9. BCS theory at T=0: Cooper pair formation

TOPICS

Introduction: Experimental information about low-temperature superconductors. Cooper pairs, pairing gap.

Vibrations of metallic lattice, longitudinal compressional waves (acoustic sound waves), Lagrange and Hamilton density, canonical quantization → phonons.

Free phonons, theory of specific heat (Debye temperature and Debye frequency).

Electron-phonon interaction, Feynman diagram → static limit: attractive electron-electron interaction.

Cooper's model: consider 2 electrons (with small attractive force) in filled Fermi sea; "Pauli blocking" of Fermi sea levels is crucial for Cooper pair formation!

Thermodynamic potential at T=0, BCS Hamiltonian. Solution via a) variational approach (1957, BCS); b) canonical transformation to quasi-particles (1958, Bogoliubov). Gap equation, properties of normal and superconducting ground state.

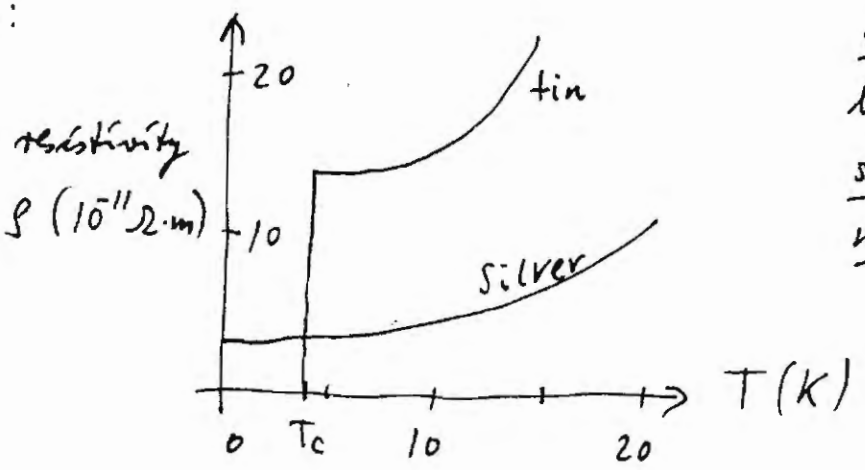
Brief discussion of pair formation in atomic nuclei: HF+BCS

Theory of low-T_c superconductivity

Introduction

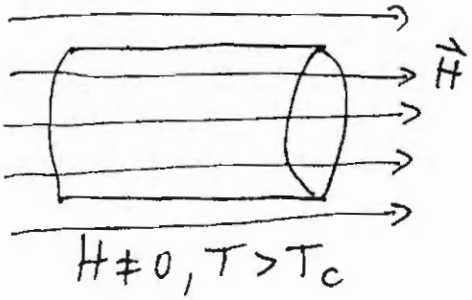
Cit: Eisberg & Resnick, Quantum Physics, Chapt. 14

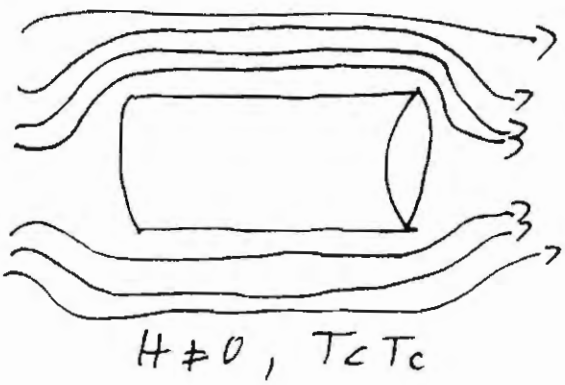
In 1911, Kammerlingh-Onnes observes experimentally that the electrical resistance of solid mercury abruptly drops to an immeasurably small value if cooled below a certain "critical" temperature $T_c = 4.2\,K$. Many other elements, many compounds and alloys have since been found to be superconductors with critical temperatures up to 23 K. This phenomenon of low-T_c superconductivity is observed in many metals, but not in all of them:



tin is supercond. below ~3.8K, but silver remains a normal conductor.

In 1933, Meissner & Ochsenfeld observed the exclusion of magnetic flux

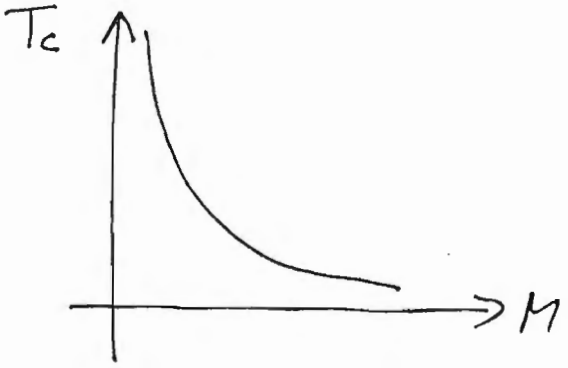




below T_c

This phenomenon is directly related to the first one: an ext. magn. field $\vec{H}$ does not penetrate the interior of a supercond. substance because the "superconducting" electrons inside the material produce an additional counteracting magnetic field. It is necessary to have a persisting (resistanceless) current to maintain the flux exclusion over longer periods of time when the external H-field is on!

In 1950, an important exp. established the "isotope effect":



$$T_c = \frac{\text{const}}{\sqrt{M}}$$

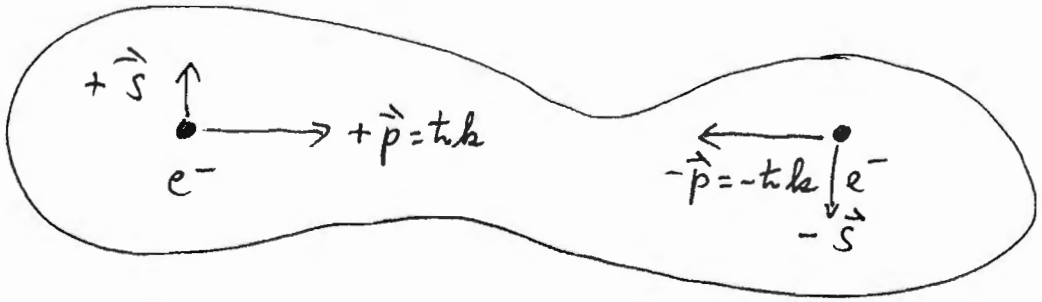
M = isotopic mass of solid

[crystals made from different isotopes of same element]

Exp. suggests that lattice ions play a role in low-T_c superconductivity.

In the same year (1950) Fröhlich explains the isotope effect as a result of interaction between electrons and phonons (=quantized lattice vibrations).

A breakthrough occured in 1956 when Cooper used the existence of the tiny electron-phonon interaction (attractive) to explain the basics of superconductivity in terms of "Cooper pairs".



Note: very weakly bound pair, size = 10^4 Å

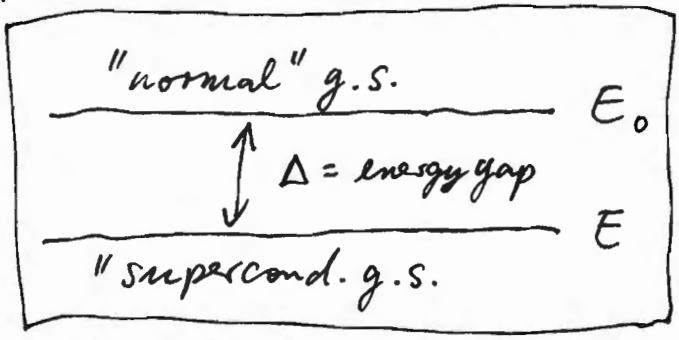
i.e. 10^4 times typical lattice spacing!

Only one year later, in 1957, Bardeen, Cooper and Schrieffer developed the detailed theory of superconductivity now known as the "BCS theory". They started a variational approach using a model g.s. for the superconductor:

$$|\phi_0^{BCS}\rangle = \prod_{k=1}^{\infty} (u_k + v_k \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow})|0\rangle$$

supercond. g.s. — prob. amplitudes — "Cooper pair" — vacuum

where u_k^2 (v_k^2) is the prob. that the s.p. level $\vec{k}$ is unfilled (filled) with a Cooper pair. BCS theory predicts a pairing gap



For mercury:

$\Delta(T=0) = 1.1 \times 10^{-3}$ eV tiny!

Compare to $E_F = 10$ eV.

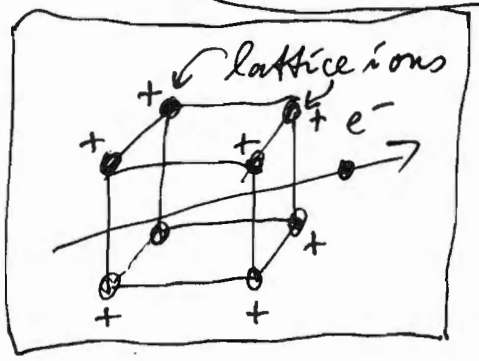
$$\frac{E_F}{\Delta} = 10^4$$ also $$\frac{\text{Cooper pair size}}{\text{lattice spacing}} = 10^4$$

$$\frac{\text{conduction } e^- \text{ density (normal g.s.)}}{\text{Cooper pair density (supercond. g.s.)}} = \frac{10^{22}/\text{cm}^3}{10^{18}/\text{cm}^3} = 10^4$$

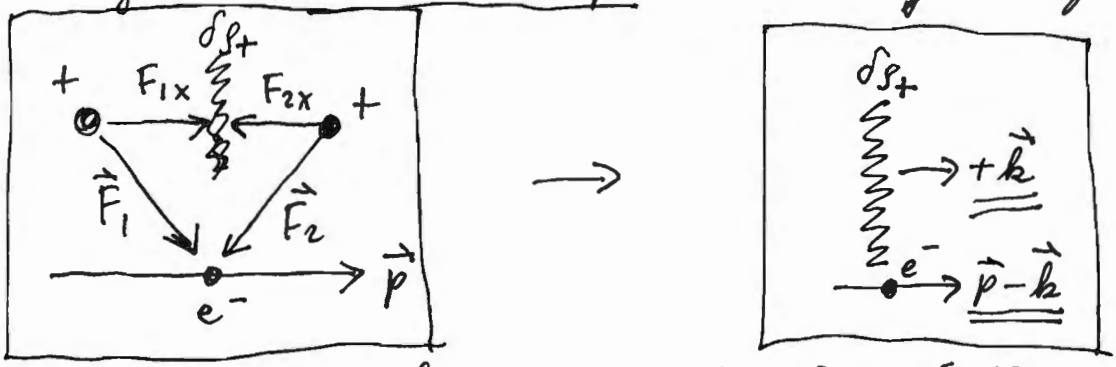
In 1986, high-T_c superconductivity ($T_c = 130$K) was discovered experimentally by Bednorz & Müller at IBM research lab in Switzerland, for metal oxides:

$$Y\,Ba_2\,Cu_3\,O_7.$$

Lattice vibrations → acoustic sound waves
→ quantize → phonons



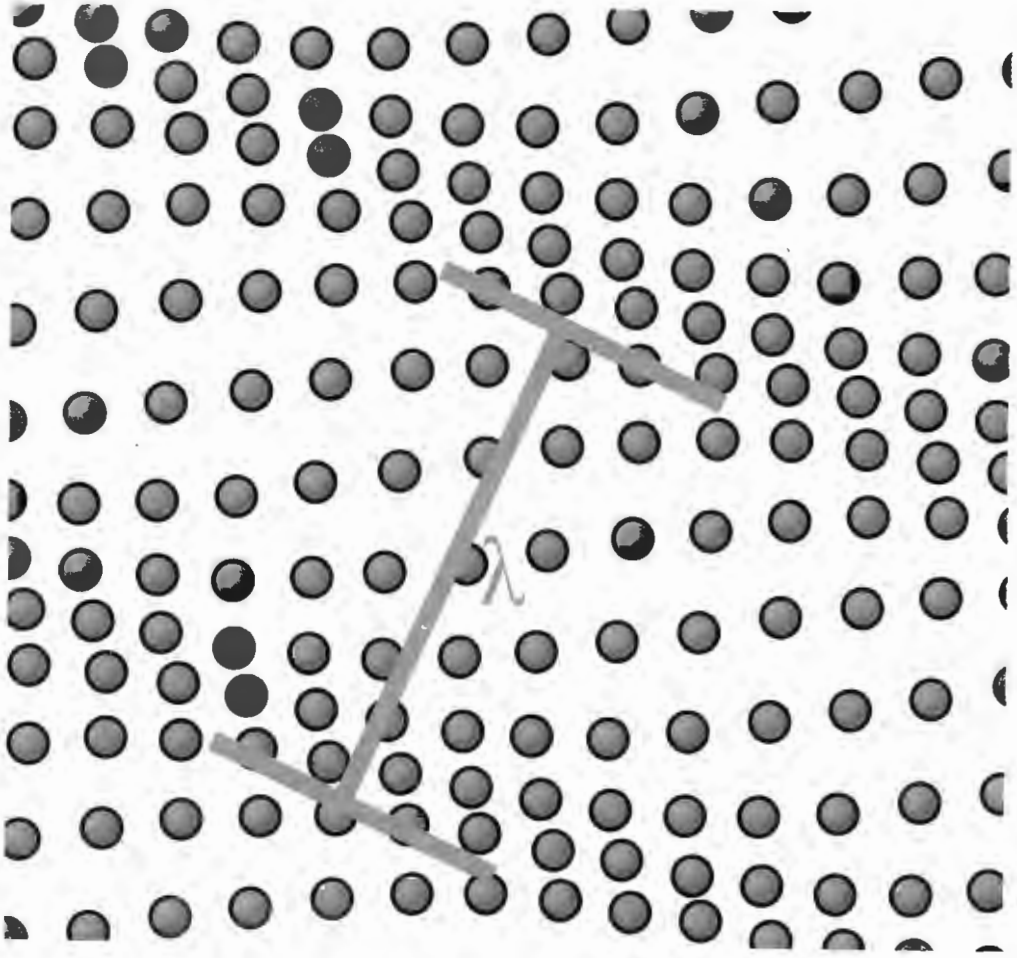
It is easy to understand how electrons moving through the metallic lattice can produce sound waves: the attractive Coulomb interaction between an electron moving with momentum $\vec{p}$ and 2 neighboring lattice ions



produces an enhanced density δs_+ in the region between the 2 ions. If the electron imparts some momentum, $+\vec{k}$, to this region of enhanced positive density, it will travel through the metallic lattice due to the electrostatic coupling of all the ions. This density disturbance is a sound wave (longitudinal compressional wave). Because of the large mass M of the ionic cores, these waves have low frequency f, and hence large wavelengths $\lambda = \frac{c}{f}$:

$$\lambda \text{ (acoustic sound waves)} >> \text{lattice spacing } d$$

The compressional wave has many characteristics of a



Phonon propagating through a square lattice

Source: Wikipedia, Search for "phonon".

particle (momentum $\hbar\vec{k}$, energy $E_{\vec{k}}$, ...) and is therefore often called a "quasiparticle". These quasiparticles are called phonons (Greek: phoné = sound). Similar to real particles, the phonons may "collide" with each other and with conduction electrons.

Because $\lambda >> d$, the acoustic phonons cannot resolve the metallic lattice structure: as before, it may be replaced by a uniform positive background density, g_0^+.

Theory of longitudinal compressional waves and phonons

Ref: Fetter & Walecka, chapter 12, p. 389 – 393

The uniform medium is described by the density ρ_0^+; add a small density perturbation $\delta\rho^+$ due to compressional sound wave

$$\rho^+(\vec{r},t) = \rho_0^+ + \delta\rho^+(\vec{r},t)$$

The theory starts from classical continuum mechanics (see e.g. the "Classical Mechanics" textbook by Fetter & Walecka). Using the Euler equation for non-viscous fluids and the continuity eq., one can derive a classical wave eq. for the density compression $\delta\rho^+$:

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right]\delta\rho^+(\vec{r},t) = 0 \qquad (FW, 44.2)$$

The density disturbance $\delta\rho^+$ may be parametriced in terms of a longitudinal displacement vector $\vec{d}(\vec{r},t)$ defined via

$$\delta\rho^+(\vec{r},t) = \rho_0\left(-\nabla\cdot\vec{d}(\vec{r},t)\right) \qquad (FW, 44.5)$$

which also satisfies the above wave eq.

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right]\vec{d}(\vec{r},t) = 0 \qquad (FW, 44.6)$$

The speed of sound, c, of the longitudinal waves is determined by the bulk modulus B:

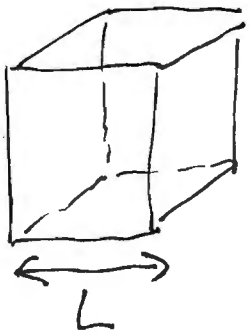
$$c = \sqrt{\frac{B}{\rho_0^+}} \quad \text{with} \quad B = -V\left(\frac{\partial P}{\partial V}\right)_{S=\text{const}}$$

(P ← pressure; S ↓ entropy)

Using the interacting Fermi gas model discussed earlier, one calculates

$$c \approx 1.1 \times 10^5 \ \frac{\text{cm}}{\text{s}} \quad \text{(metallic sodium)}$$

which agrees with exp. within a factor of 2.



