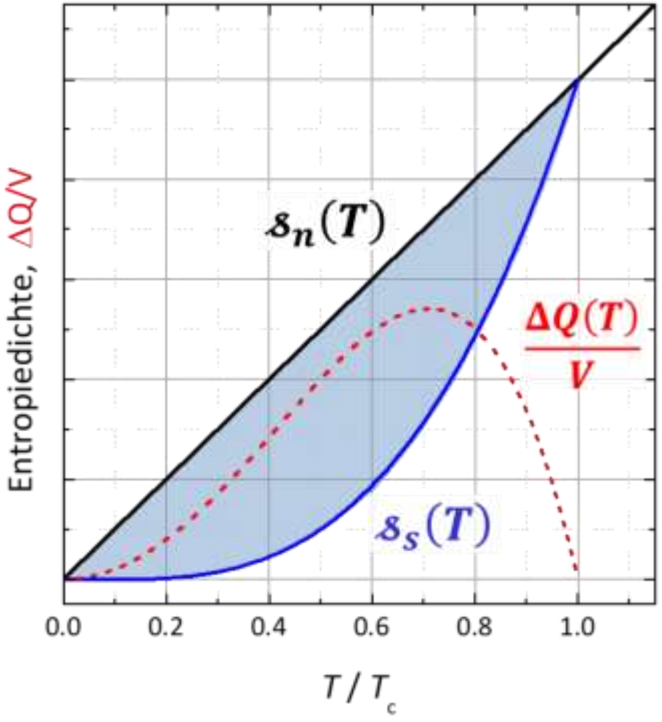
M. A. Biondi, A. T. Forrester, M. P. Garfunkel, C. B. Satterthwaite, Rev. Mod. Phys. **30**, 1109-1136 (1958)

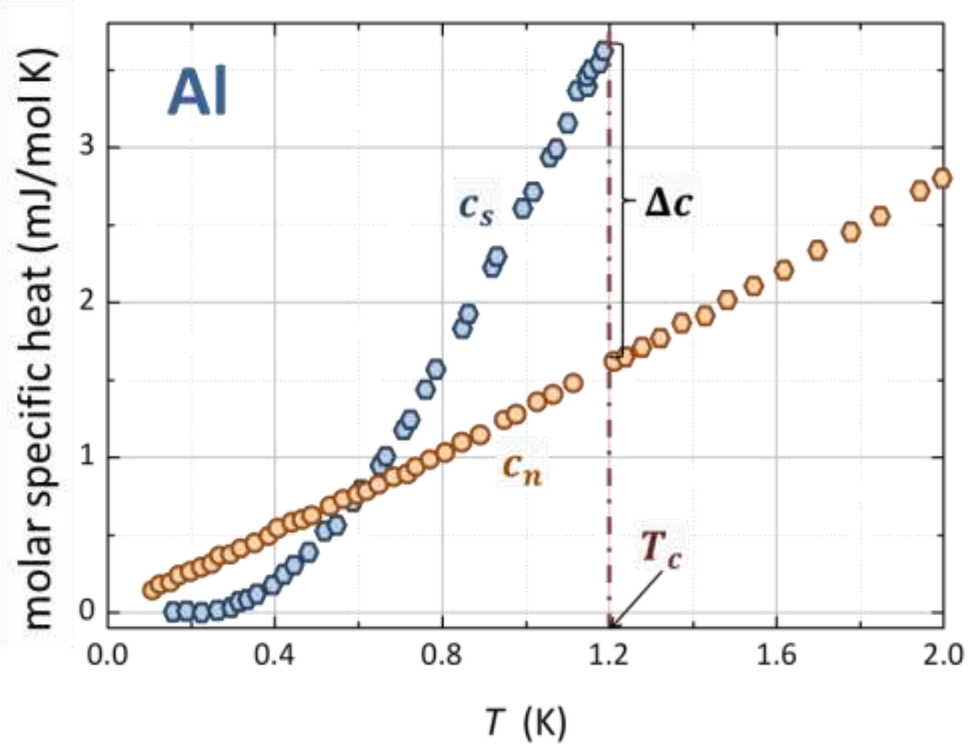
4.3 Thermodynamic Quantities

ii. $0.5 < T/T_c < 1$:

$\Delta(T)$ decreases with increasing T ➔ there is a rapid increase of the number of thermally excited quasiparticles

➔ $\frac{\partial S_s}{\partial T} > \frac{\partial S_n}{\partial T} \Rightarrow$ ***C_s is getting larger than C_n***





4.3 Thermodynamic Quantities

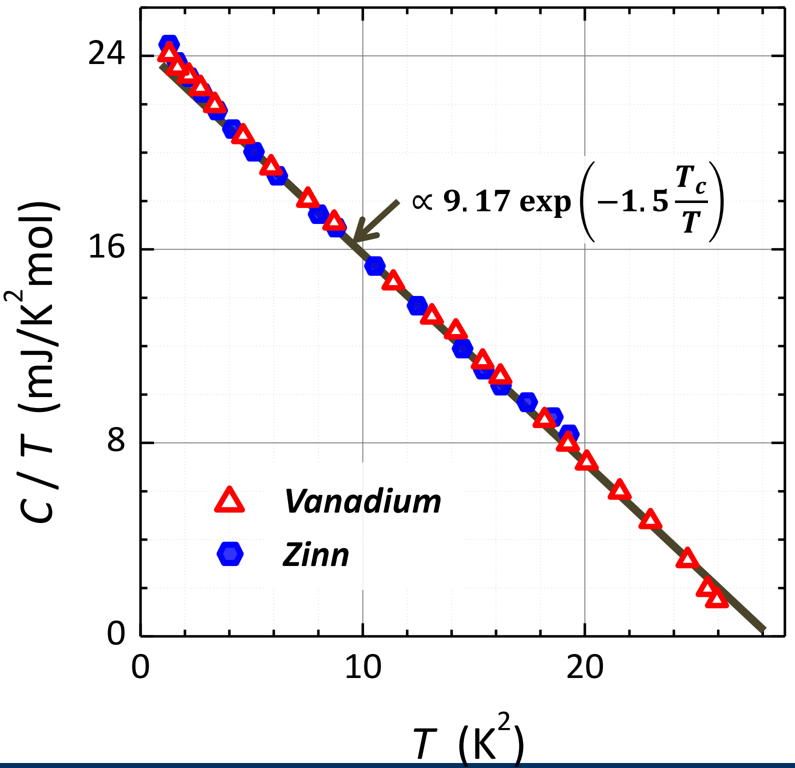
iii. $T \simeq T_c$:

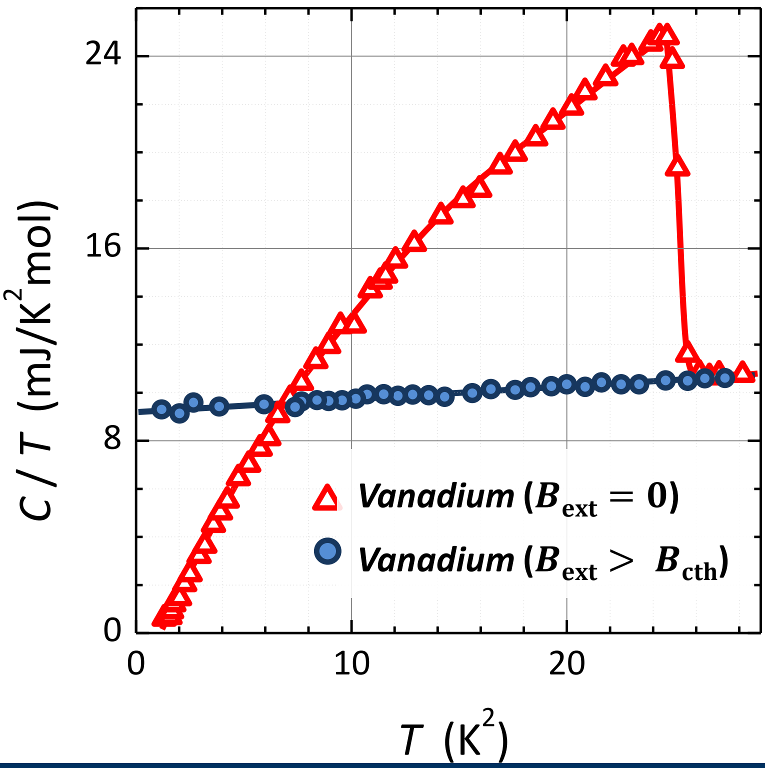
$\Delta(T) \to 0$ ➔ we can replace $E_{\mathbf{k}}$ by $|\xi_{\mathbf{k}}|$:

$$C_s = \underbrace{\frac{2}{T}\sum_{\mathbf{k}} -\frac{\partial f(\xi_{\mathbf{k}})}{\partial \xi_{\mathbf{k}}}\left(\xi_{\mathbf{k}}^2\right.}_{} - \underbrace{\left.\frac{1}{2}T\frac{\mathrm{d}\Delta^2(T)}{\mathrm{d}T}\right)}_{}$$

normal state specific heat $C_n = \frac{\pi^2}{3}D(E_F)k_B^2T$

finite for $T < T_c$
zero for $T > T_c$ } *jump of specific heat*





M. A. Biondi *et al.*,
Rev. Mod. Phys. **30**, 1109-1136 (1958)

4.3 Thermodynamic Quantities

iii. ***$T \simeq T_c$: jump of specific heat*** (we can replace $E_{\mathbf{k}}$ by $|\xi_{\mathbf{k}}|$)

$$\Delta C = (C_s - C_n)_{T=T_c} = \frac{2}{T}\sum_{\mathbf{k}} -\frac{\partial f(\xi_{\mathbf{k}})}{\partial \xi_{\mathbf{k}}}\left(-\frac{1}{2}T\frac{\mathrm{d}\Delta^2(T)}{\mathrm{d}T}\right)_{T=T_c}$$

$$\Delta C = D(E_\mathrm{F})\left(-\frac{\mathrm{d}\Delta^2(T)}{\mathrm{d}T}\right)_{T=T_c}\underbrace{\int_{-\infty}^{\infty} -\frac{\partial f(\xi_{\mathbf{k}})}{\partial \xi_{\mathbf{k}}}\,\mathrm{d}\xi_{\mathbf{k}}}_{=1}$$

we use $\Delta(T) \simeq 1.74\left(1-\frac{T}{T_c}\right)^{1/2}$ for T close to T_c and $\Delta(0) = 1.76\,k_\mathrm{B}T_c$ and obtain

$$\Delta C \simeq 4.7\,D(E_\mathrm{F})k_\mathrm{B}^2 T_c$$

with $C_n(T_c) = \frac{\pi^2}{3}\,D(E_\mathrm{F})k_\mathrm{B}^2 T_c = \gamma T_c$ we finally obtain

$$\left(\frac{\Delta C}{C_n}\right)_{T=T_c} \simeq \frac{4.7}{\pi^2/3} = 1.43$$

further key prediction of BCS theory

(in good agreement with experiment)