We work in a periodicity cube of length L; using periodic B.C.'s results in discrete wave vectors:

$$\vec{k} = \frac{2\pi}{L}\vec{n}, \qquad \vec{n} = (n_x, n_y, n_z), \quad n_i = \text{integers}$$

The plane-wave solutions of the wave eq. have the form

$$\vec{d}(\vec{r},t) = \sum_{\vec{k}} \vec{e}_{\vec{k}} \left[A_{\vec{k}}\, e^{i(\vec{k}\cdot\vec{r} - \omega_k t)} + A^*_{\vec{k}}\, e^{-i(\vec{k}\cdot\vec{r} - \omega_k t)} \right]$$

$\vec{e}_{\vec{k}} \parallel \vec{k}/k$ (long. wave!)

The classical theory now proceeds by introducing classical Lagrange / Hamilton densities

$$L = \int d^3r\, \mathcal{L}$$

(L: Lagrange function; $\mathcal{L}$: Lagrange density)

$$H = \int d^3r\, \mathcal{H}$$

(H: Hamilton function; $\mathcal{H}$: Hamilton density)

The Lagrange density has to be constructed such that the Euler-Lagrange eqs of motion correspond to the wave eq. for the displacement vector $\vec{d}$. One finds

$$\mathcal{L}\left(d_i, \frac{\partial d_i}{\partial t}, \frac{\partial d_i}{\partial x_j}\right) = \frac{1}{2}\rho_0^+\left(\frac{\partial \vec{d}(\vec{r},t)}{\partial t}\right)^2 - \frac{1}{2}B\left(\nabla\cdot\vec{d}(\vec{r},t)\right)^2$$

(FW, 44.11b)

The kinetic energy of the continuous mechanical system is described by the density ρ_0^+ and the displacement velocity $\dot{\vec{d}}$, and the bulk modulus B of the material determines its potential energy.

The displacement vector $\vec{d}(\vec{r},t)$ may be viewed as a classical field [similar to $\vec{E}(\vec{r},t)$ in E&M].

In analogy to classical mechanics of point particles, one defines the classical field momentum via

$$\vec{\pi}(\vec{r},t) = \frac{\partial \mathcal{L}}{\partial(\partial\vec{d}/\partial t)} = \rho_0^+\frac{\partial \vec{d}}{\partial t}. \qquad (FW, 44.12)$$

From the Lagrange density and $\vec{\pi}(\vec{r},t)$, one derives the classical Hamilton density

$$\mathcal{H}(\vec{d},\vec{\pi}) = \frac{\vec{\pi}^2(\vec{r},t)}{2\rho_0^+} + \frac{1}{2}B\left(\nabla\cdot\vec{d}(\vec{r},t)\right)^2$$

The Cartesian components d_i and π_i $(i=1,2,3)$ satisfy the following Poisson bracket relations:

$$\left[d_i(\vec{r},t),\ d_j(\vec{r}',t) \right]_{P.B.} = 0 = \left[\pi_i(\vec{r},t), \pi_j(\vec{r}',t) \right]_{P.B.}$$

$$\left[d_i(\vec{r},t), \pi_j(\vec{r}',t) \right]_{P.B.} = \delta_{ij}\, \delta(\vec{r}-\vec{r}')$$

Field quantization → phonons

Replace the Poisson brackets for the class. quantities by commutators for corresponding operators:

$$\text{e.g. } \left[d_i(\vec{r},t), \pi_j(\vec{r}',t) \right]_{P.B.} \longrightarrow \frac{1}{i\hbar} \left(\hat{d}_i \hat{\pi}_j - \hat{\pi}_j \hat{d}_i \right)$$

$$= \frac{1}{i\hbar} \left[\hat{d}_i, \hat{\pi}_j \right]_{Q.M.}$$

Hence:

$$\underbrace{\vec{\pi}(\vec{r},t),\ \vec{d}(\vec{r},t)}_{\text{classical fields}} \longrightarrow \underbrace{\hat{\vec{\pi}}(\vec{r},t),\ \hat{\vec{d}}(\vec{r},t)}_{\text{quantum fields}}$$

As a result of field quantization, the continuous classical amplitudes $A_{\vec{k}}$ in the expression for classical $\vec{d}(\vec{r},t)$, see page 8, become quantized:

$$\underbrace{A_{\vec{k}}}_{\text{classical}} \longrightarrow \underbrace{\hat{A}_{\vec{k}} = \frac{1}{i}\sqrt{\frac{\hbar}{\varepsilon_0 2\omega_k L^3}}\, \hat{c}_{\vec{k}}}_{\text{quantum}}$$

$$A^*_{\vec{k}} \longrightarrow \hat{A}^+_{\vec{k}} = i\sqrt{\frac{\hbar}{\varepsilon_0 2\omega_k L^3}}\, \hat{c}^+_{\vec{k}}$$

FW (44.15)

where the commutation relations for the boson operators are

$$\left[\hat{c}_{\vec{k}}, \hat{c}_{\vec{k}'} \right] = 0 = \left[\hat{c}^+_{\vec{k}}, \hat{c}^+_{\vec{k}'} \right], \text{ but } \left[\hat{c}_{\vec{k}}, \hat{c}^+_{\vec{k}'} \right] = \delta_{\vec{k}\vec{k}'}.$$

These follow from the comm. relations for $\hat{\vec{\pi}}(\vec{r},t)$ and $\hat{\vec{d}}(\vec{r},t)$.

The creation and annihilation operators $\hat{c}^{+}_{\vec{k}}$ / $\hat{c}_{\vec{k}}$ describe phonons with momentum $\hbar\vec{k}$.

One finds for the energy of the lattice vibrational waves

$$\hat{H}_{lattice} = \hat{H}_{phonon} = \int d^3r\, \hat{\mathcal{H}} =$$

$$= \sum_{\vec{k}} \hbar\omega_{\vec{k}} \left(\hat{c}^{+}_{\vec{k}} \hat{c}_{\vec{k}} + \frac{1}{2} \right)$$

$\hat{c}^{+}_{\vec{k}} \hat{c}_{\vec{k}}$ = phonon # operator

lattice vibrations → longitudinal compression waves → phonons

i.e. we obtain a system of uncoupled harmonic oscillators describing the free phonons moving through the metallic lattice!

Application of free phonon theory: Debye theory of specific heat

Ref: Fetter & Walecka, p. 393 - 395

One may wonder how realistic our free phonon model is? Main approximation used is uniform background, no lattice ions. In a uniform medium, there is no upper limit for wave freq. ω. But for a real crystal, there is a max. frequency $\omega_{max} \overset{def}{=} \omega_D$ (= Debye frequency) which

we will now determine. The total number of degrees of freedom in the crystal is $3N$, where N = number of ions. Hence, we can enumerate the allowed wave numbers, from the lowest value, up to k_{max}:

(# occupied quantum states)

$$3N \overset{!}{=} \sum_{\vec{k}} \Theta(k_{max} - k) \to \frac{L^3}{(2\pi)^3} \int d^3k\, \Theta(k_{max} - k)$$

$$\Rightarrow 3N = \frac{L^3}{8\pi^3} \int_0^{k_{max}} k^2 dk \underbrace{\int d\Omega_k}_{=4\pi} = \frac{L^3}{2\pi^2} \frac{1}{3} k_{max}^3$$

Use $k_{max} = \frac{\omega_{max}}{c} \overset{def}{=} \frac{\omega_D}{c} \Rightarrow 3N = \frac{L^3}{2\pi^2} \frac{1}{3} \frac{\omega_D^3}{c^3}$.

Solve for ω_D:

Max. frequency $\omega_{max} = \omega_D$ = Debye frequency of phonons in crystal:

$$\omega_D = \sqrt[3]{18\pi^2 n_0} \cdot c \qquad \left(n_0 = \frac{N}{L^3} = \text{number density}\right)$$

with $c = \sqrt{\frac{B}{M n_0}}$ (B = bulk modulus, M = ionic mass)

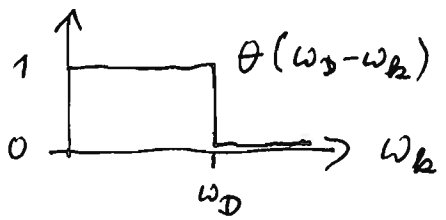
(c ↑ speed of sound)

The Debye freq. ω_D defines, in turn, the Debye temperature Θ which represents the thermal energy

$$\boxed{k_B \cdot \Theta = \hbar \omega_D} \qquad (k_B = \text{Boltzmann const.})$$

associated with the max. frequency ω_D of lattice vibrations. The Debye freq. ω_D will be of crucial importance for the electron-phonon interaction to be discussed later.

It will provide a <u>frequency cut-off</u>:



<u>Using ω_D and Θ for real crystals</u> in connection with thermodynamics and stat. mech. of the <u>free phonon system</u>, one can <u>explain</u> the <u>specific heat C_V</u> of metallic crystals:

$$C_V \overset{\text{def}}{=} \left(\frac{\partial E}{\partial T}\right)_V \quad \text{spec. heat}$$

$$E = -T^2 \frac{\partial}{\partial T}\left(\frac{\Omega_0}{T}\right)_V \quad \text{energy}$$

$$\Omega_0 = -(k_B T)\ln \text{trace}\left[\exp\left(-\frac{\hat{H}_{\text{phonon}}}{k_B T}\right)\right] \quad \text{thermodyn. potential}$$

From these 3 equations one can compute the specific heat in terms of the Debye temp. Θ:

$$C_V = 9 N k_B \left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} \frac{e^u u^4}{(e^u - 1)^2}\, du \qquad (FW\ 44.29)$$

with the limiting cases

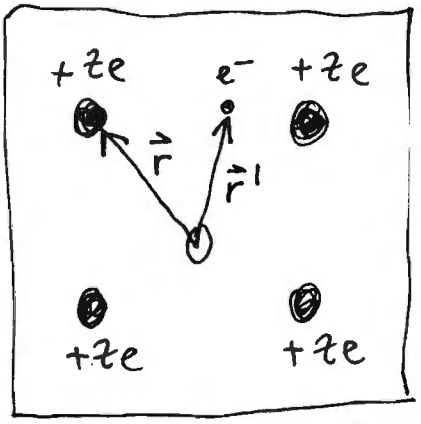
$$C_V = 3 N k_B = \text{const} \quad (T \to \infty) \quad \rightarrow \text{classical equipartition of energy}$$

$$C_V = \frac{12\pi^4}{5} N k_B \left(\frac{T}{\Theta}\right)^3 \quad (T \to 0) \quad \rightarrow \text{"Debye law"} \ (C_V \propto T^3).$$

Excellent agreement with exp. for metallic crystals (see FW, p. 395).

The electron-phonon interaction

Ref: Fetter & Walecka, p. 396 – 399



Early on, we investigated the interacting electron gas in a metallic lattice; the positive ionic cores of charge $(+Ze)$ were approximated by a uniform background charge ρ_0^+. The Hamiltonian has the structure (Born-Oppenheimer approx., ions at rest):

$$H_{el\,gas} = T_{e^-} + V^{(2)}_{e^-e^-} + V^{(1)}_{e^-ion} + V_{ion\text{-}ion}. \qquad (1)$$

Let us consider the Coulomb interaction terms involving the ions

$$V^{(1)}_{e^-ion} = \int d^3r \int d^3r' \, \frac{\rho_{e^-}(\vec{r})\,\rho_{ion}(\vec{r}')}{|\vec{r}-\vec{r}'|} \,. \qquad (2)$$

$$V_{ion\text{-}ion} = \underbrace{\frac{1}{2}}_{\text{self-energy!}} \int d^3r \int d^3r' \, \frac{\rho_{ion}(\vec{r})\,\rho_{ion}(\vec{r}')}{|\vec{r}-\vec{r}'|} \qquad (3)$$

Now we allow longitudinal compressional waves (→ phonons) which modify the density distr. as follows

$$\boxed{\rho_{ion}(\vec{r}) \longrightarrow \rho_0^+ + \delta\rho^+(\vec{r},t)} \qquad (4)$$

(ρ_0^+: uniform background; $\delta\rho^+(\vec{r},t)$: density fluctuation)

Insert (4) into (2):

$$V_{e^- ion} = \int d^3r \int d^3r' \frac{\rho_{e^-}(\vec{r})\,[\rho_0^+ + \delta\rho^+(\vec{r}')]}{|\vec{r}-\vec{r}'|} =$$

$$V_{e^- ion} = \underbrace{\int d^3r \int d^3r' \frac{\rho_{e^-}(\vec{r})\,\rho_0^+}{|\vec{r}-\vec{r}'|}}_{= H^0_{e^-b}\ \text{electron-background}} + \underbrace{\int d^3r \int d^3r' \frac{\rho_{e^-}(\vec{r})\,\delta\rho^+(\vec{r}')}{|\vec{r}-\vec{r}'|}}_{= H_{e^-\text{phonon}}} \quad (5)$$

The first term is already included in Hel gas, and the 2nd term represents the important <u>electron-phonon interaction!</u>

The self-energy of the positive background charges, with density fluctuations, becomes (insert (4) in (3)):

$$\left\{ \begin{aligned} V_{ion-ion} &= \frac{1}{2} \int d^3r \int d^3r' \frac{[\rho_0^+ + \delta\rho^+(\vec{r})][\rho_0^+ + \delta\rho^+(\vec{r}')]}{|\vec{r}-\vec{r}'|} = \\ &= \frac{1}{2} \int d^3r \int d^3r' \frac{(\rho_0^+)^2}{|\vec{r}-\vec{r}'|} \quad \left(= H^0_b, \text{included in Hel-gas}\right) \\ &+ \frac{1}{2} \int d^3r \int d^3r' \frac{\rho_0^+[\delta\rho^+(\vec{r}) + \delta\rho^+(\vec{r}')]}{|\vec{r}-\vec{r}'|} \quad \left(\rightarrow \text{vanishes, see below}\right) \\ &+ \frac{1}{2} \int d^3r \int d^3r' \frac{\delta\rho^+(\vec{r})\,\delta\rho^+(\vec{r}')}{|\vec{r}-\vec{r}'|} \quad \left(\rightarrow \text{neglect terms } O(\delta\rho^2)\right) \end{aligned} \right. \quad (6)$$

Here, <u>the 2nd term vanishes</u>. <u>To show this</u> we use the def. of the displacement vector, p.7: $\delta\rho^+(\vec{r}) = \rho_0^+(-\nabla\cdot\vec{d}(\vec{r}))$

$$\searrow \text{2nd term} \propto \int_V d^3r\, \delta\rho^+(\vec{r}) \propto \int_V d^3r\, \nabla\cdot\vec{d} = \left(\begin{matrix}\text{divergence}\\ \text{theorem}\end{matrix}\right) =$$

$$= \int_S (\vec{d}\cdot\vec{n})\,da = 0 \quad (\text{no flow at } \infty \text{ distance}).$$

The Coulomb energies involving the ions have the form (eqns 5 and 6):

$$V_{e^-\text{ion}} + V_{\text{ion ion}} \approx H^{\circ}_{e\text{-}b} + H_{e\text{-phonon}} + H^{\circ}_{b} \qquad (7)$$

Adding the electron Hamiltonian

$$H_{e^-} = T_{e^-} + V_{e^-e^-}$$

and the quantized lattice vibrations, H_{phonon}, we arrive at the model Hamiltonian of the system in the form

$$H_{\text{system}} \approx \underbrace{\left(T_{e^-} + V_{e^-e^-} + H^{\circ}_{b} + H^{\circ}_{e\text{-}b}\right)}_{= H_{\text{el gas}} \text{ (see FW §3)}} + H_{\text{phonon}} + H_{e^-\text{phonon}} \qquad (8)$$

System Hamiltonian in occupation # representation

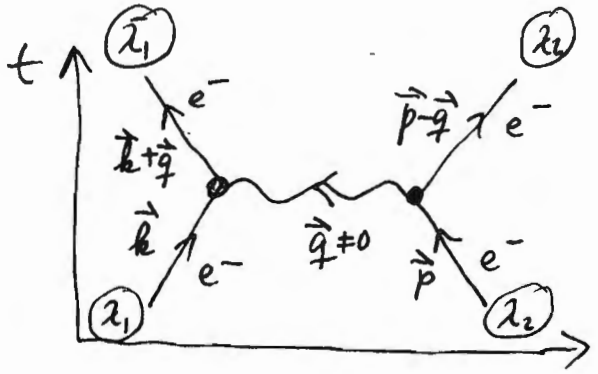
Ref: Fetter & Walecka, §45, p. 396 - 398

$$\hat{H}_{\text{system}} = \hat{H}_{\text{el gas}} + \hat{H}_{\text{phonon}} + \hat{H}_{\text{el phonon}} \qquad (9)$$

with (lecture notes, ch. 5, p. 9):

$$\hat{H}_{\text{el gas}} = \underbrace{\sum_{\vec{k},\lambda} \frac{\hbar^2 \vec{k}^2}{2m_e} \hat{a}^{+}_{\vec{k}\lambda} \hat{a}_{\vec{k}\lambda}}_{\text{kin. energy of electrons}} + \underbrace{\frac{e^2}{2V} \sum_{\vec{k},\vec{p}} \sum_{\vec{q}\neq 0} \sum_{\lambda_1,\lambda_2} \frac{4\pi}{\vec{q}^2} \hat{a}^{+}_{\vec{k}+\vec{q},\lambda_1} \hat{a}^{+}_{\vec{p}-\vec{q},\lambda_2} \hat{a}_{\vec{p}\lambda_2} \hat{a}_{\vec{k}\lambda_1}}_{\text{electron-electron int. for finite mom. transfer}} \qquad (10)$$