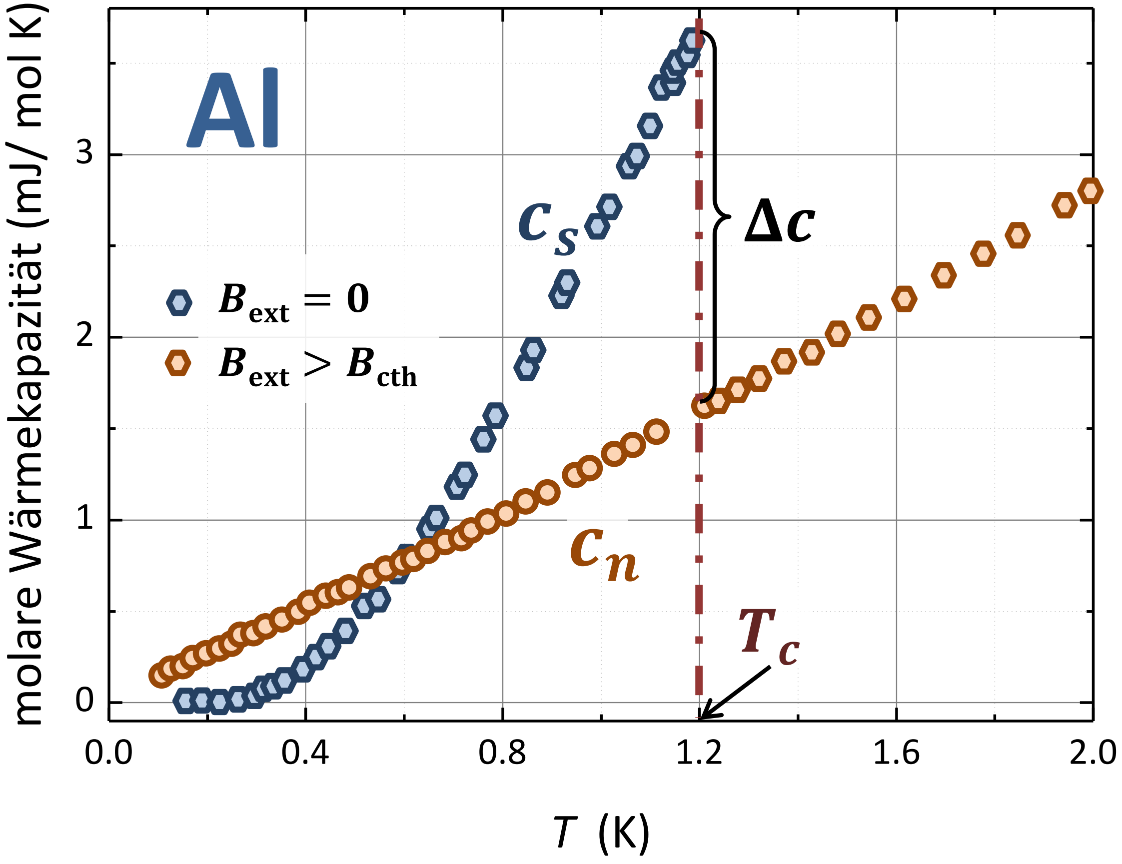
result from phenomenological treatment:

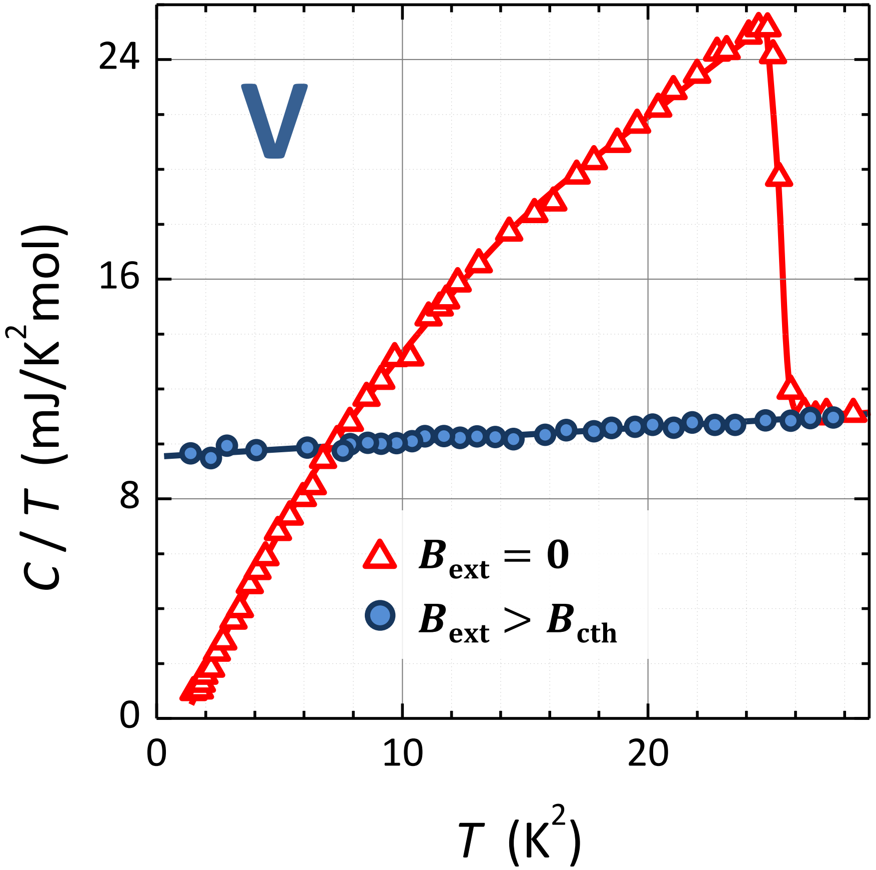
$$\left(\frac{\Delta C}{C_n}\right)_{T=T_c} = \frac{1}{C_n}\frac{T_c}{\mu_0}\left(\frac{\partial B_\mathrm{cth}}{\partial T}\right)^2_{T=T_c} = \frac{1}{C_n}\frac{8}{T_c}\frac{B^2_\mathrm{cth}(0)}{2\mu_0} = \frac{8}{\gamma T_c^2}\underbrace{\frac{B^2_\mathrm{cth}(0)}{2\mu_0}}_{\frac{1}{4}D(E_\mathrm{F})\,\Delta^2(0)} = \frac{6}{\pi^2}\left(\frac{\Delta(0)}{k_\mathrm{B}T_c}\right)^2 = \frac{6}{\pi^2}(1.76)^2 = 1.88$$

(Rutgers formula)

difference comes from $B_\mathrm{cth}(T)$

4.3 Thermodynamic Quantities





N.E. Phillips,
Phys. Rev. **114**, 676 (1959)

M. A. Biondi et al.,
Rev. Mod. Phys. **30**, 1109-1136 (1958)

4.4 Determination of the Energy Gap

- energy gap determines excitation spectrum of superconductors

  ➔ **we can use quantities that depend on excitation spectrum to determine Δ**

1. **specific heat**
2. **tunneling conductance**
3. **microwave and infrared absorption**
4. **ultrasound attenuation**
5. **…..**

- we concentrate on tunneling spectroscopy in the following

  (specific heat already discussed in previous subsection)

4.4.2 Tunneling Spectroscopy

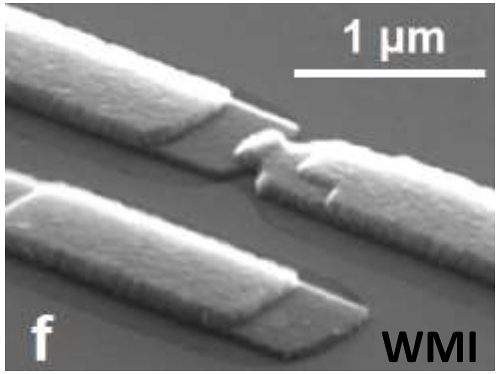
tunneling of quasiparticle excitations between two superconductors separated by thin tunneling barrier

- SIS tunnel junction:

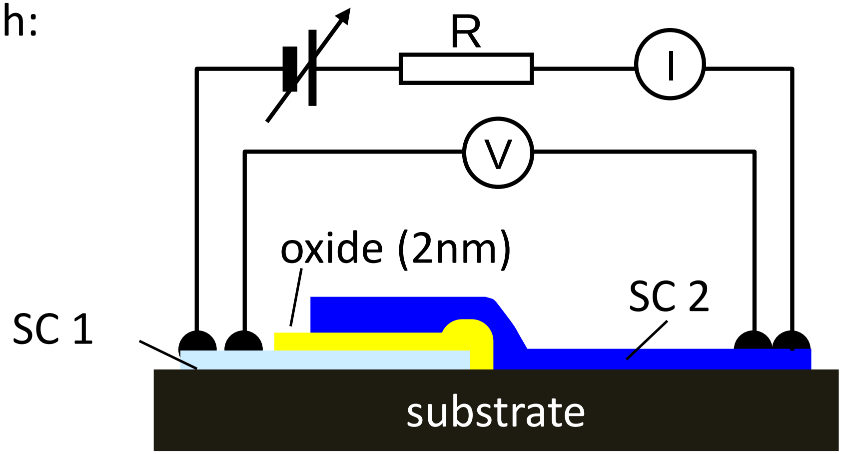
tunnel junction

- fabrication by thin film technology and patterning techniques

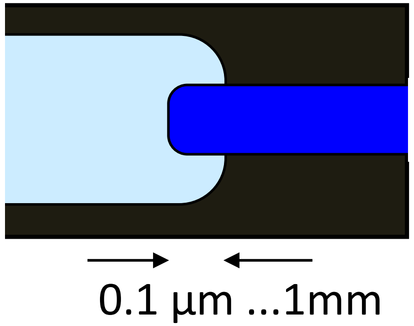
by shadow masks	(≈ mm)
by optical lithography	(≈ µm)
by e-beam lithography	(≈ 10 nm)



- sketch:



top view:



4.4.2 Tunneling Spectroscopy

- tunneling processes result in finite coupling of SC 1 and SC 2, described by tunneling hamiltonian

$$\mathcal{H}_{\mathrm{tun}} = \sum_{\mathbf{kq}\sigma} \underbrace{T_{\mathbf{kq}}}\ \underbrace{c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{q}\sigma}} + c.c.$$

tunnel matrix element

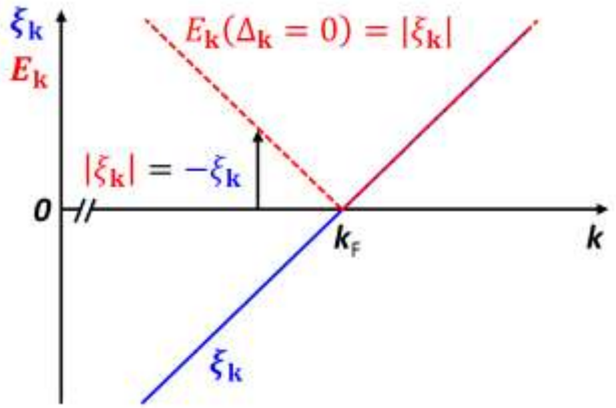
describes the creation of electron $|\mathbf{k}\sigma\rangle$ in one SC and the annihilation of electron $|\mathbf{q}\sigma\rangle$ in the other

- tunneling into state $|\mathbf{k}\sigma\rangle$ only possible if pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ is empty

  → resulting tunneling probability is $\propto |u_{\mathbf{k}}|^2 \left|T_{\mathbf{kq}}\right|^2$

- for each state $|\mathbf{k}\sigma\rangle$ there exists a state $|\mathbf{k}'\sigma\rangle$ with $E_{\mathbf{k}} = E_{\mathbf{k}'}$ but with $\xi_{\mathbf{k}'} = -\xi_{\mathbf{k}}$

  → resulting tunneling probability is $\propto |u_{\mathbf{k}'}|^2 \left|T_{\mathbf{k}'\mathbf{q}}\right|^2 \underbrace{=}_{|u(-\xi_{\mathbf{k}})|=|v(\xi_{\mathbf{k}})|} |v_{\mathbf{k}}|^2 \left|T_{\mathbf{k}'\mathbf{q}}\right|^2$



total tunneling probability $\propto \left(|\mathbf{u_k}|^2 + |\mathbf{v_k}|^2\right)\left|\mathbf{T_{kq}}\right|^2 = \left|\mathbf{T_{kq}}\right|^2$ **does not depend on coherence factors**

→ ***simple „semiconductor model“ for quasiparticle tunneling is applicable***

4.4.2 Tunneling Spectroscopy

elastic tunneling between two metals (NIN):

$$I_{1\to 2} = C \int_{-\infty}^{\infty} |T|^2 \quad \underbrace{D_1(E) f(E)}_{\text{occupied states in } \mathrm{N}_1} \quad \underbrace{D_2(E+eV)\,[1 - f(E+eV)]}_{\text{empty states in } \mathrm{N}_2} \; \mathrm{d}E$$

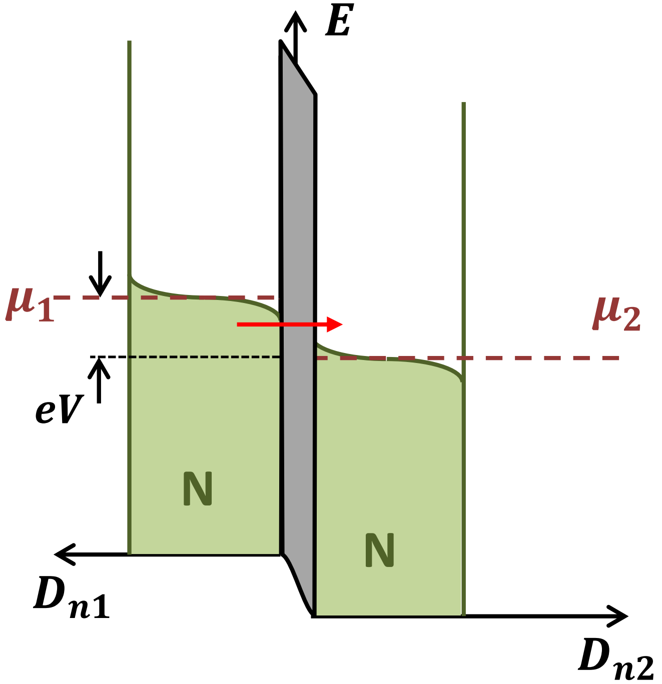
- net tunneling current:

$$I_{nn}(V) = C \int_{-\infty}^{\infty} |T|^2 D_1(E) D_2(E+eV)\,[f(E) - f(E+eV)]\,\mathrm{d}E$$

- for $eV \ll \mu$ and $\mu \simeq E_\mathrm{F}$ we can use $D_n(E+eV) \simeq D_n(E_\mathrm{F}) = const.$

$$I_{nn}(V) = C|T|^2 D_{n1}(E_\mathrm{F}) D_{n2}(E_\mathrm{F}) \underbrace{\int_{-\infty}^{\infty} [f(E) - f(E+eV)]\,\mathrm{d}E}_{=eV}$$

$$\boxed{I_{nn}(V) = C|T|^2 D_{n1}(E_\mathrm{F}) D_{n2}(E_\mathrm{F})\, e\,V = G_{nn}\,V}$$



4.4.2 Tunneling Spectroscopy

elastic tunneling between N and S (NIS junction):

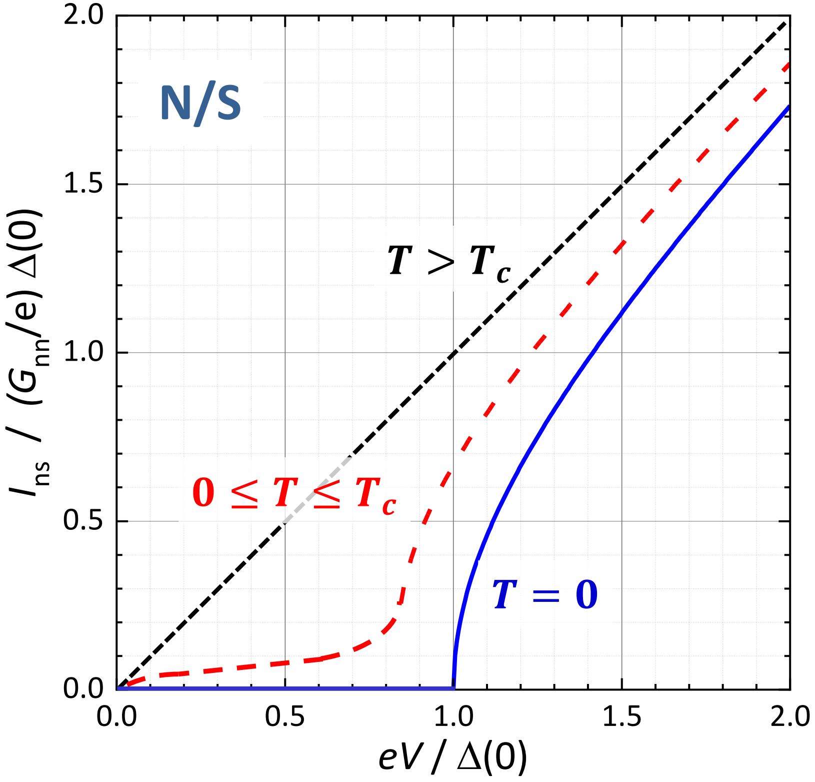
$$I_{ns}(V) = \underbrace{C|T|^2 D_{n1}(E_F) D_{n2}(E_F)}_{=G_{nn}/e} \int_{-\infty}^{\infty} \frac{D_{s2}(E)}{D_{n2}(E_F)} [f(E) - f(E+eV)]\, \mathrm{d}E$$

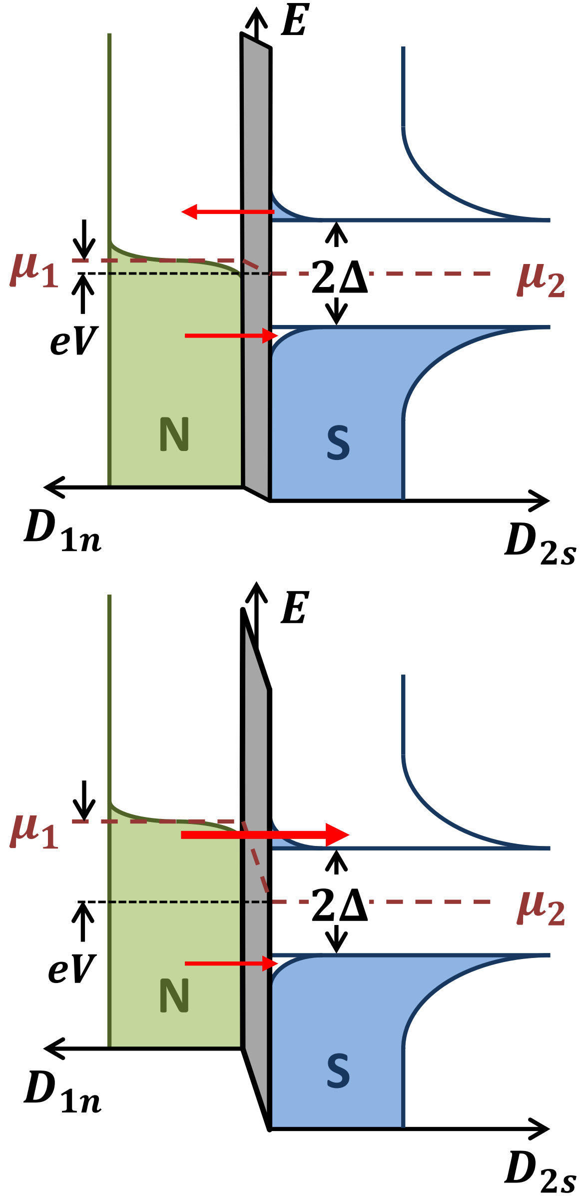
$$I_{ns}(V) = \frac{G_{nn}}{e} \int_{-\infty}^{\infty} \frac{D_{s2}(E)}{D_{n2}(E_F)} [f(E) - f(E+eV)]\, \mathrm{d}E$$

- analytical solution for $T = 0$

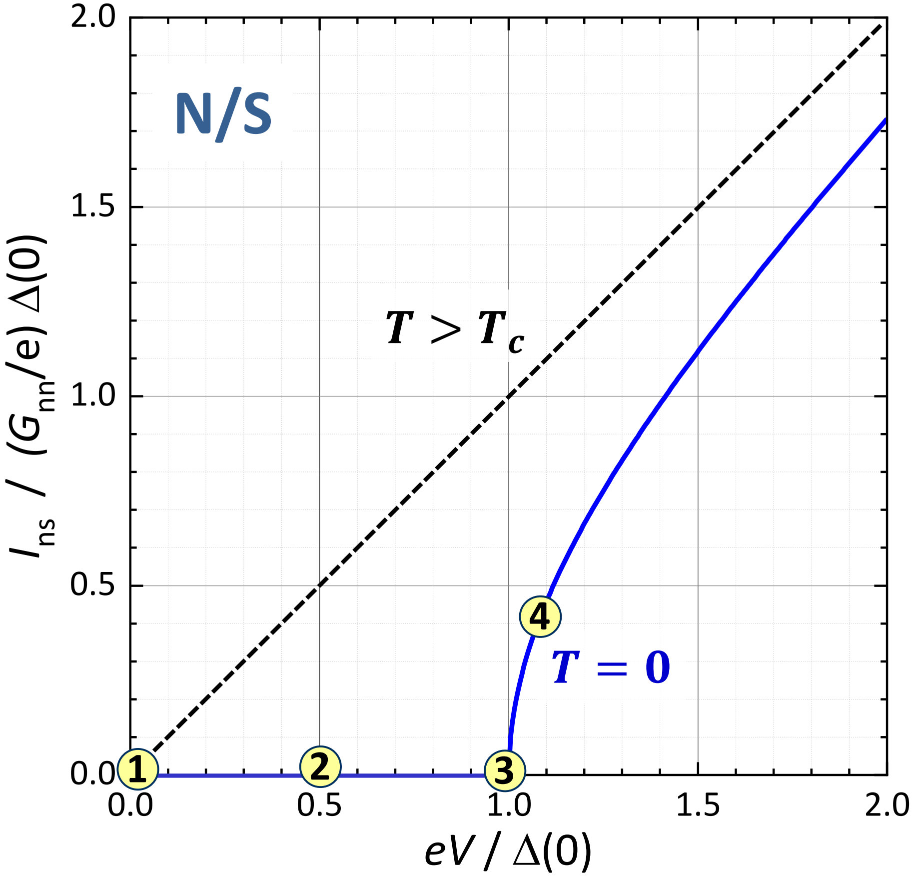
$$I_{ns}(V) = \frac{G_{nn}}{e} \int_{-\infty}^{\infty} \frac{|E|}{|E^2 - \Delta^2|^{1/2}} [f(E) - f(E+eV)]\, \mathrm{d}E$$

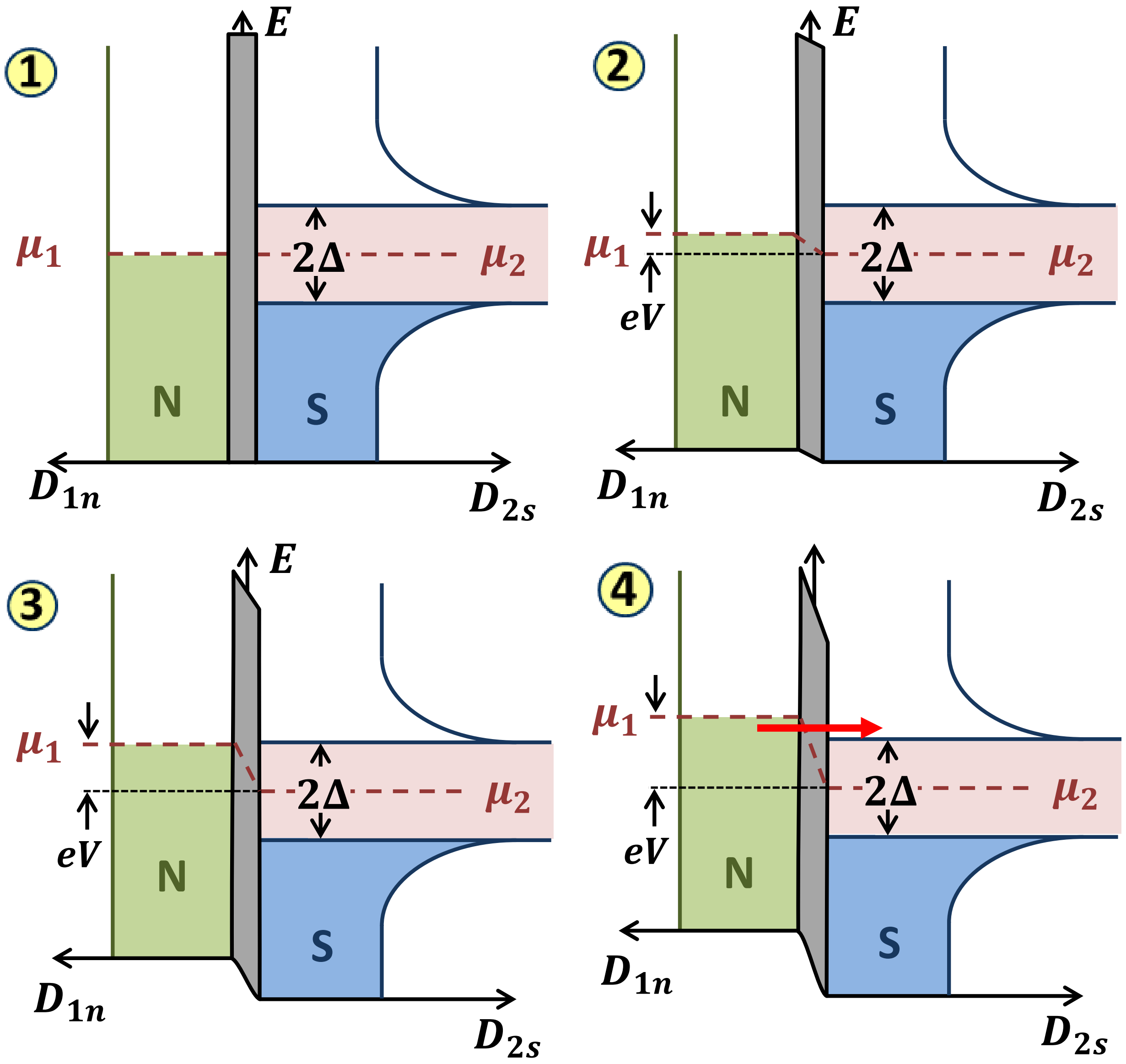
$$I_{ns}(V) = \begin{cases} 0 & |eV| < \Delta \\ \frac{G_{nn}}{e}[(eV)^2 - \Delta^2]^{1/2} & |eV| \geq \Delta \end{cases}$$





4.4.2 Tunneling Spectroscopy





4.4.2 Tunneling Spectroscopy

differential tunneling conductance of NIS junction

$$I_{ns}(V) = \frac{G_{nn}}{e} \int_{-\infty}^{\infty} \frac{D_{s2}(E)}{D_{n2}(E_\mathrm{F})} [f(E) - f(E+eV)] \, \mathrm{d}E$$

$$G_{ns}(V) = \frac{\partial I_{ns}(V)}{\partial V} = G_{nn} \int_{-\infty}^{\infty} \frac{D_{s2}(E)}{D_{n2}(E_\mathrm{F})} \underbrace{\left[-\frac{\partial f(E+eV)}{\partial\,(eV)}\right]} \mathrm{d}E$$

$$\mathrm{d}E = e\,\mathrm{d}V$$

Bell-shaped weighting function with width $\simeq 4k_\mathrm{B}T$ peaked peaked at $E = eV$
→ approaches δ-function for $T \rightarrow 0$

⇨ $$\boxed{G_{ns}(V) = G_{nn} \frac{D_{s2}(eV)}{D_{n2}(E_\mathrm{F})}}$$ @ $T = 0$