We can depict $V^{(2)}_{ee^-}(\vec{q}\neq 0)$ by a "Feynman-like" graph:



The free phonon Hamiltonian was given in this chapter, p. 11:

$$\hat{H}_{phonon} = \sum_{\vec{q}\,(q<\frac{\omega_D}{c})} \hbar\omega_q \left(\hat{c}^+_{\vec{q}}\,\hat{c}_{\vec{q}} + \tfrac{1}{2}\right) \qquad (11)$$

(phonons)

Now consider the electron-phonon interaction (notes, p. 15):

$$\hat{H}_{el\text{-}ph} = \int d^3r \int d^3r' \, \frac{\hat{\rho}_{el}(\vec{r})\,\hat{\sigma}^+(\vec{r}')}{|\vec{r}-\vec{r}'|} \qquad (12)$$

We evaluate the electron charge density operator from the field creation/annih. operators:

$$\hat{\rho}_{el}(\vec{r}) = (-e)\,\hat{\psi}^+(\vec{r})\,\hat{\psi}(\vec{r}) = (-e)\left(\sum_{\vec{k}_1\lambda_1} \hat{a}^+_{\vec{k}_1\lambda_1} \frac{1}{\sqrt{V}} e^{-i\vec{k}_1\cdot\vec{r}}\,\eta^+_{\lambda_1}\right)$$

$$\cdot\left(\sum_{\vec{k}_2\lambda_2} \hat{a}_{\vec{k}_2\lambda_2} \frac{1}{\sqrt{V}} e^{+i\vec{k}_2\cdot\vec{r}}\,\eta_{\lambda_2}\right) =$$

$$= \frac{(-e)}{V} \sum_{\vec{k}_1,\vec{k}_2} \sum_{\lambda_1,\lambda_2} \hat{a}^+_{\vec{k}_1\lambda_1}\,\hat{a}_{\vec{k}_2\lambda_2}\, e^{i(\vec{k}_2-\vec{k}_1)\cdot\vec{r}}\, \underbrace{\eta^+_{\lambda_1}\eta_{\lambda_2}}_{=\delta_{\lambda_1\lambda_2}}$$

Relabel $\lambda_1 = \lambda \Rightarrow$

$$\hat{\rho}_{el}(\vec{r}) = \frac{(-e)}{V} \sum_{\vec{k}_1,\vec{k}_2} \sum_{\lambda=\uparrow\downarrow} \hat{a}^+_{\vec{k}_1\lambda}\,\hat{a}_{\vec{k}_2\lambda}\, e^{i(\vec{k}_2-\vec{k}_1)\cdot\vec{r}} \qquad (13)$$

(electrons)

Now we calculate density fluctuation operator $\hat{\delta\rho}^{+}(\vec{r})$ in (11); from notes on p. 7

$$\hat{\delta\rho}^{+}(\vec{r}) = \rho_0^{+}\left(-\nabla\cdot\hat{\vec{d}}(\vec{r})\right) = \left(+ze\,n_0\right)\left(-\nabla\cdot\hat{\vec{d}}(\vec{r})\right) \qquad (14)$$

($+ze$: ion charge; n_0: number density)

The operator for the displacement vector is obtained from notes on p. 8 and p. 10 [use time-indep. Schrödinger picture]:

$$\hat{\vec{d}}(\vec{r}) = \sum_{\vec{k}} \frac{\vec{k}}{k}\sqrt{\frac{\hbar}{\rho_0^{+}\,2\omega_k V}}\left[-i\,\hat{c}_{\vec{k}}\,e^{i\vec{k}\cdot\vec{r}} + i\,\hat{c}^{+}_{\vec{k}}\,e^{-i\vec{k}\cdot\vec{r}}\right]\theta\left(\frac{\omega_D}{c}-k\right) \qquad (15)$$

($\theta\left(\frac{\omega_D}{c}-k\right)$: introduce Debye cut-off)

From the def. of the divergence

$$\nabla\cdot\hat{\vec{d}}(\vec{r}) = \frac{\partial\hat{d}_x}{\partial x} + \frac{\partial\hat{d}_y}{\partial y} + \frac{\partial\hat{d}_z}{\partial z}$$

we obtain for the x-component

$$\frac{\partial\hat{d}_x}{\partial x} = \sum_{\vec{k}} \frac{k_x}{k}\sqrt{\frac{\hbar}{\rho_0^{+}\,2\omega_k V}}\left\{\left[-i\,\hat{c}_{\vec{k}}\,\frac{\partial}{\partial x}\left(e^{i\vec{k}\cdot\vec{r}}\right) + i\,\hat{c}^{+}_{\vec{k}}\,\frac{\partial}{\partial x}\left(e^{-i\vec{k}\cdot\vec{r}}\right)\right]\right.$$
$$\left.\cdot\,\theta\left(\frac{\omega_D}{c}-k\right)\right\}$$

The partial derivatives are

$$\frac{\partial}{\partial x}\left(e^{\pm i\vec{k}\cdot\vec{r}}\right) = e^{\pm i\vec{k}\cdot\vec{r}}\left(\pm i k_x\right)$$

insert above:

$$\frac{\partial\hat{d}_x}{\partial x} = \sum_{\vec{k}} \underbrace{\frac{k_x}{k}}\sqrt{\cdots}\left\{\left[-i\,\hat{c}_{\vec{k}}\,e^{i\vec{k}\cdot\vec{r}}\underbrace{\left(+i k_x\right)} + i\,\hat{c}^{+}_{\vec{k}}\,e^{-i\vec{k}\cdot\vec{r}}\cdot\underbrace{\left(-i k_x\right)}\right]\theta\left(\frac{\omega_D}{c}-k\right)\right\}$$

Combine underlined terms

$$\frac{\partial \hat{d}_x}{\partial x} = \sum_{\vec{k}} \frac{k_x^2}{k} \sqrt{\frac{\hbar}{\varepsilon_0^+ 2\omega_k V}} \left[\hat{c}_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}} + \hat{c}_{\vec{k}}^{+} e^{-i\vec{k}\cdot\vec{r}} \right] \theta\left(\frac{\omega_D}{c} - k\right)$$

Similarly, we calculate the y- and z-components of $\nabla\cdot\hat{\vec{d}}$; we get factors $(k_y^2 + k_z^2)$ such that

$$\frac{k_x^2}{k} \rightarrow \frac{k_x^2 + k_y^2 + k_z^2}{k} = \frac{k^2}{k} = k \Rightarrow$$

$$\nabla\cdot\hat{\vec{d}}(\vec{r}) = \sum_{\vec{k}} k \sqrt{\frac{\hbar}{\varepsilon_0^+ 2\omega_k V}} \left[\hat{c}_{\vec{k}}\, e^{i\vec{k}\cdot\vec{r}} + \hat{c}_{\vec{k}}^{+} e^{-i\vec{k}\cdot\vec{r}} \right] \theta\left(\frac{\omega_D}{c} - k\right) \qquad (16)$$

From eqns (14) and (16) we find, with $\vec{r} \rightarrow \vec{r}'$ and $\vec{k} \rightarrow \vec{q}$:

$$\delta\hat{\rho}^+(\vec{r}') = (-ze\,n_0)\,\nabla'\cdot\hat{\vec{d}}(\vec{r}') = (-ze\,n_0) \sum_{\vec{q}} \sqrt{\frac{\hbar q^2}{\varepsilon_0^+ 2\omega_q V}} \cdot \left\{ \cdot \left[\hat{c}_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}'} + \hat{c}_{\vec{q}}^{+} e^{-i\vec{q}\cdot\vec{r}'} \right] \theta\left(\frac{\omega_D}{c} - q\right) \right\}$$

The underlined factors can be simplified as follows

$$(-ze\,n_0) \sqrt{\frac{\hbar q^2}{\varepsilon_0^+ 2\omega_q V}} = (-ze) \sqrt{\frac{n_0^2 \hbar (\omega_q/c)^2}{(M n_0) 2\omega_q \cdot V}} = \left(-\frac{ze}{c}\right) \sqrt{\frac{n_0 (\hbar\omega_q)}{M \cdot 2V}}$$

which leads to

$$\delta\hat{\rho}^+(\vec{r}') = -\left(\frac{ze}{c}\right) \sqrt{\frac{n_0}{M}} \sum_{\vec{q}} \sqrt{\frac{\hbar\omega_q}{2V}} \left[\hat{c}_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}'} + \hat{c}_{\vec{q}}^{+} e^{-i\vec{q}\cdot\vec{r}'} \right] \theta\left(\frac{\omega_D}{c} - q\right)$$

- $\delta\hat{\rho}^+(\vec{r}')$: density fluctuation
- M: ionic mass
- $\hat{c}_{\vec{q}}$, $\hat{c}_{\vec{q}}^{+}$: phonon operators
- $\theta\left(\frac{\omega_D}{c} - q\right)$: Debye cut-off

(17)

We insert eq. (17) for $\hat{\rho}^{+}_{\vec{q}}(\vec{r}')$ and eq. (113) for $\hat{\rho}_{ee}(\vec{r})$ into expression (12) for the electron-phonon int:

$$\hat{H}_{el\text{-}ph} = \int d^3r \int d^3r' \frac{1}{|\vec{r}-\vec{r}'|} \hat{\rho}_{ee}(\vec{r}) \hat{\rho}^{+}_{\vec{q}}(\vec{r}') =$$

$$= \int d^3r \int d^3r' \frac{1}{|\vec{r}-\vec{r}'|} \left[\left(-\frac{e}{V}\right) \sum_{\vec{k}_1,\vec{k}_2} \sum_{\lambda} \hat{a}^{+}_{\vec{k}_1\lambda} \hat{a}_{\vec{k}_2\lambda} e^{-i(\vec{k}_2-\vec{k}_1)\cdot\vec{r}} \right]$$

$$\times \left(-\frac{Ze}{c}\right) \sqrt{\frac{n_0}{M}} \sum_{\vec{q}} \sqrt{\frac{\hbar\omega_q}{2V}} \left[\hat{c}_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}'} + \hat{c}^{+}_{\vec{q}}\, e^{-i\vec{q}\cdot\vec{r}'} \right] \theta(\omega_D - \omega_q)$$

We proceed now like in Chapter 3 (FW p. 23) or my lecture notes (ch. 5, p. 4 previous) and introduce the new variables

$$\vec{y} = \vec{r} - \vec{r}' \;,\; \vec{x} = \vec{r}'$$

Shifting the origin due to translational invariance of the system, one obtains

$$\boxed{\int d^3r \int d^3r' \frac{1}{|\vec{r}-\vec{r}'|}\, e^{i(\vec{k}_2-\vec{k}_1)\cdot(\vec{y}+\vec{x})}\, e^{\pm i\vec{q}\cdot\vec{x}} \longrightarrow}$$

$$\int d^3x \int d^3y \, \frac{1}{y}\, e^{i(\vec{k}_2-\vec{k}_1)(\vec{y}+\vec{x})}\, e^{\pm i\vec{q}\cdot\vec{x}} =$$

$$= \underbrace{\int d^3x\, e^{i(\vec{k}_2-\vec{k}_1\pm\vec{q})\cdot\vec{x}}}_{= V\,\delta_{-\vec{k}_2+\vec{k}_1\pm\vec{q}}} \underbrace{\int d^3y \, \frac{1}{y}\, e^{i(\vec{k}_2-\vec{k}_1)\cdot\vec{y}}}_{= \frac{4\pi}{(\vec{k}_2-\vec{k}_1)^2} = \text{F.T. of Coul. pot}}$$

$$\boxed{= V \cdot \delta_{-\vec{k}_2+\vec{k}_1\pm\vec{q}}\, \frac{4\pi}{\vec{q}^{\,2}}} \qquad (*)$$

Inserting (*) into $\hat{H}_{el\text{-}ph}$ above, and we obtain

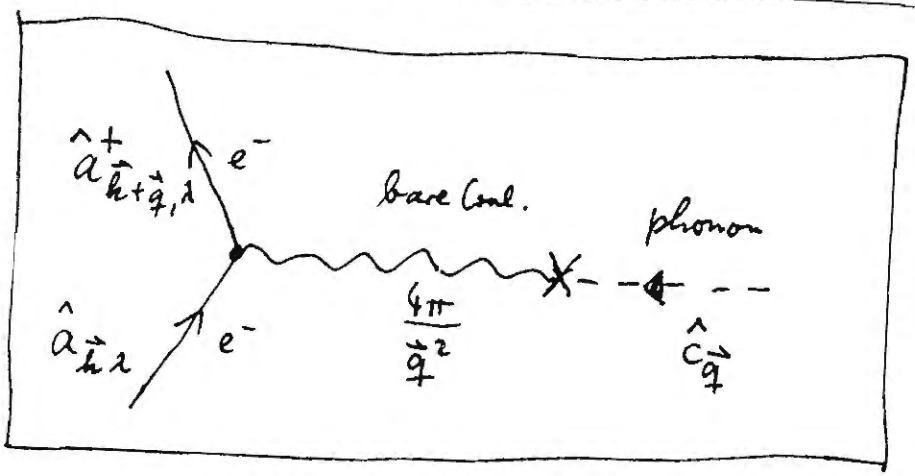
$$\hat{H}_{el-ph} = \sum_{\vec{k}_1,\vec{k}_2} \sum_{\lambda} \sum_{\vec{q}} \left(-\frac{e}{V}\right)\left(-\frac{Ze}{c}\right)\sqrt{\frac{\hbar}{M}}\sqrt{\frac{\hbar\omega_q}{2V}}\,\frac{4\pi}{q^2}\,V \cdot \theta\left(\frac{\omega_D}{c}-\frac{q}{\hbar}\right)\left[\delta_{\vec{k}_1,\vec{k}_2+\vec{q}}\;\hat{a}^{+}_{\vec{k}_1\lambda}\,\hat{a}_{\vec{k}_2\lambda}\,\hat{c}_{\vec{q}} + \delta_{\vec{k}_2,\vec{k}_1+\vec{q}}\;\hat{a}^{+}_{\vec{k}_1\lambda}\,\hat{a}_{\vec{k}_2\lambda}\,\hat{c}^{+}_{\vec{q}}\right]$$

$$\hat{H}_{el-ph} = +\frac{Ze^2}{c}\sqrt{\frac{\hbar}{M}}\sum_{\vec{q},\lambda}\sqrt{\frac{\hbar\omega_q}{2V}}\,\frac{4\pi}{q^2}\left[\sum_{\vec{k}_2}\hat{a}^{+}_{\vec{k}_2+\vec{q},\lambda}\,\hat{a}_{\vec{k}_2\lambda}\,\hat{c}_{\vec{q}} + \sum_{\vec{k}_1}\hat{a}^{+}_{\vec{k}_1\lambda}\,\hat{a}_{\vec{k}_1+\vec{q},\lambda}\,\hat{c}^{+}_{\vec{q}}\right]\theta\left(\frac{\omega_D}{c}-\frac{q}{\hbar}\right)$$

Finally, replacing the dummy indices $\vec{k}_1$ and $\vec{k}_2$ with $\vec{k}$, we obtain [FW eq. 45.6b]:

$$\hat{H}_{el-ph} = +\left(\frac{Ze^2}{c}\right)\sqrt{\frac{\hbar}{M}}\sum_{\vec{k},\lambda}\sum_{\vec{q}}\sqrt{\frac{\hbar\omega_q}{2V}}\,\frac{4\pi}{\vec{q}^2}\,\theta\left(\frac{\omega_D}{c}-\frac{q}{\hbar}\right)\cdot\left[\hat{a}^{+}_{\vec{k}+\vec{q},\lambda}\,\hat{a}_{\vec{k}\lambda}\,\hat{c}_{\vec{q}} + \hat{a}^{+}_{\vec{k}\lambda}\,\hat{a}_{\vec{k}+\vec{q},\lambda}\,\hat{c}^{+}_{\vec{q}}\right]$$

Graphical representation of first term:



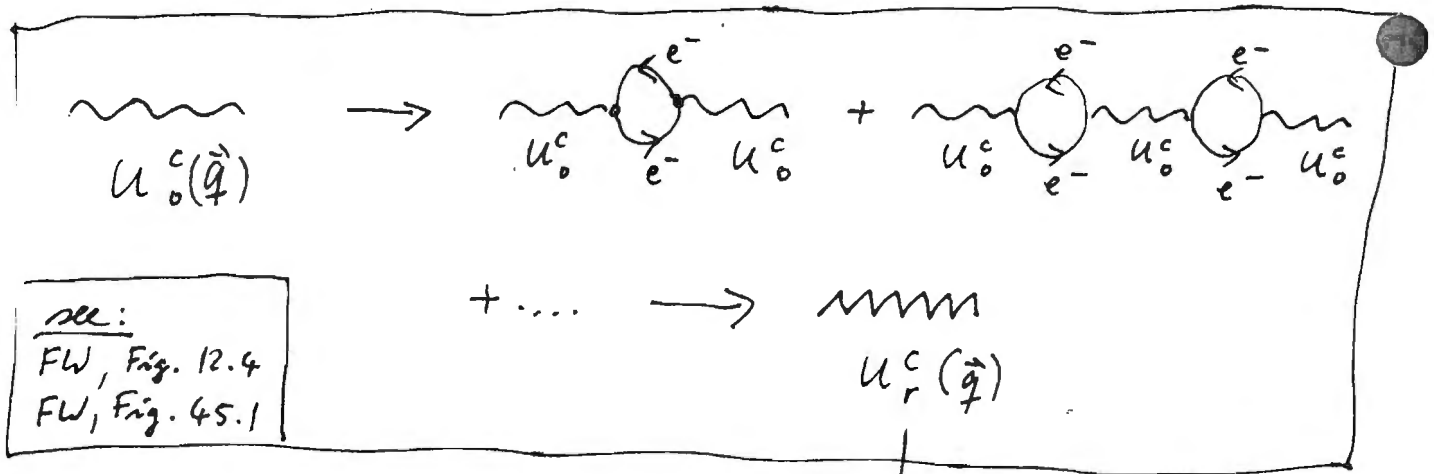
FW, Fig. 45.1

It turns out that using the "bare" (infinite-range) Coulomb interaction in the medium is not very realistic. The "effective" interaction between 2 charges in the medium is modified by the dielectric constant. The modified Coul. int. takes the form

$$U^c(\vec{q}) = \underbrace{\frac{4\pi e^2}{\vec{q}^2}}_{= U_0^c(\vec{q})} \cdot \frac{1}{K(\vec{q})}$$

modified Coul. ↑ describes dielectric properties

Using Feynman perturbation theory, one can evaluate $K(q)$ by summing "ring diagrams"; these diagrams look like the vacuum polarization diagrams in QED and describe the polarization of the medium:



see:
FW, Fig. 12.4
FW, Fig. 45.1

For details about ring diagram calculation, see FW, chapter 12.

"ring diagram" (r) approx. of "effective" Coul. int.

In ring approx., one finds the following result in momentum space

$$\boxed{U_r^c(\vec{q}) = \frac{4\pi e^2}{\vec{q}^2 + \mu^2}} \quad (\text{for } q \ll k_F)$$

which, in coordinate space, is equivalent to a screened Coul. int.

of range $r_c = 1/\mu$ [illegible]

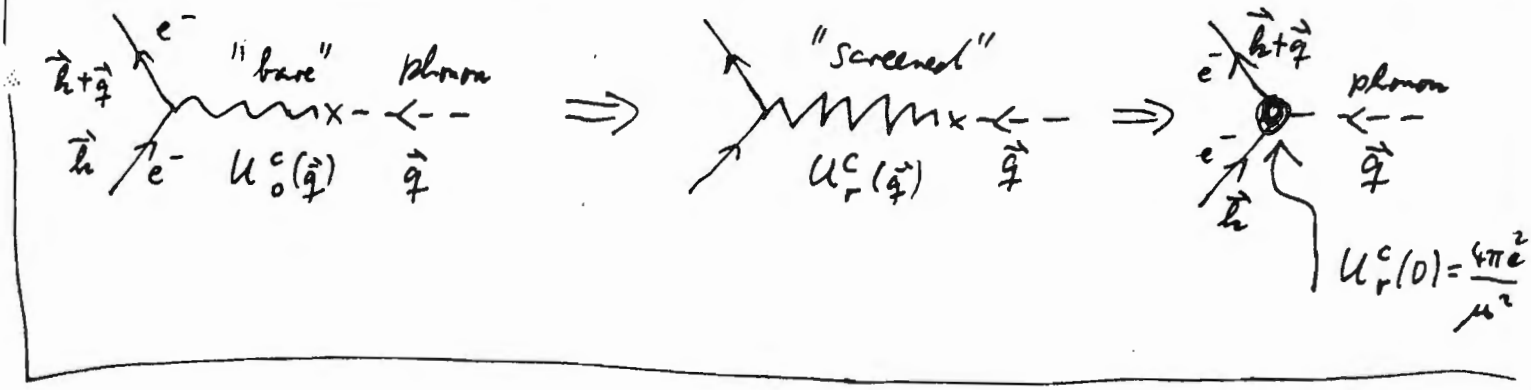
$$V_r^c(r) \sim \frac{e^{-\mu r}}{r}$$

One can show that in the expression for $\hat{H}_{el-ph}$ on p. 21, one can replace

$$\sum_{\vec{q}} \underbrace{\frac{4\pi e^2}{\vec{q}^2}}_{= U_0^c(\vec{q})} \longrightarrow \sum_{\vec{q}} \underbrace{\frac{4\pi e^2}{\vec{q}^2+\mu^2}}_{= U_r^c(\vec{q})} \longrightarrow \approx \underbrace{\frac{4\pi e^2}{\mu^2}}_{= U_r^c(\vec{q}=0)} \sum_{\vec{q} \neq 0} \dots$$

"bare" — "screened" — "screened" int. at zero momentum transfer

or in graphical form (FW, fig. 45.1):



We apply now the last approx. to $\hat{H}_{el-ph}$ on p. 21; replacing the expression

$$\frac{ze^2}{c}\sqrt{\frac{n_0}{M}} \sum_{\vec{q}} \frac{4\pi}{\vec{q}^2} \rightarrow \underbrace{\frac{ze^2}{c}\sqrt{\frac{n_0}{M}} \frac{4\pi}{\mu^2}}_{= \text{def.} = \gamma} \sum_{\vec{q}}$$

we obtain the coupling constant γ of the electron-phonon int.:

$$\hat{H}_{el-ph} = \gamma \sum_{\vec{k},\lambda} \sum_{\vec{q}} \sqrt{\frac{\hbar\omega_{\vec{q}}}{2V}}\, \theta\left(\frac{\omega_D}{c} - |\vec{q}|\right) \left[\hat{a}^+_{\vec{k}+\vec{q},\lambda}\, \hat{a}_{\vec{k}\lambda}\, \hat{c}_{\vec{q}} + \hat{a}^+_{\vec{k}\lambda}\, \hat{a}_{\vec{k}+\vec{q},\lambda}\, \hat{c}^+_{\vec{q}} \right]$$

Ring diagram theory yields the result (FW 45.8 and 45.9)

$$\frac{4\pi}{\mu^2} = \frac{\pi^2 a_0}{k_F} \qquad (a_0 = \text{Bohr radius})$$

and here for the electron-phonon coupling constant γ (see FW 45.12):

$$\gamma = \frac{Ze^2}{c}\sqrt{\frac{n_0}{M}}\,\frac{\pi^2 a_0}{k_F}$$

Replacing the speed of sound c in terms of the bulk modulus B and ionic mass M and number density n_0 we set

$$\frac{1}{c} = \sqrt{\frac{M n_0}{B}}\,, \quad \text{resulting in}$$

$$\boxed{\gamma = \frac{Ze^2 n_0 \pi^2 a_0}{k_F}\,\frac{1}{\sqrt{B}} \overset{a_0 = \frac{\hbar^2}{me^2}}{=\!=\!=\!=\!\Rightarrow} \frac{Z\hbar^2 n_0 \pi^2}{m k_F}\,\frac{1}{\sqrt{B}}} \quad \text{FW (45.12)}$$

We see that the electron-phonon coupling constant γ depends on the density of the electron gas (n_0), the Fermi momentum k_F of the electrons, the charge Z of the ionic cores and on the bulk modulus B of the metal.
Note that γ does not depend on the mass M of the ionic cores.

However, the phonon frequency spectrum depends on M because

$$(\hbar\omega_k)_{\text{phonon}} = \hbar k \cdot c = \hbar k \sqrt{\frac{B}{M n_0}}\,.$$

Coupled electron-phonon field theory and static limit: attractive electron-electron int.

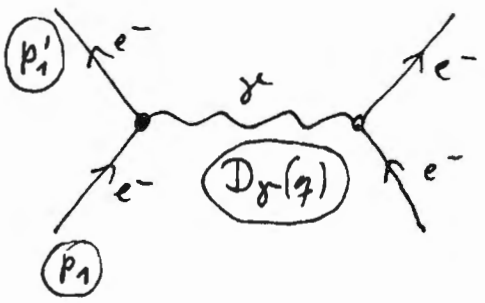
Lit: FW, p. 399-401

One starts from the system Hamiltonian $\hat{H} = H_{\text{el-gas}} + \hat{H}_{\text{ph}} + \hat{H}_{\text{el-ph}}$

To obtain the equivalent e^-e^- interaction from the phonon propagator, one follows the same steps as in QED:

QED: how to obtain $V_{coul}(r) = \frac{e^2}{r}$ from photon propagator

Feynman diagram for e^-e^- scattering in QED



photon propagator: $D_\gamma^{(q)} = -i\frac{g_{\mu\nu}}{q^2} \sim \frac{1}{-q^2} = \frac{1}{-q_0^2+\vec{q}^2}$,

where the 4-d mom. transfer is given by $q = p_1' - p_1$.

In the static limit we have $q_0 = 0$ because

$$q_0 = E_1' - E_1 \approx m_e c^2 - m_e c^2 = 0$$

↓ zero kin. energy!

resulting in

$$D_\gamma(q_0 = 0, \vec{q}) \sim \frac{1}{\vec{q}^2}.$$ Photon-prop. in static limit ($q_0 = 0$)

If we multiply the photon prop. in the static lit ($q_0 = 0$) with the coupling constant $\alpha \sim e^2$, we obtain the Fourier transform of the static Coulomb potential:

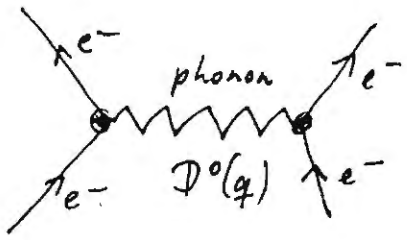
$$V_{coul}(\vec{q}) \sim e^2 D_\gamma(q_0 = 0, \vec{q}) \sim \frac{e^2}{\vec{q}^2}.$$

The inverse F.T. yields

$$V_{coul}(\vec{r}) = \frac{e^2}{|\vec{r}|}$$!!!

Static $e^- e^-$ interaction for phonon exchange

Feynman diagram



(FW Fig. 46.3)

phonon propagator:

$$D^0(q) = D^0(q_0, \vec{q}) = D^0(q_0, \omega_q = |\vec{q}|\cdot c) = \\ = \hbar \frac{\omega_{\vec{q}}^2}{q_0^2 - (\omega_{\vec{q}} - i\eta)^2}\, \theta(\omega_D - \omega_{\vec{q}})$$

FW (46.6)

static limit ($q_0 = 0$):

speed of sound

$$D^0(q_0 = 0, \vec{q}) = -\hbar\theta(\omega_D - \omega_{\vec{q}}) = -\hbar\theta(\omega_D - |\vec{q}|\cdot c)$$

Fourier transform of equivalent electron-electron potential:

$$U_0(\vec{q}) = \frac{\gamma^2}{\hbar} D^0(q_0 = 0, \vec{q}) = -\gamma^2 \theta(\omega_D - |\vec{q}|\cdot c)$$

Inverse F.T. yields the equiv. potential in coord. space

$$V_{eq}(\vec{r}) = (2\pi)^{-3} \int d^3q\, U_0(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}$$

Let us leave out the Debye cutoff factor $\theta(\ldots)$ for a moment. In this case we obtain

$$V_{eq}(\vec{r}) \approx \underbrace{(2\pi)^{-3} \int d^3q\, e^{i\vec{q}\cdot\vec{r}}}_{= \delta(\vec{r})} (-\gamma^2) = -\gamma^2 \delta(\vec{r})$$

(without Debye-factor).

If one includes the Debye cutoff factor, one obtains a finite-range attractive interaction:

$$V_{eq}(\vec{r}) = -\gamma^2 f(|\vec{r}|)$$

↑ finite-range

γ = electron-phonon coupling constant, FW (45.12)

This discovery by Fröhlich, in 1950, of a weak attractive $e^- e^-$ interaction due to phonon exchange was an important stepping stone towards Cooper's model (1956) and the full BCS theory (1957).

But there is still a big mystery: the electron-phonon coupling constant ($-\gamma^2$) is very small, therefore perturbation theory should be applicable. But how can a small perturbation cause a huge "response", i.e. a phase transition from "normal" state of matter to superconducting state? Many physicists, including Feynman tried and failed to understand this.
Finally, in 1956 Leon Cooper developed an ingenious model which avoids the use of perturbation theory.
He found the surprising result that the pairing gap Δ depends exponentially on the coupling constant γ^2.
That's why perturbation theory fails miserably!!

Note: because of page renumbering, the next page is page 107a.

Cooper's model assumptions (1956)

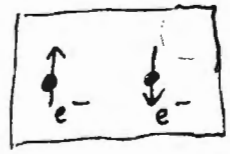
1) The model considers 2 electrons only which interact via a 2-body potential λV; λ = coupling constant. The electrons are treated as distinguishable particles, because of opposite spin, using a simple product WF, i.e. no antisymmetry:

2 free electrons:

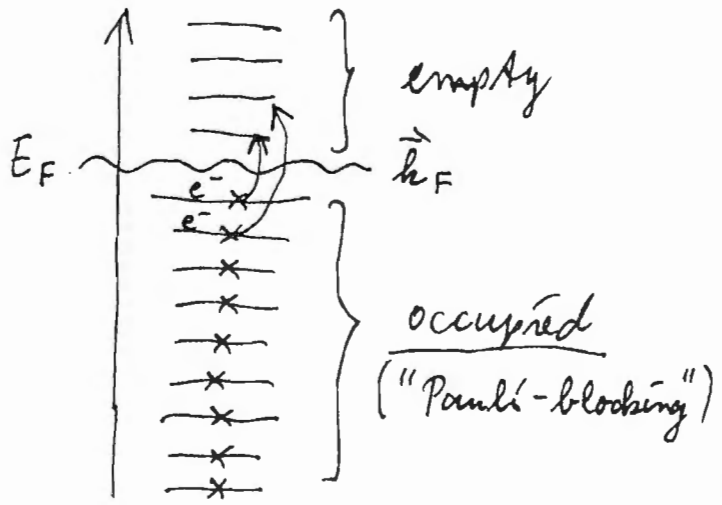
$$H_0 = -\frac{\hbar^2}{2m}\nabla^2_{\vec{x}_1} - \frac{\hbar^2}{2m}\nabla^2_{\vec{x}_2}, \quad H_0\,\varphi_n(\vec{x}_1,\vec{x}_2) = E_n^0\,\varphi_n(\vec{x}_1,\vec{x}_2)$$

with

$$\varphi_n(\vec{x}_1,\vec{x}_2) \equiv \varphi_{\vec{k}_1,\vec{k}_2}(\vec{x}_1,\vec{x}_2) = \frac{e^{i\vec{k}_1\cdot\vec{x}_1}}{L^{3/2}}\,\frac{e^{i\vec{k}_2\cdot\vec{x}_2}}{L^{3/2}}$$



2) The "medium" (metal) is approximated by a non-interacting Fermi gas of electrons. The medium manifests itself primarily through the Pauli principle:



The interaction potential, λV, can scatter the electrons only into unoccupied states with $E > E_F$, or equivalently, momenta $|\vec{k}_1| > k_F$, $|\vec{k}_2| > k_F$.

We will see that the Pauli blocking is crucial for Cooper pair formation!