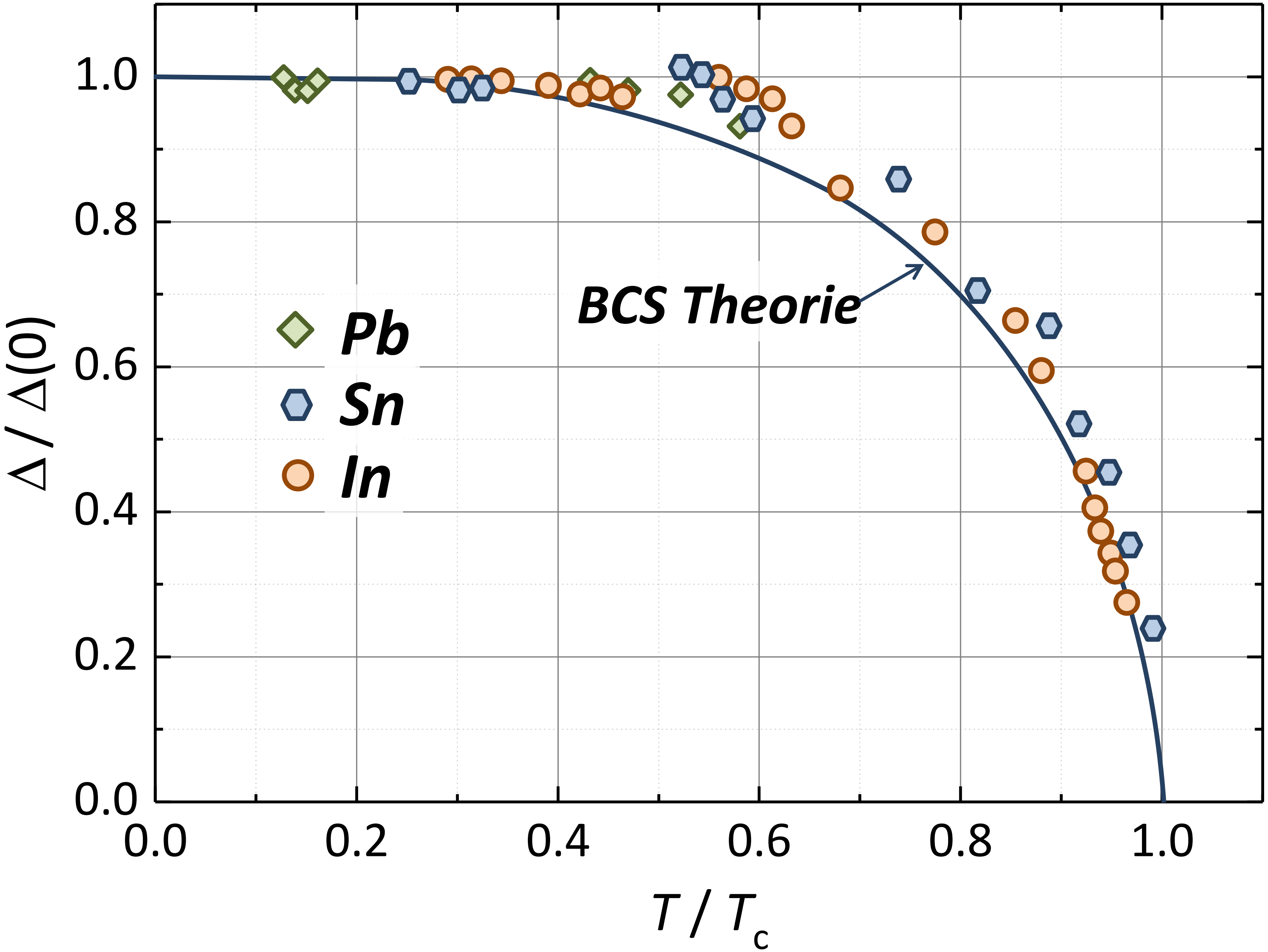
measurement of $G_{ns}(V)$ allows determination of $D_{s2}(eV)$ and Δ, for $T > 0$, $G_{ns}(V)$ measures DOS smeared out by $\pm k_\mathrm{B}T$

- at $T > 0$: finite conductance at $eV \ll \Delta$ due to smeared Fermi distribution, calculation yields

$$\boxed{\left.\frac{G_{ns}}{G_{nn}}\right|_{eV \ll \Delta} = \left(\frac{2\pi\Delta}{k_\mathrm{B}T}\right) \mathrm{e}^{-\Delta/k_\mathrm{B}T}}$$

exponential T-dependence can be used for temperature measurement, particle detectors, …

4.4.2 Tunneling Spectroscopy

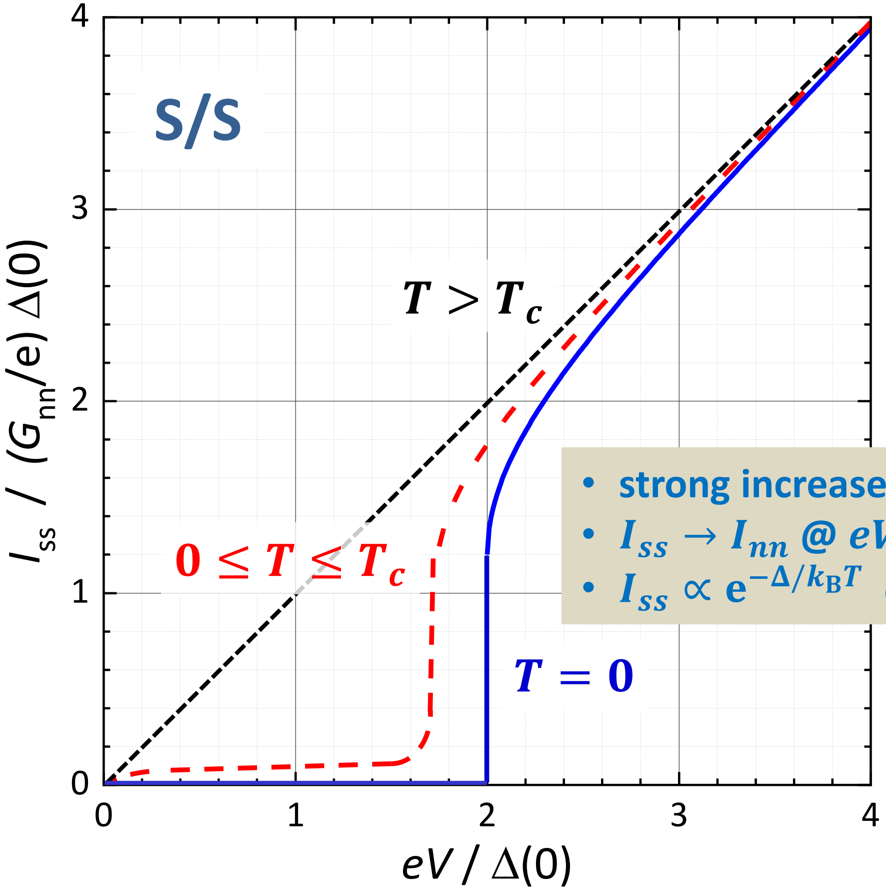


I. Giaever, K. Megerle,
Phys. Rev. **122**, 1101-1111 (1961)

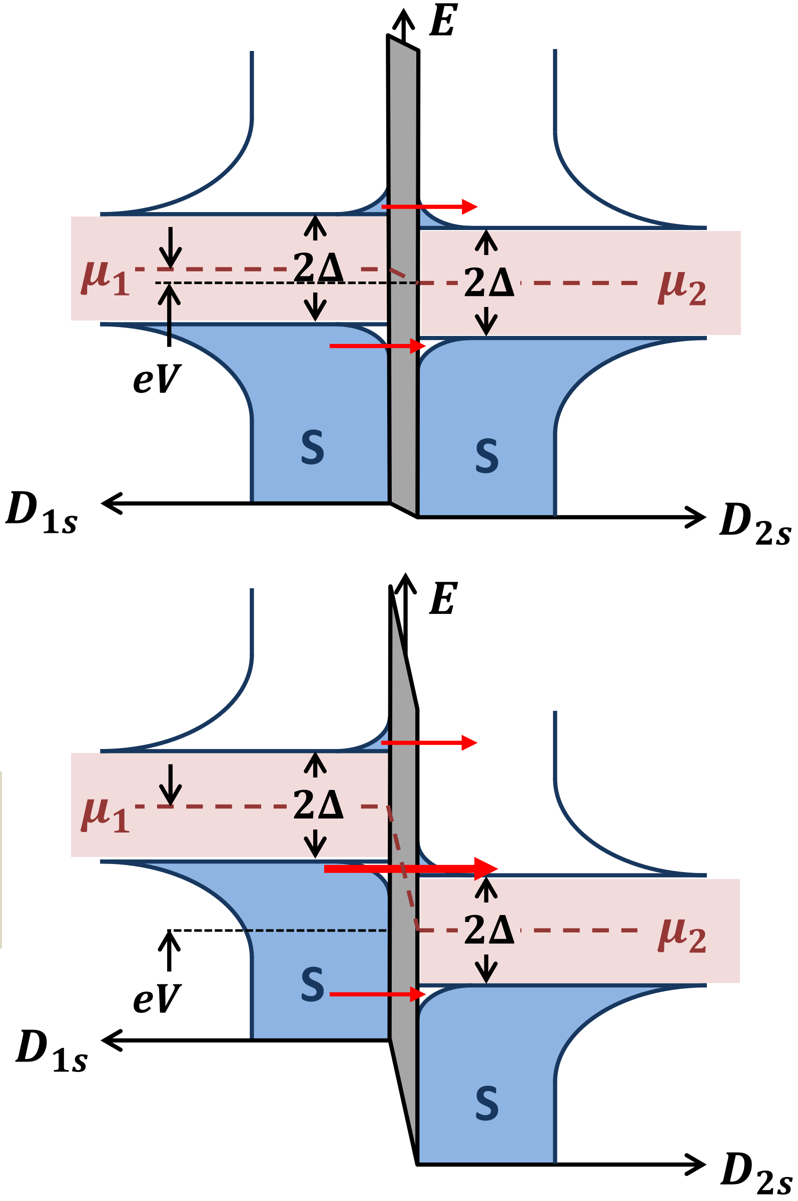
4.4.2 Tunneling Spectroscopy

elastic tunneling between two superconductors: SIS junction

$$I_{ss}(V) = \frac{G_{nn}}{e} \int_{-\infty}^{\infty} \frac{D_{s1}(E+eV)}{D_{n1}(E_\mathrm{F})} \frac{D_{s2}(E)}{D_{n2}(E_\mathrm{F})} [f(E) - f(E+eV)]\,\mathrm{d}E$$