It is useful to separate the center-of-mass motion, we introduce

$$\vec{P} = \vec{k}_1 + \vec{k}_2 \quad = \text{total pair momentum}$$

$$2\vec{k} = \vec{k}_1 - \vec{k}_2 \quad = \text{rel. momentum of pair}$$

$$\vec{R} = \frac{m\vec{x}_1 + m\vec{x}_2}{2m} = \frac{1}{2}(\vec{x}_1 + \vec{x}_2) = \text{c.m. coordinate}$$

$$\vec{x} = \vec{x}_1 - \vec{x}_2 \quad = \text{relative coordinate}$$

Inverting these relations, one finds

$$\vec{k}_1 = \vec{k} + \frac{\vec{P}}{2}\,, \quad \vec{k}_2 = -\vec{k} + \frac{\vec{P}}{2}\,, \quad \vec{x}_1 = \vec{R} + \frac{\vec{x}}{2}\,, \quad \vec{x}_2 = \vec{R} - \frac{\vec{x}}{2}$$

Using these relations, we can express the WF for <u>2 free electrons</u> in the form

$$\varphi_n(\vec{x}_1, \vec{x}_2) \equiv \varphi_{\vec{k}_1, \vec{k}_2}(\vec{x}_1, \vec{x}_2) \longrightarrow \varphi_{\vec{P}, \vec{k}}(\vec{R}, \vec{x}) = \frac{e^{i\vec{P}\cdot\vec{R}}}{L^{3/2}} \frac{e^{i\vec{k}\cdot\vec{x}}}{L^{3/2}}$$

The energy of the <u>free</u> pair can be written as

$$E^0_{n=0} \equiv E^0_{\vec{k}_1 \vec{k}_2} = \frac{\hbar^2}{2m}(\vec{k}_1^{\,2} + \vec{k}_2^{\,2}) = \frac{\hbar^2 k^2}{m} + \frac{\hbar^2 \vec{P}^2}{4m}$$

Consider now <u>2 interacting electrons:</u>

$$\left[H_0 + \lambda V(\vec{x}_1 - \vec{x}_2)\right] \psi(\vec{x}_1, \vec{x}_2) = E\,\psi(\vec{x}_1, \vec{x}_2)$$

↑ coupling constant ($\lambda > 0$ repulsive, $\lambda < 0$ attractive)

or in bra-ket notation: $[H_0 + \lambda V]\,|\psi\rangle = E\,|\psi\rangle$

$\Rightarrow (E - H_0)\,|\psi\rangle = \lambda V\,|\psi\rangle$, take inverse of operator:

$$|\psi\rangle = (E - H_0)^{-1}\,\lambda V\,|\psi\rangle$$

Insert completeness relation

$$\sum_n |\varphi_n\rangle\langle\varphi_n| = 1 \quad , \text{ where } H_0|\varphi_n\rangle = E_n|\varphi_n\rangle$$

$$\Rightarrow |\psi\rangle = \sum_n (E - H_0)^{-1} |\varphi_n\rangle\langle\varphi_n| \lambda V|\psi\rangle$$

We split up the terms into the lowest s.p. state $n=0$ and the excited states $n \neq 0$:

$$\boxed{|\psi\rangle = \frac{|\varphi_0\rangle\langle\varphi_0|\lambda V|\psi\rangle}{E - E_0} + \sum_{n\neq 0} \frac{|\varphi_n\rangle\langle\varphi_n|\lambda V|\psi\rangle}{E - E_n}} \qquad (1)$$

We show now that $\boxed{\langle\varphi_0|\lambda V|\psi\rangle = E - E_0}$ (2)

Proof:

$$(H_0 + \lambda V)|\psi\rangle = E|\psi\rangle \quad | \times \langle\varphi_0|$$

$$\langle\varphi_0|H_0 + \lambda V|\psi\rangle = E\langle\varphi_0|\psi\rangle$$

$$E_0\langle\varphi_0|\psi\rangle + \langle\varphi_0|\lambda V|\psi\rangle = E\langle\varphi_0|\psi\rangle$$

$$\Rightarrow \langle\varphi_0|\lambda V|\psi\rangle = (E - E_0)\underbrace{\langle\varphi_0|\psi\rangle}_{\stackrel{!}{=} 1 \text{ (normal. cond. for } \psi)} = E - E_0 \quad \text{q.e.d.}$$

Inserting (2) into (1) yields

$$\boxed{|\psi\rangle = |\varphi_0\rangle + \sum_{n\neq 0} \frac{|\varphi_n\rangle\langle\varphi_n|\lambda V|\psi\rangle}{E - E_n}} \qquad (3)$$

We separate now relative and total momentum for the 3 different types of WFs, $|\varphi_0\rangle$, $|\varphi_{n\neq 0}\rangle$ and $|\psi\rangle$:

$$|\varphi_0\rangle = |\varphi_{\vec{k}_1,\vec{k}_2}\rangle \hat{=} |\varphi_{\vec{P},\vec{k}}\rangle \Rightarrow \varphi_{\vec{P},\vec{k}}(\vec{R},\vec{x}) = \frac{e^{i\vec{P}\cdot\vec{R}}}{L^{3/2}} \frac{e^{i\vec{k}\cdot\vec{x}}}{L^{3/2}}$$

$$|\varphi_{n\neq 0}\rangle = |\varphi_{\vec{t}_1,\vec{t}_2}\rangle \hat{=} |\varphi_{\vec{P},\vec{t}}\rangle \Rightarrow \varphi_{\vec{P},\vec{t}}(\vec{R},\vec{x}) = \frac{e^{i\vec{P}\cdot\vec{R}}}{L^{3/2}} \frac{e^{i\vec{t}\cdot\vec{x}}}{L^{3/2}}$$

$$|\psi\rangle \hat{=} \psi_E(\vec{R},\vec{x}) = \frac{e^{i\vec{P}\cdot\vec{R}}}{L^{3/2}} \frac{\psi^{(E)}_{\vec{P},\vec{k}}(\vec{x})}{L^{3/2}}$$

$\psi^{(E)}_{\vec{P},\vec{k}}(\vec{x})$ — unknown, to be computed

Remarks: a) The total momentum $\vec{P}$ of the pair is always conserved in this model because the pair does not interact with the rest of the "Fermi sea".

b) $|\psi\rangle$ is the quantum state of the 2 interacting electrons. The notation $\psi^{(E)}_{\vec{P},\vec{k}}(\vec{x})$ means that the interacting pair has energy E, and without the interaction λV it has the rel. momentum $\vec{k}$.

Now calculate the matrix element in (3):

$$\langle \varphi_{n\neq 0}|\lambda V|\psi\rangle = \int d^3x \int d^3R \; \frac{e^{-i\vec{P}\cdot\vec{R}}\, e^{-i\vec{t}\cdot\vec{x}}}{L^3} \lambda V(\vec{x}) \cdot \frac{e^{i\vec{P}\cdot\vec{R}}\, \psi^{(E)}_{\vec{P},\vec{k}}(\vec{x})}{L^3} =$$

$$= \int d^3x \; \frac{e^{-i\vec{t}\cdot\vec{x}}}{L^3} \lambda V(\vec{x}) \psi^{(E)}_{\vec{P},\vec{k}}(\vec{x}) \underbrace{\int d^3R \frac{1}{L^3}}_{=1}$$

$$\Rightarrow \langle \varphi_{n\neq 0}|\lambda V|\psi\rangle = \frac{\lambda}{L^3} \int d^3x \, e^{-i\vec{t}\cdot\vec{x}} V(\vec{x}) \psi^{(E)}_{\vec{P},\vec{k}}(\vec{x})$$

$$\boxed{\langle \varphi_{n\neq 0}|\lambda V|\psi\rangle = \frac{\lambda}{L^3} \langle \vec{t}|V|\psi^{(E)}_{\vec{P},\vec{k}}\rangle} \quad (4)$$

Insert the matrix element (4) and the expressions for $|\varphi_0\rangle$, $|\varphi_{n\neq 0}\rangle$ and $|\psi\rangle$ into (107c)

eq. (3): $|\psi\rangle = |\varphi_0\rangle + \sum_{n\neq 0} \frac{|\varphi_n\rangle\langle\varphi_n|\lambda V|\psi\rangle}{E - E_n} \Rightarrow$

$$\mathcal{L}^{-3} e^{i\vec{P}\cdot\vec{R}} \psi^{(E)}_{\vec{P},\vec{k}}(\vec{x}) = \mathcal{L}^{-3} e^{i\vec{P}\vec{R}} e^{i\vec{k}\cdot\vec{x}} + \mathcal{L}^{-3} e^{i\vec{P}\cdot\vec{R}} \cdot \sum_{|\vec{t}_1|,|\vec{t}_2|>k_F} e^{i\vec{t}\cdot\vec{x}} \frac{1}{E - E_{\vec{t}_1,\vec{t}_2}} \frac{\lambda}{\mathcal{L}^3} \langle \vec{t}|V|\psi^{(E)}_{\vec{P},\vec{k}}\rangle$$

↑ Note: Pauli blocking!

$$\psi^{(E)}_{\vec{P},\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + \frac{1}{\mathcal{L}^3} \sum_{\substack{|\vec{t}+\frac{\vec{P}}{2}|>k_F \\ |\vec{t}-\frac{\vec{P}}{2}|>k_F}} e^{i\vec{t}\cdot\vec{x}} \frac{\langle t|\lambda V|\psi^{(E)}_{\vec{P},\vec{k}}\rangle}{E - E_{\vec{t},\vec{P}}}$$

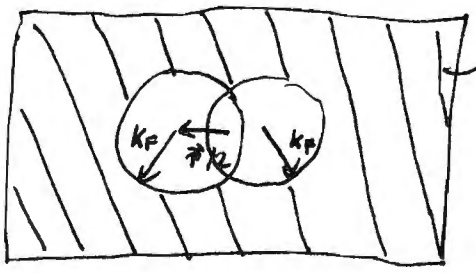
Using the expression on p. 107b, the energy denominator can be written in the form

(5) $$E - E_{\vec{t},\vec{P}} = \left(\frac{\hbar^2\vec{K}^2}{m} + \frac{\hbar^2\vec{P}^2}{4m}\right) - \left(\frac{\hbar^2\vec{t}^2}{m} + \frac{\hbar^2\vec{P}^2}{4m}\right) = \frac{\hbar^2}{m}(\vec{K}^2 - \vec{t}^2)$$

where the quantity $\vec{K}^2$ parametrizes the unknown Cooper pair energy with interaction λV.

Replacing the sum by an integral: $\frac{1}{\mathcal{L}^3}\sum_{\Gamma} \to \int_{\Gamma} \frac{d^3t}{(2\pi)^3}$

where Γ defines the integration region in momentum space:



$$\Gamma = |\vec{t} \pm \tfrac{\vec{P}}{2}| > k_F$$

We observe the "Pauli blocking" of the 2 overlapping spheres from the integration region!

Using the shorthand notation $\boxed{v(\vec{x}) = \frac{m}{\hbar^2} V(\vec{x})}$

we finally arrive at the famous "Bethe-Goldstone" eqn:

$$\boxed{\psi^{(E)}_{\vec{P},\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} + \int_\Gamma \frac{d^3t}{(2\pi)^3} e^{i\vec{t}\cdot\vec{x}} \frac{1}{\kappa^2 - t^2} \langle t|\lambda v|\psi_{\vec{P},\vec{k}}\rangle} \quad (6)$$

It is the Schrödinger eq. for 2 electrons (fermions) in a medium which manifests its existence through restrictions on integration in momentum space. The electrons interact via $\lambda V(\vec{x}) = \lambda \frac{\hbar^2}{m} v(\vec{x})$.

We observe that the Bethe-Goldstone eq. contains the same state vector $|\psi^{(E)}_{\vec{P},\vec{k}}\rangle$ on both sides (underlined); therefore, it must be solved by iteration:

$$|\psi^{(E)}_{\vec{P},\vec{k}}\rangle = |\vec{k}\rangle + \lambda \int_\Gamma \frac{d^3t}{(2\pi)^3} |\vec{t}\rangle \frac{1}{\kappa^2 - t^2} \langle \vec{t}|v|\psi^{(E)}_{\vec{P},\vec{k}}\rangle$$

We now iterate on the RHS:

$$|\psi^{(E)}_{\vec{P},\vec{k}}\rangle = |\vec{k}\rangle + \lambda \int_\Gamma \dots$$

$$|\psi^{(E)}_{\vec{P},\vec{k}}\rangle = |\vec{k}\rangle + \lambda \int_\Gamma \frac{d^3t}{(2\pi)^3} |\vec{t}\rangle \frac{1}{\kappa^2 - t^2} \langle t|v|\vec{k}\rangle + \underbrace{O(\lambda^2)}_{\approx 0}$$

and we neglect terms of order λ^2 and higher because the coupling constant λ is assumed to be small.

From eq. (2) we have: $(E - E_0) = \langle \varphi_0|\lambda V|\psi\rangle$

Inserting eqns (4) and (5) for the special case $\kappa = 0$, i.e. $\vec{t} \to \vec{k}$:

$$(E - E_0) \overset{(5)}{=} \frac{\hbar^2}{m}(\kappa^2 - k^2) = \langle \varphi_0|\lambda V|\psi\rangle \overset{(4)}{=} \frac{\lambda}{L^3} \langle \vec{k}|V|\psi^{(E)}_{\vec{P},\vec{k}}\rangle$$

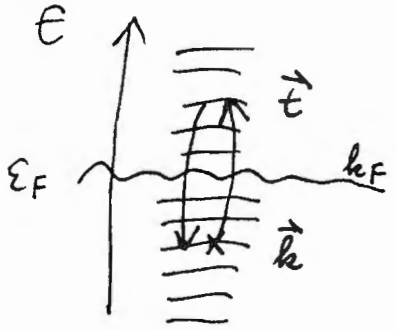
or $$\boxed{(\kappa^2 - k^2) = \frac{\lambda}{L^3} \langle \vec{k}\left|\underbrace{\frac{mV}{\hbar^2}}_{=v}\right|\psi^{(E)}_{\vec{P},\vec{k}}\rangle} \quad (7)$$

Inserting the Bethe-Goldstone eqn. (in first iteration on RHS)

$$|\psi^{(E)}_{\vec{p},\vec{k}}\rangle = |\vec{k}\rangle + \lambda \int_\Gamma \frac{d^3t}{(2\pi)^3} |\vec{t}\rangle \frac{1}{K^2 - t^2} \langle \vec{t}|\underline{\underline{v}}|\vec{k}\rangle + \dots$$

into eq. (7) yields

$$(K^2 - k^2) = \frac{\lambda}{L^3}\left[\langle \vec{k}|v|\vec{k}\rangle + \lambda \int_\Gamma \frac{d^3t}{(2\pi)^3} \frac{\langle \vec{k}|v|\vec{t}\rangle\langle \vec{t}|v|\vec{k}\rangle}{K^2 - t^2}\right]$$



2-step virtual scattering by interaction λv: from $\vec{k}$ → $\vec{t}$ → $\vec{k}$

↓ below k_F ↓ above k_F ↓ below k_F

Using $\langle \vec{t}|v|\vec{k}\rangle = \langle \vec{k}|v|\vec{t}\rangle^*$, the last eq. can be rewritten

$$(K^2 - k^2) = \frac{\lambda}{L^3}\langle \vec{k}|v|\vec{k}\rangle + \lambda \int_\Gamma \frac{d^3t}{(2\pi)^3} \frac{1}{K^2 - t^2}\left\{\frac{\lambda}{L^3}\left|\langle \vec{k}|v|\vec{t}\rangle\right|^2\right\} \qquad (8)$$

This equation determines the energy shift of the electron pair due to the interaction λV:

$$\Delta E_{pair} = E - E_0 \overset{(5)}{=} \left(\frac{\hbar^2 K^2}{m} + \frac{\hbar^2 p^2}{4m}\right) - \left(\frac{\hbar^2 k^2}{m} + \frac{\hbar^2 p^2}{4m}\right)$$

$$= \frac{\hbar^2}{m}(K^2 - k^2) \qquad (9)$$

free electrons E_0

$\Delta E = \frac{\hbar^2}{m}(K^2 - k^2)$

Cooper pair E

Equation (8) for the energy shift $(k^2 - h^2)$ cannot be solved analytically without further approximations. However, one can solve (8) graphically if one generalizes the interaction $\lambda v(\vec{x})$ to a "nonlocal separable" potential of the form

$$\boxed{v(\vec{x}) \to v(\vec{x},\vec{x}') = u(|\vec{x}|)\, u(|\vec{x}'|)^* = u(x)\, u(x')^*.} \quad (10)$$

local — nonlocal — separable (in $\vec{x},\vec{x}'$)

One should not read too much physics into the last eq.; its only purpose for is to get an analytical solution! (Ultimately, it has to be justified by more accurate numerical approach).

$$\Rightarrow \langle \vec{h}|v|\vec{t}\rangle \equiv \int d^3x\, \varphi_{\vec{h}}^*(\vec{x})\, v(\vec{x})\, \varphi_{\vec{t}}(\vec{x}) \xrightarrow{\text{nonlocal}}$$

$$\int d^3x \int d^3x'\, \varphi_{\vec{h}}^*(\vec{x})\, \underbrace{v(\vec{x},\vec{x}')}_{u(x)\,u(x')^*}\, \varphi_{\vec{t}}(\vec{x}') =$$

$$= \underbrace{\int d^3x\, e^{-i\vec{h}\cdot\vec{x}}\, u(x)}_{=u(h)} \quad \underbrace{\int d^3x'\, e^{+i\vec{t}\cdot\vec{x}'}\, u(x')^*}_{=u^*(t)}$$

Hence: $$\boxed{\langle \vec{h}|v|\vec{t}\rangle = u(h)\, u^*(t)} \quad (11)$$ for non-local separable potential u

Insert (11) into (8):

$$(k^2 - h^2) = \frac{\lambda}{L^3}\,|u(h)|^2 + \lambda \int_\Gamma \frac{d^3t}{(2\pi)^3}\, \frac{1}{k^2 - t^2} \underbrace{\left\{\frac{\lambda}{L^3}\,|u(h)|^2\right\}}_{=(k^2-h^2)} |u(t)|^2 \quad (12)$$

↳ because from (8): $k^2 - h^2 = \frac{\lambda}{L^3}\langle \vec{h}|\vec{v}|\vec{h}\rangle + O(\lambda^2) = \frac{\lambda}{L^3}|u(h)|^2 + O(\lambda^2)$

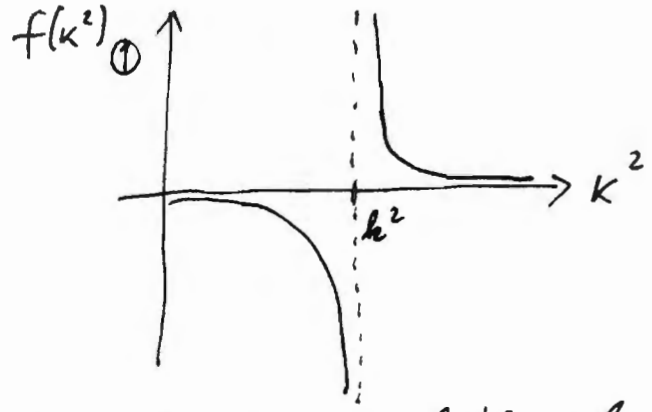
Divide eq. (12) by

$$\lambda \cdot (k^2 - h^2) \quad \Rightarrow$$

$$\frac{1}{\lambda} = \frac{1}{C^3}\frac{|u(k)|^2}{(K^2-k^2)} + \int_\Gamma \frac{d^3t}{(2\pi)^3}\frac{|u(t)|^2}{K^2-t^2} \equiv f(K^2) \qquad (13)$$