- strong increase of I_{ss} @ $eV = 2\Delta$
- $I_{ss} \rightarrow I_{nn}$ @ $eV \gg 2\Delta$
- $I_{ss} \propto \mathrm{e}^{-\Delta/k_\mathrm{B}T}$ @ $eV < 2\Delta$

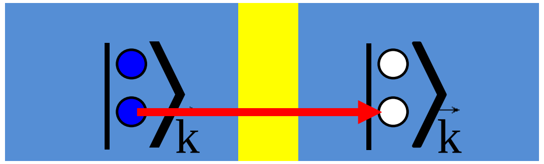


4.4.2 Tunneling Spectroscopy

interpretation of tunneling in SIS junction at $T = 0$

- single electron tunnels from left to right:

before tunneling



occupied and empty pair state

after tunneling

two quasiparticles

- energy balance: $-E_{\mathrm{F}}^{(\mathrm{left})} + E_{\mathbf{k}}^{(\mathrm{left})} + E_{\mathrm{F}}^{(\mathrm{right})} + E_{\mathbf{k}}^{(\mathrm{right})}$

e⁻ moves from left to right

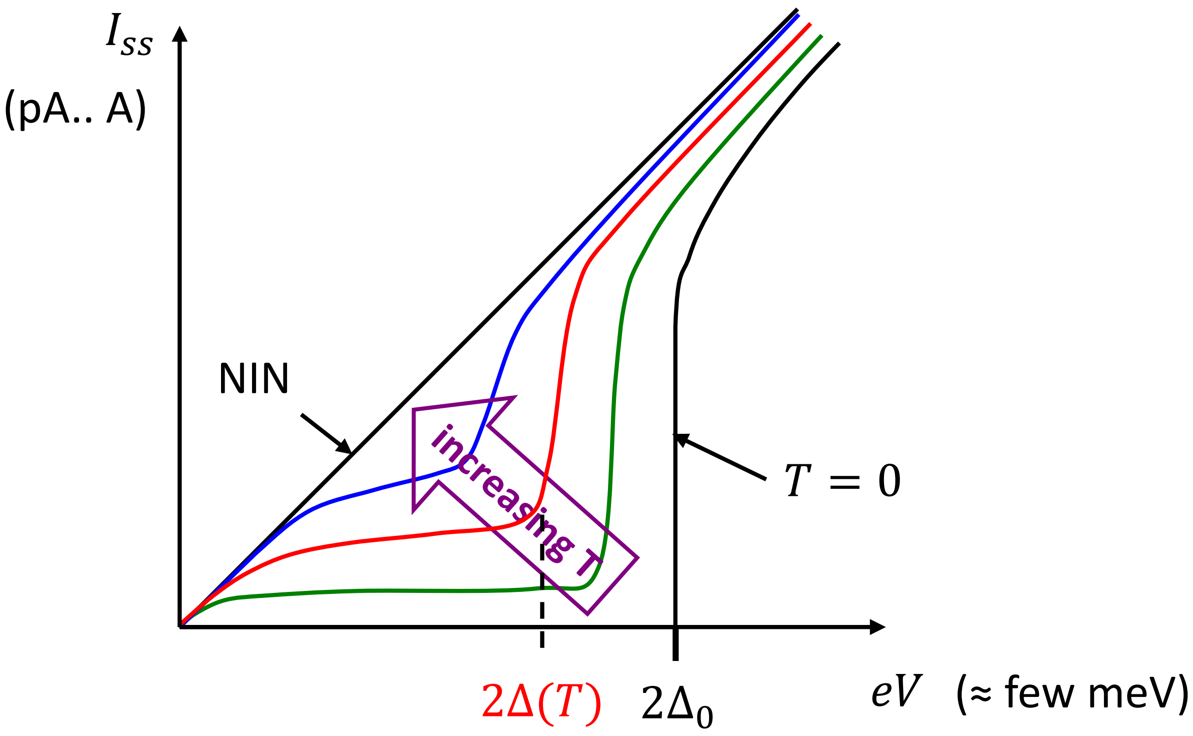
generation of two qp

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}$$

- required voltage: $\mathrm{e}V = E_{\mathbf{k}}^{(\mathrm{left})} + E_{\mathbf{k}}^{(\mathrm{right})}$
- minimal voltage: $eV = \Delta_1 + \Delta_2 = 2\Delta \quad \text{for } \Delta_1 = \Delta_2$

4.4.2 Tunneling Spectroscopy

current-voltage characteristics of SIS junction at finite temperatures



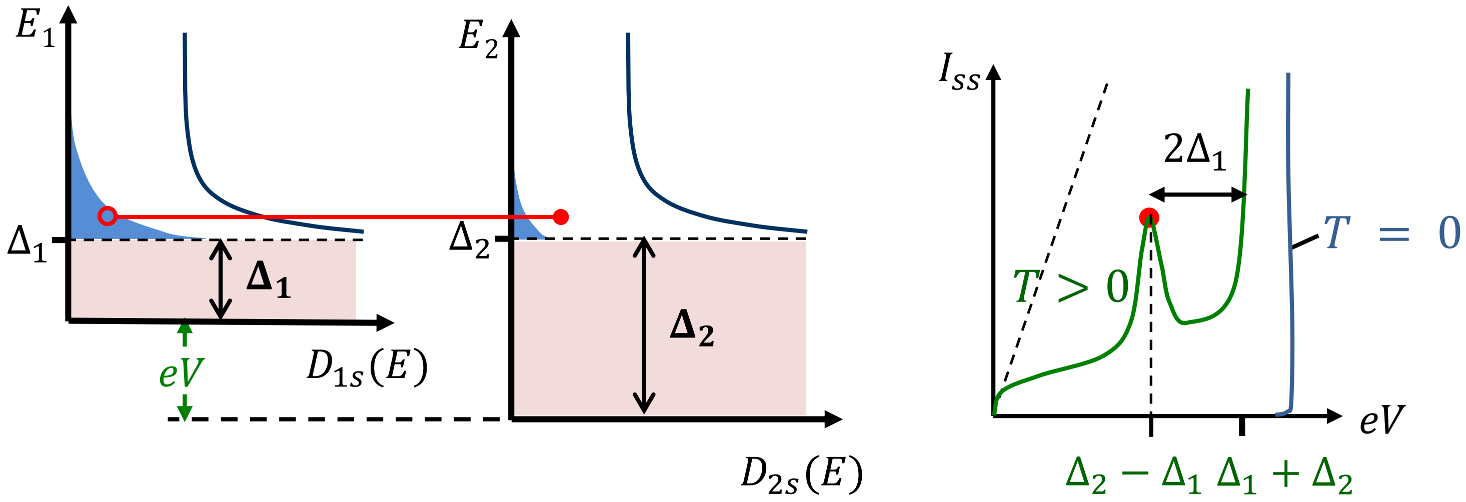
4.4.2 Tunneling Spectroscopy

special case: SIS tunnel junction with $\Delta_1 \neq \Delta_2$

- at $eV = \Delta_2 - \Delta_1$ the two singularities in the DOS are facing each other

$\Rightarrow$ maximum of the tunneling current

$\Rightarrow$ negative differential resistance



4.5 Coherence Effects

- description of an external perturbation on the electrons in a metal

$$\mathcal{H}_1 = \sum_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} P_{\mathbf{k}'\sigma',\mathbf{k}\sigma}\; c^\dagger_{\mathbf{k}'\sigma'}\; c_{\mathbf{k}\sigma}$$

interaction hamiltonian

$\left|P_{\mathbf{k}'\sigma',\mathbf{k}\sigma}\right|^2$ corresponds to transition probability

- description of the external perturbation on the electrons in a superconductor

➔ more complicated since there is a coherent superposition of occupied one-electron states

$$\left.\begin{aligned} \hat{c}^\dagger_{\mathbf{k}\uparrow} &= u^\star_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}} + v_{\mathbf{k}}\,\beta_{-\mathbf{k}} \\ \hat{c}_{-\mathbf{k}\downarrow} &= -v^\star_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}} + u_{\mathbf{k}}\beta_{-\mathbf{k}} \\ \hat{c}_{\mathbf{k}\uparrow} &= u_{\mathbf{k}}\alpha_{\mathbf{k}} + v^\star_{\mathbf{k}}\beta^\dagger_{-\mathbf{k}} \\ \hat{c}^\dagger_{-\mathbf{k}\downarrow} &= -v_{\mathbf{k}}\alpha_{\mathbf{k}} + u^\star_{\mathbf{k}}\beta^\dagger_{-\mathbf{k}} \end{aligned}\right\}$$

$$c^\dagger_{\mathbf{k}'\uparrow}\, c_{\mathbf{k}\uparrow} = \left(u^\star_{\mathbf{k}'}\alpha^\dagger_{\mathbf{k}'} + v_{\mathbf{k}'}\beta_{-\mathbf{k}'}\right)\left(u_{\mathbf{k}}\alpha_{\mathbf{k}} + v^\star_{\mathbf{k}}\beta^\dagger_{-\mathbf{k}}\right)$$

$$c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} = \left(-v_{\mathbf{k}}\alpha_{\mathbf{k}} + u^\star_{\mathbf{k}}\beta^\dagger_{-\mathbf{k}}\right)\left(-v^\star_{\mathbf{k}'}\alpha^\dagger_{\mathbf{k}'} + u_{\mathbf{k}'}\beta_{-\mathbf{k}'}\right)$$

connect the same qp states

➔ matrix elements $\left|P_{\mathbf{k}'\sigma',\mathbf{k}\sigma}\right|^2$ have to be multiplied by so-called coherence factors