$(\hat{=}$ FW 36.22)

First term of $f(K^2)$ has pole at $K^2 = k^2$



To obtain the location of the pole in the second term, we write the integral in spherical coordinates

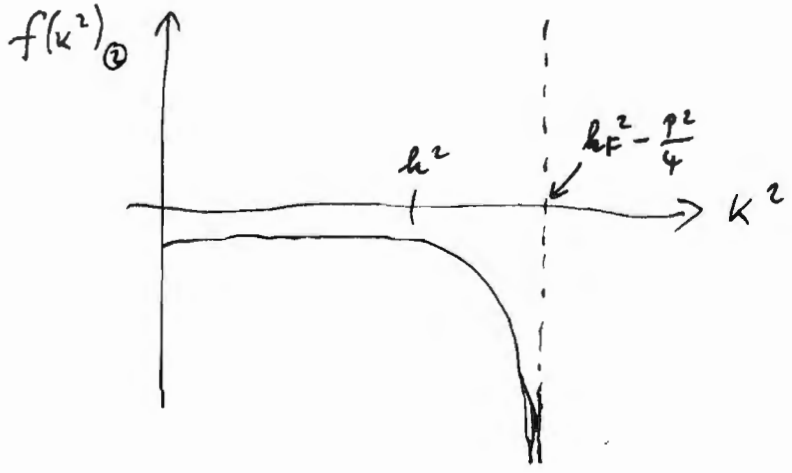
$$\int_\Gamma \frac{d^3t}{(2\pi)^3}\frac{|u(t)|^2}{K^2-t^2} = \int_{t_{min}}^{\infty} \frac{t^2 dt}{(2\pi)^3}\frac{|u(t)|^2}{K^2-t^2}\underbrace{\int d\Omega_t}_{=4\pi} \qquad (14)$$

where t_{min} is obtained from the expression for Γ, see p. 107e:

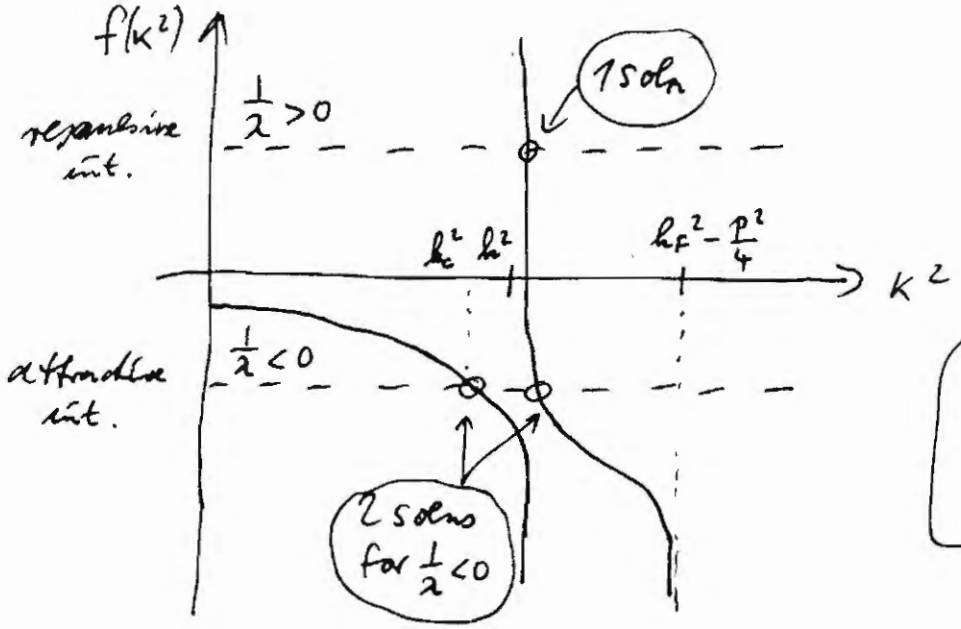
$$\Gamma = \left|\vec{t} \pm \frac{\vec{p}}{2}\right| > k_F$$

② Pole at $K^2 = t_{min}^2$, with $t_{min}^2 = k_F^2 - \frac{p^2}{4}$,

hence $K^2 = k_F^2 - \frac{p^2}{4}$ for second pole



Adding both terms together, we get the following "graphical soln"



FW, Fig. 36.2

Eigenvalue cond. for Bethe-Goldstone equation

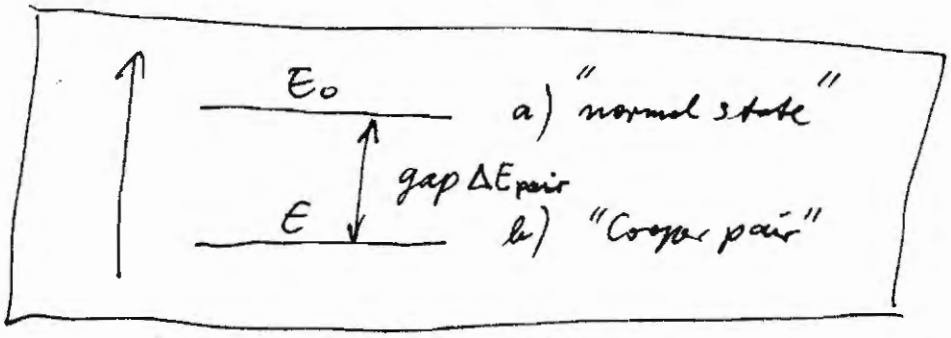
We observe: For a repulsive residual int. ($\lambda>0$), there is only one solution

$$k^2 \approx k^2 \quad , \text{ i.e. } \underline{E-E_0 \approx 0} \, ,$$

but for an attractive interaction, there are two solns:

a) $k^2 \approx k^2$, i.e. $E \approx E_0$

b) $k^2 = k_c^2 < k^2$, i.e. $E < E_0$



Let's study the "Cooper pair" soln with $k^2 = k_c^2$ in more detail. The 1st term in $f(k^2)$ is negligible near $k^2 = k_c^2$ (see graphs) and we have, for $\lambda<0$:

$$\frac{1}{\lambda} \simeq \int_\Gamma \frac{d^3t}{(2\pi)^3} \frac{|u(t)|^2}{k^2-t^2} \quad \text{with} \rightarrow \Gamma = \left|\frac{\vec{P}}{2} \pm \vec{t}\right| > k_F$$

Thus: $\frac{1}{|\lambda|} = -\frac{1}{\lambda} \overset{(14)}{=} \int_{t_{min}}^{\infty} \frac{t^2 dt}{(2\pi)^3} \frac{|u(t)|^2 4\pi}{t^2 - k^2}$.

$\uparrow$ $\lambda < 0$

Consider now the special case

$$\boxed{\vec{P} = \text{total pair mom.} = \vec{0}}$$

$\Rightarrow t_{min}^2 = k_F^2 - \frac{P^2}{4}^{=0} = k_F^2$

$\Rightarrow \underline{t_{min} = k_F}$

Assume that $|u(t)|^2$ contributes mostly near $t_{min} = k_F$:

$$|u(t)|^2 \approx |u(k_F)|^2$$

and take it outside the integral

$$\frac{1}{|\lambda|} = \frac{4\pi}{8\pi^3} |u(k_F)|^2 \int_{k_F}^{\infty} \frac{t^2 dt}{t^2 - k^2} = \frac{|u(k_F)|^2}{2\pi^2} \int_{k_F}^{\infty} \frac{t^2 dt}{t^2 - k^2}$$

Inserting an approximate soln. for the integral, one finds

$$\frac{1}{|\lambda|} = \frac{|u(k_F)|^2}{2\pi^2} \left[\frac{1}{2} k_F \ln\left(\frac{k_F^2}{k_F^2 - K^2} \right) \right] \qquad (\text{for } \vec{P} = 0)$$

Solving for $-\ln(\dots)$, we obtain:

$$-\frac{4\pi^2}{k_F |\lambda| |u(k_F)|^2} = -\ln\left(\frac{k_F^2}{k_F^2 - K^2} \right) = +\ln\left(\frac{k_F^2 - K^2}{k_F^2} \right)$$

Exponentiation yields

$$\exp\left(-\frac{4\pi^2}{k_F |\lambda| |u(k_F)|^2} \right) = \frac{k_F^2 - K^2}{k_F^2} = \frac{\frac{\hbar^2 k_F^2}{m} - \frac{\hbar^2 K^2}{m}}{\frac{\hbar^2 k_F^2}{m}} \overset{\text{def}}{=} \frac{2(\varepsilon_{k_F} - \varepsilon_K)}{2\varepsilon_{k_F}} \equiv \Delta$$

Defining the "pairing gap Δ" via $\boxed{\Delta \overset{\text{def}}{=} 2(\varepsilon_{k_F} - \varepsilon_K)}$ (15a)

results in the expression

$$\boxed{\Delta = (2\varepsilon_{k_F}) \exp\left(-\frac{4\pi^2}{k_F |\lambda| |u(k_F)|^2} \right)} \quad (15b)$$

Δ: pairing gap; $2\varepsilon_{k_F}$: Fermi energy; $|\lambda|$: coupling constant; $|u(k_F)|^2$: F.T. of nonlocal int.

Finally, we express the energy shift of the Cooper pair in terms of Δ:

$$\Delta E_{pair} = E - E_0 \overset{(9)}{=} \frac{\hbar^2}{m}(K^2 - k^2) = 2(\varepsilon_K - \varepsilon_k) =$$

$$= \underbrace{2(\varepsilon_K - \varepsilon_{k_F})}_{=-\Delta} + 2(\varepsilon_{k_F} - \varepsilon_k) \quad \Rightarrow$$

$$\boxed{\Delta E_{pair} = E - E_0 = -\Delta + 2(\varepsilon_{k_F} - \varepsilon_k)} \quad (16)$$

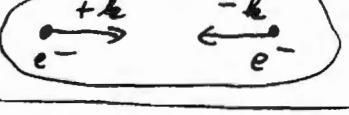
If the relative momentum k of the 2 fermions is close to the Fermi momentum k_F ($k \approx k_F \Rightarrow \varepsilon_k \approx \varepsilon_{k_F}$), we have

$$\boxed{\Delta E_{pair} = E - E_0 \approx -\Delta} \quad \text{(for } k \approx k_F\text{)} \quad (17)$$

Eq. (15b) shows that the pairing gap Δ depends exponentially on the electron-phonon int. coupling constant $\lambda = -|2|$:

$$\boxed{\Delta = \exp\left(-\frac{1}{|2|} \cdots\right)} \quad (18)$$

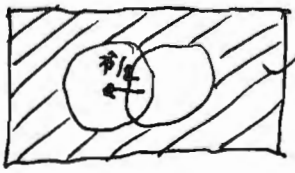
$\Rightarrow$ Pairing is a non-perturbative phenomenon (more in HF+BCS section that follows!)

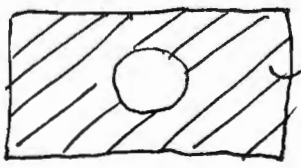
Pairing gap is largest for $\vec{P} = 0$, i.e. 

Reason: $\Delta = 2(\varepsilon_{k_F} - \varepsilon_K) = \frac{\hbar^2}{m}(k_F^2 - K^2)$, and K^2 is obtained from integral on p. 108d:

$$\frac{1}{\lambda} \approx \int_\Gamma \frac{d^3t}{(2\pi)^3} \frac{|u(t)|^2}{K^2 - t^2}, \text{ with } \Gamma = \left|\frac{\vec{P}}{2} \pm \vec{t}\right| > k_F.$$

The phase-space for this integral is maximized if $\vec{P} = 0$: (shaded area = Γ)

a) finite $\vec{P}$ 

b) $\vec{P} = \vec{0}$ 

Note finally that Cooper's model explains another "mystery": - 2 particles in free space will not form a bound state unless the strength of the potential exceeds some critical value. But Fröhlich has shown that the electron-phonon equivalent potential

$$V_{eq,el\text{-}ph}(\vec{r},\vec{r}') = -\gamma^2 \delta(\vec{r}-\vec{r}')$$

is very weak (γ^2 is very small!). So how can one get a bound pair? The answer to this question is that the medium plays a crucial role in the pair formation. There is always an energy gap Δ, even for an arbitrarily weak residual interaction:

$$\Delta = (2\varepsilon_{k_F}) \exp\left(-\frac{4\pi}{k_F |\lambda| |u(k_F)|^2}\right), \quad \text{where } |\lambda| = \gamma^2.$$

The reason is, ultimately the "Pauli blocking" of electrons in the medium, as manifested by the integration region Γ.

Interacting electron gas (metal) at temp. $T=0$; Hartree-Fock plus BCS pairing model

Lit: FW § 37, p. 326-337 — Generalize Cooper model to N electrons

The Hamiltonian of the system consists of an interacting (repulsive Coul.) electron gas with uniform ionic background charge, see FW eq. (3.19), and an additional attractive "residual" 2-body electron-phonon potential:

$$\hat{H}_{\text{system}} = \hat{H}_{\text{el-gas}} + \hat{V}^{(2)}_{\text{eq, el-ph}} \qquad (1)$$

with

$$\hat{H}_{\text{el-gas}} = \sum_{\vec{k},\lambda} \frac{\hbar^2 \vec{k}^2}{2m} \hat{a}^+_{\vec{k}\lambda} \hat{a}_{\vec{k}\lambda} + \frac{e^2}{2L^3} \sum_{\substack{\vec{k},\vec{p},\vec{q} \\ (\vec{q}\neq 0)}} \sum_{\lambda_1,\lambda_2} \frac{4\pi}{\vec{q}^2} \cdot \hat{a}^+_{\vec{k}+\vec{q},\lambda_1} \hat{a}^+_{\vec{p}-\vec{q},\lambda_2} \hat{a}_{\vec{p}\lambda_2} \hat{a}_{\vec{k}\lambda_1} \qquad (2)$$

The equivalent 2-body el-ph potential has the form, in "first quantized" ~~former~~ version:

$$V^{(2)}_{\text{eq, el-ph}} = \frac{1}{2} \sum_{\substack{i,j=1 \\ (i\neq j)}}^{N} V(\vec{x}_i, \vec{x}_j) = \begin{matrix}\text{Fröhlich, 1950} \\ \text{(FW 46.9)}\end{matrix} = \frac{1}{2} \sum_{\substack{i,j=1 \\ (i\neq j)}}^{N} -\gamma^2 \delta(\vec{x}_i - \vec{x}_j) \qquad (3)$$

(γ^2: el-ph coupling constant)

We will transform this to occup. # repr. later.

We proceed in 2 steps:

(1) solve $\hat{H}_{\text{el-gas}}$ in HF approximation

(2) consider effects of "residual" electron-phonon potential

The electron gas Hamiltonian has the form

$$\hat{H}_{\text{el-gas}} = \hat{T}^{(1)} + \hat{V}^{(2)}_{\text{coul},e^-e^-}$$

In HF approximation, we replace this by the 1-body Hamiltonian

$$\boxed{\hat{H}^{HF}_{\text{el-gas}} = \sum_{\alpha,\beta=1}^{\infty} \underbrace{\langle\beta|\, h_{HF}\,|\alpha\rangle}_{=\varepsilon^0_\alpha \delta_{\alpha\beta}} \hat{a}^+_\beta \hat{a}_\alpha = \sum_{\alpha=1}^{\infty} \varepsilon^0_\alpha \hat{a}^+_\alpha \hat{a}_\alpha} \quad (4)$$

with the HF s.p. energies (see my notes ch. 7, p. 18):

$$\varepsilon^0_\alpha = \langle\alpha|\, h_{HF}\,|\alpha\rangle = \langle\alpha|t|\alpha\rangle + \sum_{\mu=1}^{N} \langle\alpha\mu|\, v^{(2)}_{\text{coul},e^-e^-}\,|\alpha\mu-\mu\alpha\rangle \quad (5)$$

One can show that the HF s.p. wave functions are simply plane waves for a uniform interacting fermion system, i.e. same as the free UFs !! (This is due to translational invariance of the bulk medium). Hence:

$$\boxed{\varphi^{HF}_\alpha(\vec{x}) = \langle\vec{x}|\alpha\rangle \longrightarrow \langle\vec{x}|\vec{k}\lambda\rangle = \varphi_{\vec{k}\lambda}(\vec{x}) = L^{-3/2} e^{i\vec{k}\cdot\vec{x}} \eta_\lambda} \quad (6)$$

This leads to

$$\hat{H}^{HF}_{\text{el-gas}} = \sum_{\vec{k},\lambda} \varepsilon^0_k \hat{a}^+_{\vec{k}\lambda} \hat{a}_{\vec{k}\lambda} \quad (7a)$$

and one obtains for the HF s.p. energies the full expression (see FW p. 127):

$$\varepsilon_k^0 = \frac{\hbar^2 k^2}{2m} + n\,V(k=0) - \left(\frac{1}{2\pi}\right)^3 \int d^3k'\, V(\vec{k}-\vec{k}')\,\theta(k_F - k') \qquad (7b)$$

where $V(\vec{q})$ is the Fourier transform of the bare / screened repulsive Coulomb potential between the electrons.