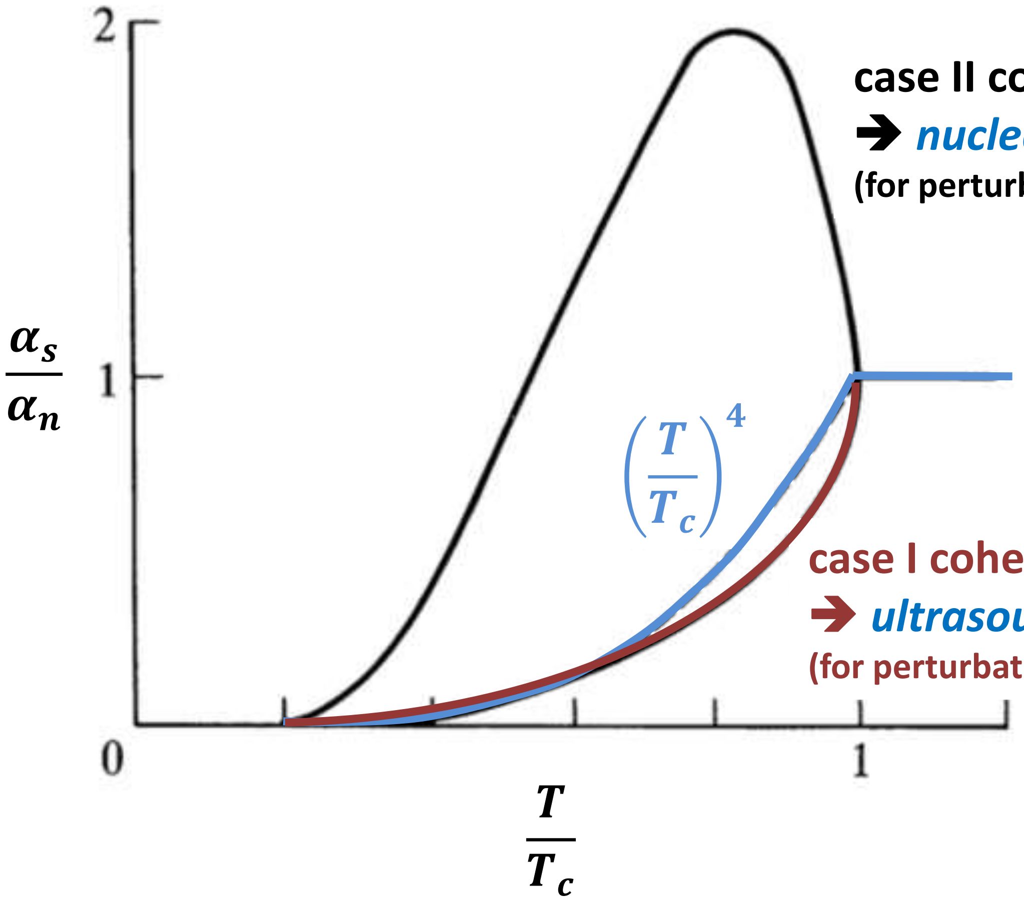
$(u_{\mathbf{k}}u_{\mathbf{k}'} \mp v_{\mathbf{k}}v_{\mathbf{k}'})^2$ for scattering of quasiparticles

$(v_{\mathbf{k}}u_{\mathbf{k}'} \pm u_{\mathbf{k}}v_{\mathbf{k}'})^2$ for creation or annihilation of quasiparticles

$u_{\mathbf{k}}, v_{\mathbf{k}}$ are assumed real
see e.g.
M. Tinkham
Introduction to Superconductivity

4.5 Coherence Effects

temperature dependence of low-frequency absorption processes in superconductors



case II coherence factor

➔ *nuclear relaxation, electromagnetic absorption*

(for perturbation which are even under time reversal)

two-fluid model

case I coherence factor

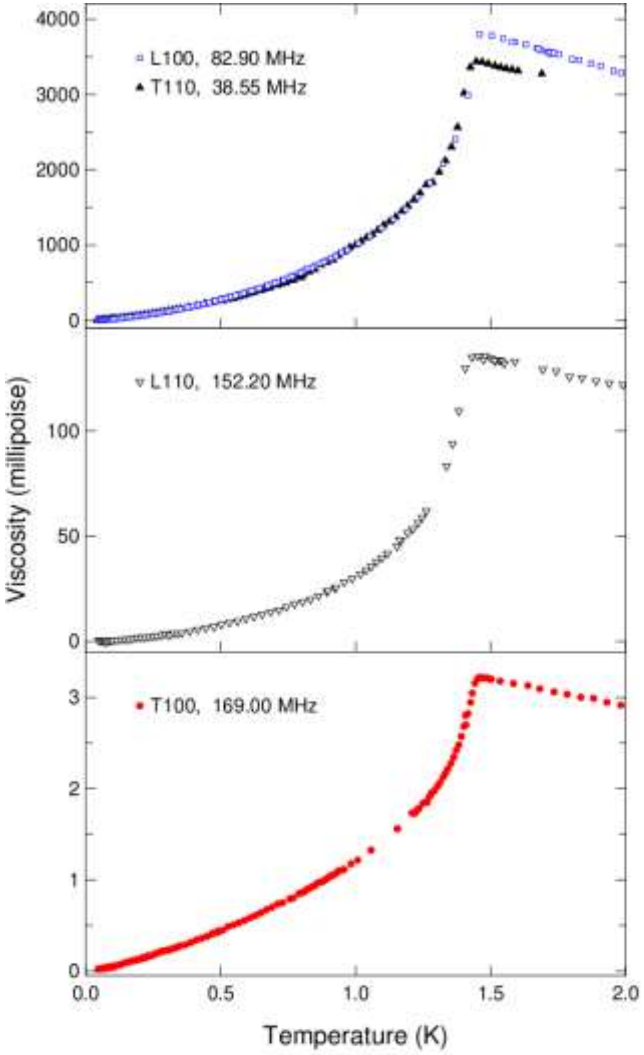
➔ *ultrasound attenuation*

(for perturbation which are odd under time reversal)

BCS theory makes prediction for coherence factors

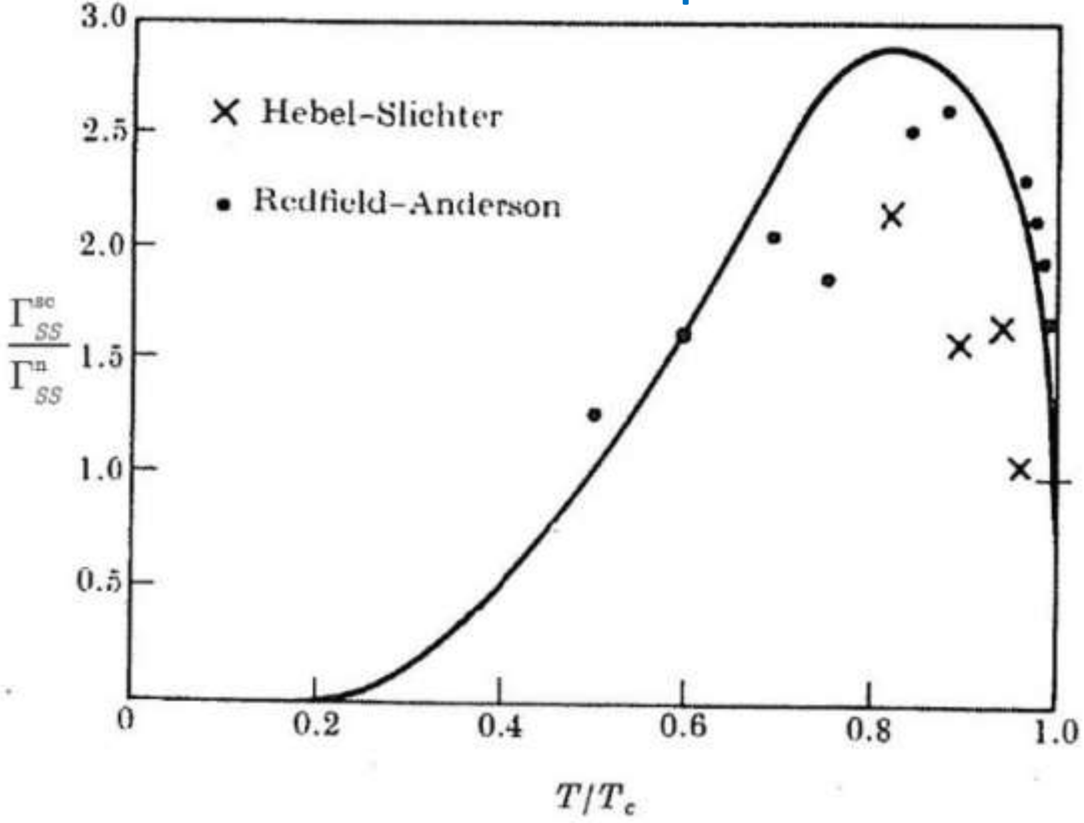
R. Gross and A. Marx , © Walther-Meißner-Institut (2004 - 2021)

4.5 Coherence Effects



Ultrasound Attenuation in Sr_2RuO_4:
An Angle-Resolved Study of the Superconducting Gap Function
C. Lupien, W. A. MacFarlane, Cyril Proust, Louis Taillefer, Z. Q. Mao, and Y. Maeno
Phys. Rev. Lett. **86**, 5986 (2001)

Hebel-Slichter peak



A.G. Redfield, *Nuclear Spin Relaxation Time in Superconducting Aluminum*.
Phys. Rev. Lett. **3**, 85–86 (1959)
L.C. Hebel, *Theory of Nuclear Spin Relaxation in Superconductors*.
Phys. Rev. **116**, 79–81 (1959).

Summary of Lecture No. 9 (1)

- ***minimization of free energy yields BCS gap equation***:

$$1 = V_0 \sum_{\mathbf{k}'} \frac{1}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_\mathrm{B}T}\right)$$

BCS gap equation

- ***analytical solution with simplifications***: $V_{\mathbf{k},\mathbf{k}'} = -V_0,\ \Delta_\mathbf{k} = \Delta,\ V_0 D(E_\mathrm{F}) \ll 1$: weak coupling approximation

$T \ll T_c$ $$\Delta(0) \simeq 2\hbar\omega_\mathrm{D}\, \mathrm{e}^{-\frac{2}{V_0 D(E_\mathrm{F})}}$$

$T \simeq T_c$ $$k_\mathrm{B}T_c = 1.13\ \hbar\omega_\mathrm{D}\, \mathrm{e}^{-\frac{2}{V_0 D(E_\mathrm{F})}}$$

⟹

$$\frac{\Delta(0)}{k_\mathrm{B}T_c} = \frac{\pi}{\mathrm{e}^\gamma} = 1.764$$

- ***condensation energy at $T = 0$*** $V_{\mathbf{k},\mathbf{k}'} = -V_0,\ \Delta_\mathbf{k} = \Delta,\ V_0 D(E_\mathrm{F}) \ll 1$: weak coupling approximation

$$E_\mathrm{kond}(0) = \langle \mathcal{H}_\mathrm{BCS} \rangle - \langle \mathcal{H}_n \rangle = -D(E_\mathrm{F})\Delta^2(0)/4$$

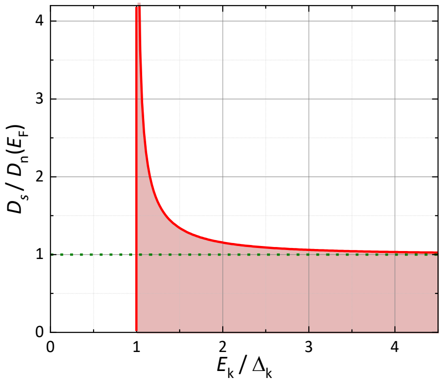
comparison to $E_\mathrm{cond}(0) = -B_\mathrm{cth}^2(0)/2\mu_0$ (thermodynamics) yields

$$\mathrm{B_{cth}}(0) = \sqrt{\frac{\mu_0 D(E_\mathrm{F})\Delta^2(0)}{2V}}$$

Summary of Lecture No. 9 (2)

- ***density of states***:

$$D_s(E_\mathbf{k}) = D_n(\xi_\mathbf{k})\frac{\mathrm{d}\xi_\mathbf{k}}{\mathrm{d}E_\mathbf{k}} = \begin{cases} D_n(E_\mathrm{F})\dfrac{E_\mathbf{k}}{\sqrt{E_\mathbf{k}^2-\Delta^2}} & \text{for} \quad E_\mathbf{k} > \Delta \\ 0 & \text{for} \quad E_\mathbf{k} < \Delta \end{cases}$$



- ***BCS prediction for thermodynamic quantities***

$$S_s = -2k_\mathrm{B}\sum_\mathbf{k}\left\{\underbrace{[1-f(E_\mathbf{k})]\ln[1-f(E_\mathbf{k})]}_{\text{hole like}} + \underbrace{f(E_\mathbf{k})\ln[f(E_\mathbf{k})]}_{\text{electron like}}\right\}$$

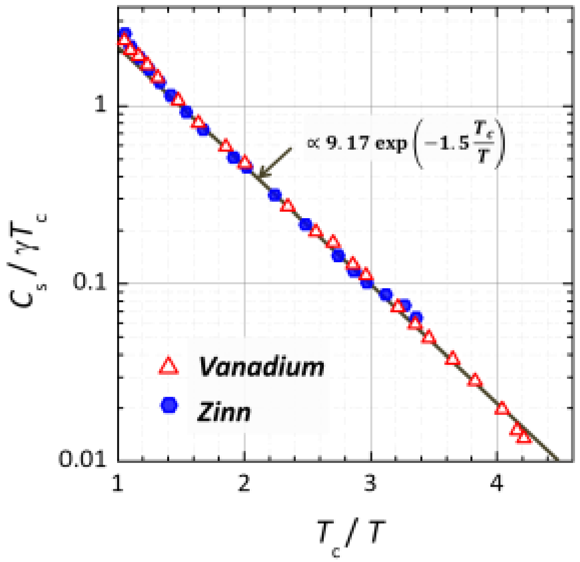
entropy

$$C_s = \frac{2}{T}\sum_\mathbf{k} -\frac{\partial f(E_\mathbf{k})}{\partial E_\mathbf{k}}\left(E_\mathbf{k}^2 - \frac{1}{2}T\frac{\mathrm{d}\Delta_\mathbf{k}^2(T)}{\mathrm{d}T}\right)$$

heat capacity

⇒ $$C_s \propto T^{-\frac{3}{2}}\mathrm{e}^{-\frac{\Delta(0)}{k_\mathrm{B}T}} \propto T^{-\frac{3}{2}}\mathrm{e}^{-1.76\frac{T}{T_c}} \quad @\, T \ll T_c$$

exponential decrease of heat capacity at low T



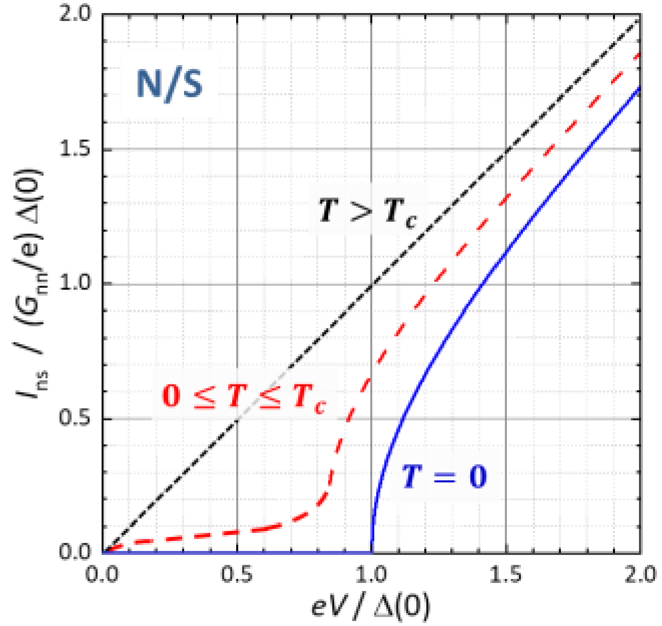
- ***determination of energy gap and DOS by tunneling spectroscopy***

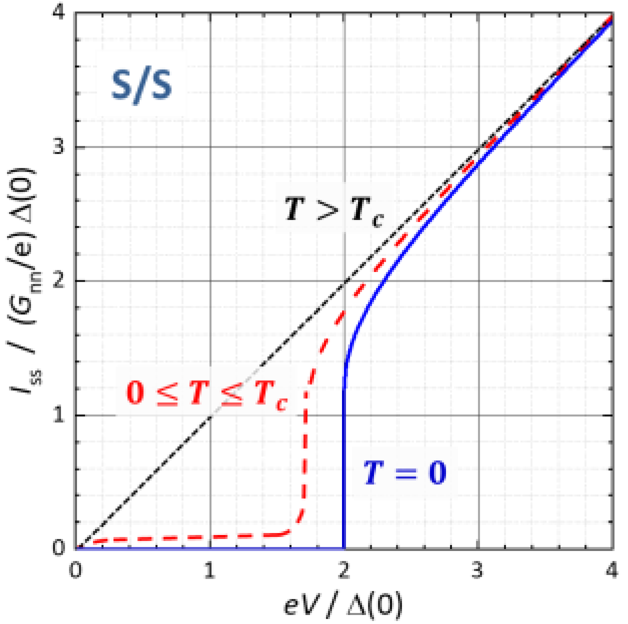
$$I_{ns}(V) = \frac{G_{nn}}{e}\int_{-\infty}^{\infty}\frac{D_{s2}(E)}{D_{n2}(E_\mathrm{F})}\,[f(E)-f(E+eV)]\,\mathrm{d}E$$

⇒ $$G_{ns}(V) = \frac{\partial I_{ns}(V)}{\partial V} = G_{nn}\frac{D_{s2}(eV)}{D_{n2}(E_\mathrm{F})} \propto D_{s2}(eV) \qquad @\, T = 0$$

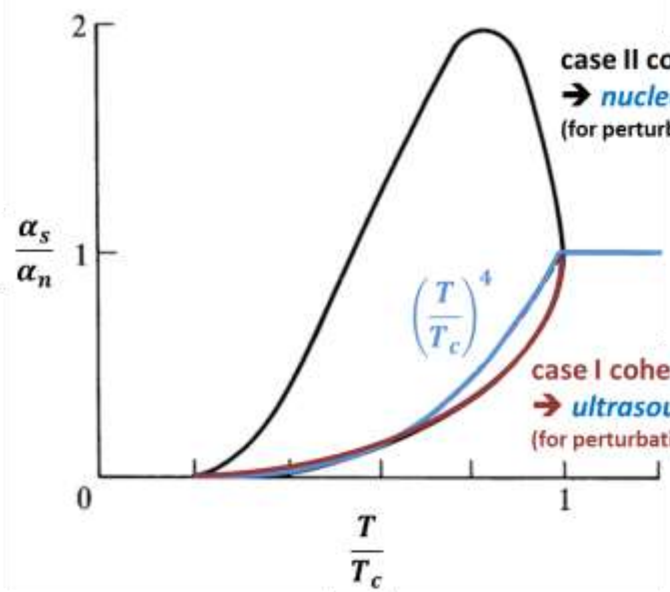
Summary of Lecture No. 9 (3)

- ***NIS and SIS tunnel junctions***





- ***BCS coherence factors***



case II coherence factor
➔ ***nuclear relaxation, electromagnetic absorption***
(for perturbation which are even under time reversal)

two-fluid model

case I coherence factor
➔ ***ultrasound attenuation***
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