The 2-body residual interaction (attractive el-ph) has the form

$$\hat{V}^{(2)}_{eff,\,el\text{-}ph} = -\frac{1}{2} \sum_{\substack{\vec{k}_1 \ldots \vec{k}_4 \\ \lambda_1 \ldots \lambda_4}} \underbrace{\langle \vec{k}_1 \lambda_1, \vec{k}_2 \lambda_2 | v | \vec{k}_3 \lambda_3, \vec{k}_4 \lambda_4 \rangle}_{= \delta_{\lambda_1 \lambda_3} \delta_{\lambda_2 \lambda_4} \langle \vec{k}_1 \vec{k}_2 | v | \vec{k}_3 \vec{k}_4 \rangle} \cdot \hat{a}^+_{\vec{k}_1 \lambda_1} \hat{a}^+_{\vec{k}_2 \lambda_2} \hat{a}_{\vec{k}_4 \lambda_4} \hat{a}_{\vec{k}_3 \lambda_3} \qquad (8)$$

where the 2-body pot. matrix elements $\langle \ldots | v | \ldots \rangle$ are assumed to be spin-independent.

Our goal here is to study the thermodynamic properties of metals at low T. The starting point is the thermodynamic potential Ω (see FW p. 34):

$$\Omega(T, V, \mu) = E - T \cdot S - \mu \cdot N \qquad (9a)$$

Ω: thermodyn. pot. — E: internal energy — T: temp. — S: entropy — μ: chem. potential — N: particle #

This is the starting point of the BCS theory at finite T, see FW § 51.

We will here study the T=0 case only

$$\Rightarrow \boxed{\Omega(T=0, V, \mu) = E - \mu N} \qquad \begin{matrix} \downarrow & \downarrow \\ \hat{K} = \text{Hermodyn. pot. op.} & = \hat{H} - \mu \hat{N} \end{matrix} \qquad \begin{matrix} \text{c-numbers} \\ \text{operators} \end{matrix} \qquad (9b)$$

Bardeen, Cooper, and Schrieffer ("BCS") start from a model g.s. $|\phi_0^{BCS}\rangle$ which is based on Cooper's model:

the BCS g.s. contains "Cooper pairs" of electrons with opposite momenta $(\vec{k}, -\vec{k})$, i.e. pair momentum $\vec{P} = 0$, and opposite spins (reduces "Pauli repulsion" of pairs):

$$|\phi_0^{BCS}\rangle = \prod_{k=1}^{\infty} (u_k + v_k \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow}) |0\rangle \qquad (10)$$

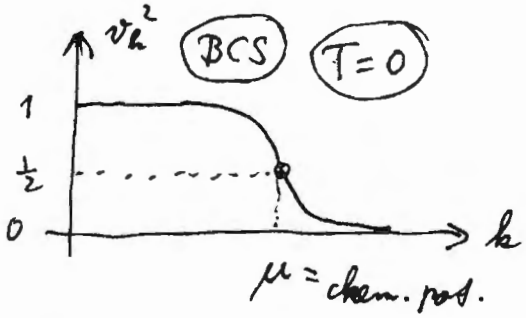
FW, p. 337

u_k, v_k: prob. amplitudes; $\hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow}$: "Cooper pair"; $|0\rangle$: vacuum (no particles)

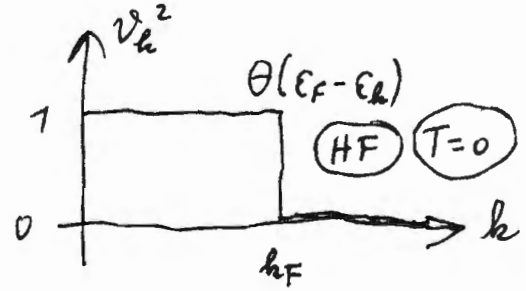
From the normal. condition $\langle \phi_0^{BCS} | \phi_0^{BCS} \rangle = 1$ one finds

$$u_k^2 + v_k^2 = 1 \qquad (11)$$

i.e. u_k^2 is the prob. that the s.p. level $\vec{k}$ is unfilled, and v_k^2 is the prob. that it is filled with a Cooper pair. We will see later that the BCS theory predicts:



i.e. there is no longer a sharp Fermi surface (particles are scattered by residual int. into unoccupied states above μ, even at $T=0$).



compare to HF g.s.

It turns out that because of approximations to the g.s., the particle # is no longer conserved in the BCS theory, in fact one finds for the particle # fluctuation, see FW, problem 10.6, p. 337:

$$\delta(N^2) = \frac{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2}{\langle \hat{N} \rangle^2} = \frac{\sum_k (u_k v_k)^2}{\left(\sum_k v_k^2\right)^2} \neq 0 \qquad (12)$$

where $\langle \hat{N} \rangle = \langle \phi_0^{BCS} | \hat{N} | \phi_0^{BCS} \rangle = \langle \phi_0^{BCS} | \sum_{k,\lambda} \hat{a}^+_{k\lambda} \hat{a}_{k\lambda} | \phi_0^{BCS} \rangle$

and

$$\langle \hat{N}^2 \rangle = \langle \phi_0^{BCS} | \hat{N} \cdot \hat{N} | \phi_0^{BCS} \rangle = \langle \phi_0^{BCS} | \sum_{\substack{k,k' \\ \lambda,\lambda'}} \hat{a}^+_{k\lambda} \hat{a}_{k\lambda} \hat{a}^+_{k'\lambda'} \hat{a}_{k'\lambda'} | \phi_0^{BCS} \rangle$$

The best one can do is "particle number conservation on average", i.e. one requires that

$$\boxed{\langle \phi_0^{BCS} | \hat{N} | \phi_0^{BCS} \rangle \doteq^{!} N} \qquad (13)$$

(N ↑ actual particle #)

The thermodyn. pot. at zero temp. is therefore given by

$$\Omega(T=0, V, \mu) = E - \mu N \iff$$

$$\boxed{\langle \phi_0^{BCS} | \hat{K} | \phi_0^{BCS} \rangle = \langle \phi_0^{BCS} | \hat{H} - \mu \hat{N} | \phi_0^{BCS} \rangle} \qquad (14)$$

Bardeen, Cooper, and Schrieffer (1957) used a variational approach (like in HF theory) to obtain u_k, v_k, energy gap, and

g.s. energy. One varies the thermodyn. pot. with respect to the quantities u_k, v_k which determine the BCS g.s. structure:

$$\delta \Big|_{u_k, v_k} \langle \phi_0^{BCS} | \hat{K} | \phi_0^{BCS} \rangle \stackrel{!}{=} 0 \qquad \hat{K} = \hat{H} - \mu \hat{N}$$

with $(u_k^2 + v_k^2 = 1)$

$\rightarrow$ result: u_k, v_k, gap Δ_k, $E_{g.s.}^{BCS}$ (15)

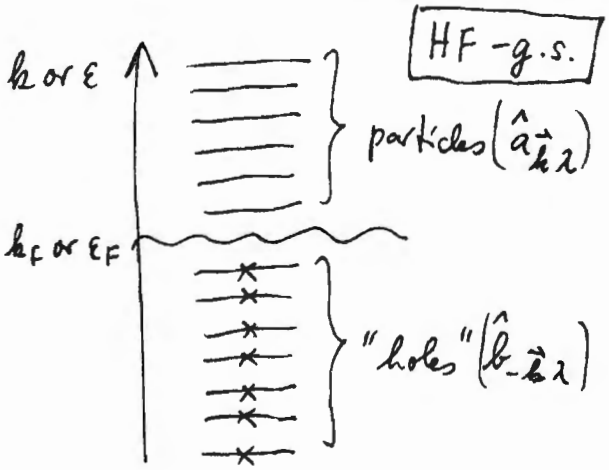
where $\hat{K} = \hat{H} - \mu \hat{N}$ has the structure

$$\hat{K} = \sum_{k,\lambda} (\varepsilon_k^0 - \mu)\, \hat{a}^+_{k\lambda} \hat{a}_{k\lambda} + \hat{V}^{(2)}_{eff,\,el\text{-}ph}$$

(ε_k^0: HF s.p. energies; μ: chem. pot.; $\hat{V}^{(2)}_{eff,\,el\text{-}ph}$: eq. (8)) (16)

Instead of following the original BCS approach, we now follow Bogoliubov's idea (1958) to solve the problem by a canonical "quasiparticle" transformation. These quasiparticles are generalized particle-hole transformations as we will show now.

Review: p-h transf. in HF formalism



See lecture notes ch. 3, p. 2-3:
Canonical transf. from original operators to p-h operators

$$\hat{c}_i \rightarrow (\hat{a}_i, \hat{b}_i)$$

$$|\phi_0^{HF}\rangle = \hat{c}_1^+ \hat{c}_2^+ \ldots \hat{c}_F^+ |0\rangle = \hat{b}_{-1} \hat{b}_{-2} \ldots \hat{b}_{-F} |0\rangle \qquad (17)$$

note: particle creation = hole destruction

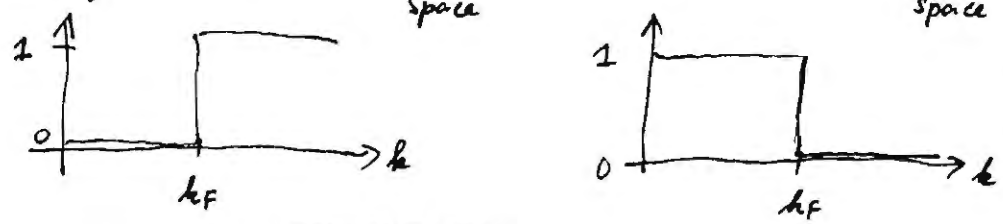
The HF-g.s. is the vacuum with respect to the "particle-hole quasiparticles":

$$\hat{a}_i \, |\phi_0^{HF}\rangle = 0 \,, \quad \hat{b}_i \, |\phi_0^{HF}\rangle = 0 \qquad \text{(FW 7.40)}$$

In the HF case, we used this "trivial" p-h quasiparticle transf (see FW eqns (7.34) and (56.8a)):

$$\hat{C}_{\vec{k}\uparrow} = \theta(k - k_F)\, \hat{a}_{\vec{k}\uparrow} + \theta(k_F - k)\, \hat{b}^{+}_{-\vec{k}\uparrow}$$

original operator — "particle" space — "hole" space

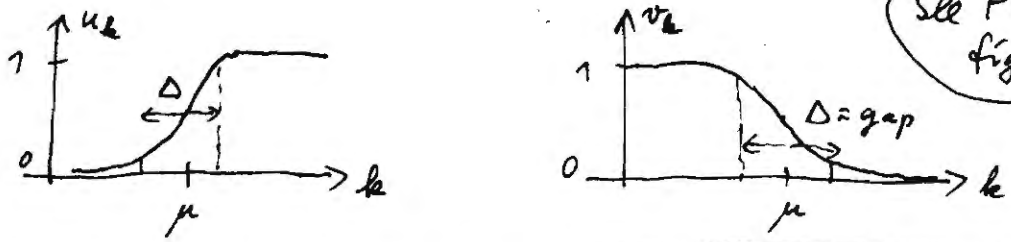


The Bogoliubov transf. is a generalization of this transf:

$$\hat{a}_{\vec{k}\uparrow} = u_k \, \hat{\alpha}_{\vec{k}} + v_k \, \hat{\beta}^{+}_{-\vec{k}}$$

original operator — "quasiparticle" space — "quasihole" space

FW 37.5a



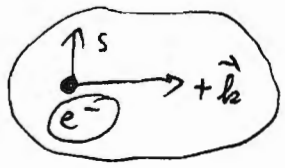
See FW fig. 37.1

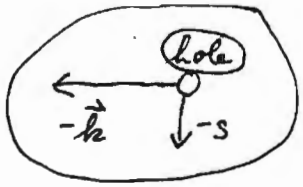
i.e. the occupation numbers are no longer 0 or 1 (step function) but represent a "smeared out" Fermi surface. The width of the occup. number distribution is given by the pairing gap Δ.

The inverse of the above transf. yields the quasiparticle operators $\hat{\alpha}_{\vec{k}}$ and $\hat{\beta}_{-\vec{k}}$:

$$\hat{\alpha}^{+}_{\vec{k}} = u_k \, \hat{a}^{+}_{\vec{k}\uparrow} - v_k \, \hat{a}_{-\vec{k}\downarrow} \qquad \text{(FW 37.1)}$$

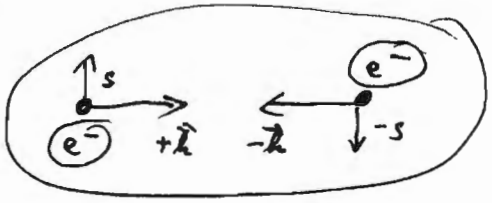
$\Rightarrow$

quasiparticle $= u_k \cdot$ 

$- v_k \cdot$ 

So, the quasiparticle is a linear superposition of particles and holes with prob. amplitudes u_k and $(-v_k)$.

Note, the quasiparticle is related to, but not identical with the Cooper pair given by

Cooper pair $= \hat{a}^{+}_{\vec{k}\uparrow} \hat{a}^{+}_{-\vec{k}\downarrow} =$ 

Note that the quasiparticles always appear as superpositions of the original state $|k\rangle$ and the time-reversed state $|\bar{k}\rangle$

$$|k\rangle = |+\vec{k},\uparrow\rangle \Rightarrow |\bar{k}\rangle = \hat{T}|k\rangle = \hat{T}|+\vec{k},\uparrow\rangle = |-\vec{k},\downarrow\rangle$$

($\hat{T}$: time-reversal op.)

simple "classical" reasoning: under $\hat{T}$ we have $\vec{r} \to \vec{r}$, $t \to -t$

$\Rightarrow \vec{p} = m\frac{d\vec{r}}{dt} \xrightarrow{\hat{T}} m\left(-\frac{d\vec{r}}{dt}\right) = -\vec{p}$ and $\vec{L} = \vec{r}\times\vec{p} \xrightarrow[\hat{T}]{} \vec{r}\times(-\vec{p}) = -\vec{L}$,

and the spin has to transform in the same way as the orbital $\vec{L}$.

We define

$$\hat{\beta}^{+}_{-k} \overset{\text{def}}{=} \hat{\alpha}^{+}_{\bar{k}}$$

↙ Ring & Schuck, p. 234

resulting in

$$\hat{\beta}^{+}_{-k} = \hat{\alpha}^{+}_{\bar{k}} = \hat{T}(\hat{\alpha}^{+}_{k}) = \text{see above} = \hat{T}\left(u_k \hat{a}^{+}_{\vec{k}\uparrow} - v_k \hat{a}_{-\vec{k}\downarrow}\right) =$$

$$= u_{\bar{k}} \, \hat{a}^{+}_{-\vec{k}\downarrow} - v_{\bar{k}} \, \hat{a}_{\vec{k}\uparrow}$$

Choosing the usual "BCS phase convention"

$$u_k = v_k = \text{real} \quad \text{and}$$

$$u_{\bar{k}} = u_k > 0\,, \quad v_{\bar{k}} = -v_k < 0$$

one obtains for the "quasihole creation" operator

$$\hat{\beta}^+_{-k} = u_k\, \hat{a}^+_{-\vec{k}\downarrow} + v_k\, \hat{a}_{\vec{k}\uparrow} \qquad \text{(FW 37.1)}$$

One straightforwardly proves that the transf.

$$\left(\hat{a}_{\vec{k}\uparrow}\,,\ \hat{a}_{-\vec{k}\downarrow}\right) \longrightarrow \left(\hat{\alpha}_k\,,\ \hat{\beta}_{k'}\right)$$

is canonical, i.e. same anticomm. relations

$$\left\{\hat{\alpha}_{\vec{k}}\,,\ \hat{\alpha}^+_{\vec{k}'}\right\} = \delta_{\vec{k},\vec{k}'} = \left\{\hat{\beta}_{\vec{k}}\,,\ \hat{\beta}^+_{\vec{k}'}\right\}$$

$$\text{all other } \{\,,\} = 0 \qquad \text{(FW 37.2)}$$

provided that $u_k^2 + v_k^2 = 1$ (37.4)

In analogy to the HF g.s., Bogolinbov assumes the BCS-gs to be the quasiparticle vacuum with respect to the $\hat{\alpha}$'s, $\hat{\beta}$'s:

$$\hat{\alpha}_{\vec{k}}\,|\phi_0^{BCS}\rangle = 0 \quad \equiv \quad \hat{\alpha}_{\vec{k}}\,|\tilde{0}\rangle = 0 \qquad \text{FW (37.8)}$$

$$\hat{\beta}_{\vec{k}}\,|\phi_0^{BCS}\rangle = 0 \quad \equiv \quad \hat{\beta}_{\vec{k}}\,|\tilde{0}\rangle = 0$$

($|\tilde{0}\rangle$ ← quasiparticle vacuum)

The (BCS)-gs can be constructed in analogy to HF case, eq.(

$$|\tilde{0}\rangle \equiv |\phi_0^{BCS}\rangle = \hat{\beta}_1\,\hat{\beta}_2 \cdots \hat{\beta}_\infty\,|0\rangle$$

($|0\rangle$ ← vacuum)

(see Ring & Schuck p. 249)

One can prove (difficult!) that this state is identical to the original BCS state vector

$$|\phi_0^{BCS}\rangle = \prod_{k=1}^{\infty} (u_k + v_k \hat{a}^+_{\vec{k}\uparrow} \hat{a}^+_{-\vec{k}\downarrow})|0\rangle$$

($|0\rangle$: vacuum)

Our goal is to compute

$$\Omega(T=0) = E - \mu N = \langle \phi_0^{BCS}| \underbrace{\hat{H} - \mu \hat{N}}_{=\hat{K}} |\phi_0^{BCS}\rangle = \langle \tilde{0}| \underbrace{\hat{H} - \mu \hat{N}}_{=\hat{K}} |\tilde{0}\rangle \quad (11)$$

Inserting the structure of $\hat{H}$, we find from eqns (16) and (8):

$$\hat{K} = \hat{H} - \mu \hat{N} = \sum_{\vec{k},\lambda} (\underbrace{\varepsilon_k^0}_{\text{HF s.p. energies}} - \underbrace{\mu}_{\text{chem. pot.}}) \hat{a}^+_{\vec{k}\lambda} \hat{a}_{\vec{k}\lambda} - \frac{1}{2} \sum_{\substack{\vec{k}_1 \ldots \vec{k}_4 \\ \lambda_1 \ldots \lambda_4}} \delta_{\lambda_1\lambda_3} \delta_{\lambda_2\lambda_4} \cdot \langle \vec{k}_1 \vec{k}_2 | v | \vec{k}_3 \vec{k}_4 \rangle \hat{a}^+_{\vec{k}_1\lambda_1} \hat{a}^+_{\vec{k}_2\lambda_2} \hat{a}_{\vec{k}_4\lambda_4} \hat{a}_{\vec{k}_3\lambda_3} \quad (12)$$

The calculation of $\langle \tilde{0}|\hat{K}|\tilde{0}\rangle$ is greatly simplified by using Wick's theorem, because all normal-ordered exp. values

$$\langle \tilde{0}| N_{\hat{\alpha},\hat{\beta}}(\ldots) |\tilde{0}\rangle = 0.$$

($|\tilde{0}\rangle$: quasiparticle vacuum)

Look at the first term in $\hat{K}$ above; it involves the calculation of

$$\hat{T}_1 = \sum_{\vec{k},\lambda} (\varepsilon_k^0 - \mu) \hat{a}^+_{\vec{k}\lambda} \hat{a}_{\vec{k}\lambda} = \sum_{\vec{k}} (\varepsilon_k^0 - \mu) [\hat{a}^+_{\vec{k}\uparrow} \hat{a}_{\vec{k}\uparrow} + \hat{a}^+_{\vec{k}\downarrow} \hat{a}_{\vec{k}\downarrow}]$$

Since we sum over <u>all</u> $\vec{k}$ (+ and −), we can change $\vec{k} \to -\vec{k}$ in the second part:

$$\hat{T}_1 = \sum_{\vec{k}} (\varepsilon^0_{\vec{k}} - \mu)\left[\hat{a}^+_{\vec{k}\uparrow}\hat{a}_{\vec{k}\uparrow} + \hat{a}^+_{-\vec{k}\downarrow}\hat{a}_{-\vec{k}\downarrow}\right] \qquad (3)$$

Using Wick's theorem for operators of the form

$$\hat{a}^+_1\hat{a}_2 = \mathcal{T}(\hat{a}^+_1\hat{a}_2) = \mathcal{N}(\hat{a}^+_1\hat{a}_2) + \hat{a}^+_1\hat{a}_2 \qquad (4)$$

$\hat{a}^+_1\hat{a}_2$: time-indep. $\mathcal{T}$: time-ordering $\mathcal{N}$: normal-ordering $\hat{a}^+_1\hat{a}_2$: contraction

where $\mathcal{T}$, $\mathcal{N}$ and $\llcorner\lrcorner$ are <u>with respect to the quasiparticles $\hat{\alpha}, \hat{\beta}$</u> which annihilate $|\tilde{0}\rangle$.

We found earlier (see notes ch. 4, p. 11):

$$\hat{a}^+_1\hat{a}_2 = \langle\tilde{0}|\hat{a}^+_1\hat{a}_2|\tilde{0}\rangle = \langle\phi_0^{BCS}|\hat{a}^+_1\hat{a}_2|\tilde{0}\rangle.$$

Let us evaluate the contraction

$$\hat{a}^+_{\vec{k}\uparrow}\hat{a}_{\vec{k}'\uparrow} = \langle\tilde{0}|\hat{a}^+_{\vec{k}\uparrow}\hat{a}_{\vec{k}'\uparrow}|\tilde{0}\rangle = \text{insert (37.5)} =$$

$$= \langle\tilde{0}|\left(u_k\hat{\alpha}^+_{\vec{k}} + v_k\hat{\beta}_{-\vec{k}}\right)\left(u_{k'}\hat{\alpha}_{\vec{k}'} + v_{k'}\hat{\beta}^+_{-\vec{k}'}\right)|\tilde{0}\rangle =$$

$$= \langle\tilde{0}|\, u_k u_{k'}\hat{\alpha}^+_{\vec{k}}\hat{\alpha}_{\vec{k}'} + v_k u_{k'}\hat{\beta}_{-\vec{k}}\hat{\alpha}_{\vec{k}'} + u_k v_{k'}\hat{\alpha}^+_{\vec{k}}\hat{\beta}^+_{-\vec{k}'} +$$

($\hat{\alpha}_{\vec{k}'}|\tilde{0}\rangle = 0$, $\hat{\beta}_{-\vec{k}}|\tilde{0}\rangle = 0$, $\langle\tilde{0}|\hat{\alpha}^+_{\vec{k}} = 0$)

$$+ v_k v_{k'}\hat{\beta}_{-\vec{k}}\hat{\beta}^+_{-\vec{k}'}|\tilde{0}\rangle =$$

$$= v_k v_{k'}\langle\tilde{0}|\underbrace{\hat{\beta}_{-\vec{k}}\hat{\beta}^+_{-\vec{k}'}}_{=\left(\delta_{\vec{k}\vec{k}'} - \hat{\beta}^+_{-\vec{k}'}\hat{\beta}_{-\vec{k}}\right)}|\tilde{0}\rangle = v_k v_{k'}\delta_{\vec{k}\vec{k}'} = v_k^2\delta_{\vec{k},\vec{k}'}$$

($\hat{\beta}_{-\vec{k}}|\tilde{0}\rangle = 0$)

i.e.

$$\boxed{\hat{a}^+_{\vec{k}\uparrow}\hat{a}_{\vec{k}'\uparrow} = v_k^2\delta_{\vec{k},\vec{k}'}} \qquad (5)$$

(see FW 37.9)

Similarly one finds the other contraction

$$\boxed{\hat{a}^{+}_{-\vec{k}\downarrow}\,\hat{a}_{-\vec{k}'\downarrow} = v_k^2\,\delta_{\vec{k}\vec{k}'}\ (\text{same})} \qquad (6) \qquad (\text{see FW } 37.10)$$

Inserting (4), (5), and (6) into (3) we obtain for the first term in the Hamiltonian

$$\boxed{\hat{T}_1 = \sum_{\vec{k}} (\varepsilon^0_k - \mu)\left[N\left(\hat{a}^{+}_{\vec{k}\uparrow}\,\hat{a}_{\vec{k}\uparrow}\right) + N\left(\hat{a}^{+}_{-\vec{k}\downarrow}\,\hat{a}_{-\vec{k}\downarrow}\right) + 2v_k^2\right]} \qquad (7)$$

The N-products with respect to $\hat{\alpha}, \hat{\beta}$ can be calculated, if desired, see FW (37.11).

The potential operator term $\hat{V} = \hat{V}_{\text{eq, el-ph}}$ in (2) involves terms of the form (see lecture notes, ch. 4, p. 12):

$$\hat{a}_1^{+}\hat{a}_2^{+}\hat{a}_4\hat{a}_3 = \underline{\text{Wick}} = T\left(a_1^{+}a_2^{+}a_4a_3\right) =$$

$$N\left(a_1^{+}a_2^{+}a_4a_3\right) + N\left(\underline{a_1^{+}a_2^{+}}\,a_4a_3\right) + N\left(a_1^{+}\underline{a_2^{+}a_4}\,a_3\right) + N\left(\underline{a_1^{+}a_2^{+}a_4}\,a_3\right) +$$

$$+ N\left(\underline{a_1^{+}a_2^{+}a_4}\,a_3\right) + N\left(a_1^{+}\underline{a_2^{+}a_4}\,a_3\right) + N\left(a_1^{+}a_2^{+}\underline{a_4a_3}\right) +$$

$$+ N\left(a_1^{+}a_2^{+}\underline{a_4a_3}\right) + N\left(\underline{a_1^{+}a_2^{+}}\,\underline{a_4a_3}\right) + N\left(\underline{a_1^{+}a_2^{+}a_4}\,a_3\right) +$$

$$+ N\left(\underline{a_1^{+}a_2^{+}a_4}\,a_3\right) \qquad (8)$$

One encounters a few new contractions in the pot. term, in particular the pairing tensor amplitudes ($\rightarrow$ homework) of the form

$$F_k^{(1)} = \hat{a}^+_{\vec{k}\uparrow}\,\hat{a}^+_{-\vec{k}\downarrow} = \langle \tilde{0}|\ldots|\tilde{0}\rangle$$

$$F_k^{(2)} = \hat{a}_{-\vec{k}\downarrow}\,\hat{a}_{\vec{k}\uparrow} = \langle \tilde{0}|\ldots|\tilde{0}\rangle$$

A lengthy and messy, but straightforward calculation yields for the thermodynamic potential operator

$$\boxed{\hat{K} = U + \hat{H}_1 + \hat{H}_2 + N(\hat{V})} \qquad \text{FW 37.20}$$

with (FW 37.26)

$$U = \text{"c-numbers"} = 2\sum_{\vec{k}} \xi_k v_k^2 + \sum_{\vec{k},\vec{k}'} v_k^2 v_{k'}^2 \langle \vec{k}\vec{k}'|\bar{V}|\vec{k}\vec{k}'\rangle - \sum_{\vec{k}} u_k v_k \Delta_k$$

$$\hat{H}_1 = \sum_{\vec{k}} \underbrace{\left(\hat{\alpha}^+_{\vec{k}}\hat{\alpha}_{\vec{k}} + \hat{\beta}^+_{-\vec{k}}\hat{\beta}_{-\vec{k}}\right)}_{\text{quasipart. number operators}} \left[(u_k^2 - v_k^2)\xi_k + 2u_k v_k \Delta_k\right]$$

$$\hat{H}_2 = \sum_{\vec{k}} \underbrace{\left(\hat{\alpha}^+_{\vec{k}}\hat{\beta}^+_{-\vec{k}} + \hat{\beta}_{-\vec{k}}\hat{\alpha}_{\vec{k}}\right)}_{\substack{\text{create/destroy } \underline{\text{two}} \\ \text{quasiparticles}}} \left[2u_k v_k \xi_k - (u_k^2 - v_k^2)\Delta_k\right]$$

$N(\hat{V})$ = normal-ordered product of $\hat{V}$, no contractions, contains up to $\underline{\underline{4}}$ quasiparticle creation/annih. operators

In these terms, we have used the foll. abbreviations

$$\xi_{\vec{k}} = (\epsilon_{\vec{k}} - \mu)$$

s.p. energy with respect to chemical potential μ

$$\epsilon_{\vec{k}} = \epsilon^0_{\vec{k}} - \sum_{\vec{k}'} \langle \vec{k}\vec{k}' | \bar{V} | \vec{k}\vec{k}' \rangle v_{\vec{k}'}^2$$

$\epsilon_{\vec{k}}$: s.p. energy; $\epsilon^0_{\vec{k}}$: HF; the sum: modification due to electron-phonon attractive pot.

$$\Delta_{\vec{k}} = \sum_{\vec{k}'} \langle \vec{k}-\vec{k} | V | \vec{k}'-\vec{k}' \rangle u_{\vec{k}'} v_{\vec{k}'}$$

energy gap

So far, we have transformed $\hat{K}$ in terms of quasiparticle operators $\hat{\alpha}, \hat{\beta}$. The canonical transf. has not yet been specified (except for the constraint $u_k^2 + v_k^2 = 1$).

We will choose u_k and v_k such that

$$\hat{H}_2 \equiv 0 \Rightarrow 2u_k v_k \xi_k - (u_k^2 - v_k^2)\Delta_k = 0 \quad (10a)$$

$\Rightarrow u_k, v_k$

Below we will see that this condition can always be fulfilled.

The thermodynamic potential operator becomes

$$\hat{K} \to U + \hat{H}_4 + N(\hat{V}) \quad (10b)$$

Note that eqns (10a,b) are still exact. We have made no approximations to $\hat{K}$.

From the normal. condition $u_k^2 + v_k^2 = 1$ and from eq. (10a) one finds after some algebra (FW, p. 330/331):

$$\boxed{v_k^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right)} \quad \text{with} \quad \boxed{E_k \overset{\text{def}}{=} \sqrt{\xi_k^2 + \Delta_k^2}} \qquad (18a)$$

We examine now the "energy gap" Δ_k defined on p. 118:

$$\Delta_k = \sum_{\vec{k}'} \langle \vec{k} - \vec{k} \,|\, v \,|\, \vec{k}' - \vec{k}' \rangle \, u_{k'} v_{k'} . \qquad (18b)$$

Solving eq. (10a) for $u_{k'} v_{k'}$ results in

$$2 u_{k'} v_{k'} \xi_{k'} = (u_{k'}^2 - v_{k'}^2)\, \Delta_{k'}$$

$$u_{k'} v_{k'} = \frac{1}{2} \frac{(u_{k'}^2 - v_{k'}^2)}{\xi_{k'}} \Delta_{k'}, \quad \text{insert } u_{k'}^2 = 1 - v_{k'}^2$$

$$u_{k'} v_{k'} = \frac{1}{2} \frac{(1 - 2 v_{k'}^2)}{\xi_{k'}} \Delta_{k'} \overset{(18a)}{=} \frac{1}{2} \frac{1 - (1 - \xi_{k'}/E_{k'})}{\xi_{k'}} \Delta_{k'}$$

$$u_{k'} v_{k'} = \frac{1}{2} \frac{1}{E_{k'}} \Delta_{k'} \overset{(18a)}{=} \frac{1}{2} \frac{\Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}} \qquad (18c)$$

Inserting (18c) into (18b) results in the "BCS gap equation"

$$\boxed{\Delta_k = \frac{1}{2} \sum_{\vec{k}'} \langle \vec{k} - \vec{k} \,|\, v \,|\, \vec{k}' - \vec{k}' \rangle \frac{\Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}}} \qquad (19)$$

Note that if we replace $\sum_{\vec{k}'} \to \int d^3k'$, (19) becomes a non-linear integral equation which is difficult to solve:

$$\boxed{\Delta_k = \frac{1}{2} \int d^3k' \ldots \frac{\Delta_{k'}}{\sqrt{\ldots + \Delta_{k'}^2}}}$$

Using the relations for u_k and v_k, we can simplify $\hat{H}_1$:

$$\hat{H}_1 = \sum_{\vec{k}} \left(\hat{\alpha}^+_{\vec{k}} \hat{\alpha}_{\vec{k}} + \hat{\beta}^+_{-\vec{k}} \hat{\beta}_{-\vec{k}} \right) \left[\underbrace{(u_k^2 - v_k^2)}_{= \xi_k / E_k} \xi_k + \underbrace{2 u_k v_k}_{= \Delta_k / E_k} \Delta_k \right]$$

$$\hat{H}_1 = \sum_{\vec{k}} \left(\hat{\alpha}^+_{\vec{k}} \hat{\alpha}_{\vec{k}} + \hat{\beta}^+_{-\vec{k}} \hat{\beta}_{-\vec{k}} \right) \frac{\xi_k^2 + \Delta_k^2}{E_k} = \frac{E_k^2}{E_k} = E_k$$

(20)

$$\hat{H}_1 = \sum_{\vec{k}} E_k \left(\hat{\alpha}^+_{\vec{k}} \hat{\alpha}_{\vec{k}} + \underbrace{\hat{\beta}^+_{-\vec{k}} \hat{\beta}_{-\vec{k}}}_{\text{sum over all } \vec{k}: \; -\vec{k} \to +\vec{k}} \right) \Rightarrow \boxed{\hat{H}_1 = \sum_{\vec{k}} E_k \left(\underbrace{\hat{\alpha}^+_{\vec{k}} \hat{\alpha}_{\vec{k}}}_{\hat{n}^{(\alpha)}_{\vec{k}}} + \underbrace{\hat{\beta}^+_{\vec{k}} \hat{\beta}_{\vec{k}}}_{\hat{n}^{(\beta)}_{\vec{k}}} \right)}$$

quasiparticle number operators $\hat{n}^{(\alpha)}_{\vec{k}}$ $\hat{n}^{(\beta)}_{\vec{k}}$

The thermodynamic potential operator $\hat{K}$ can be written in the form

$$\hat{K} = \hat{K}_0 + N(\hat{V}) \quad \text{with} \quad \hat{K}_0 = U + \hat{H}_1 = U + \sum_{\vec{k}} E_k \left(\hat{n}^{(\alpha)}_{\vec{k}} + \hat{n}^{(\beta)}_{\vec{k}} \right)$$

(21)

Let's first examine the exp. value of the $\hat{K}_0$ operator in the state $|\phi\rangle$:

Thermodyn. potential

$$\Omega_0(T=0) = \langle \phi | \hat{K}_0 | \phi \rangle = U + \sum_{\vec{k}} E_k \langle \phi | \hat{n}^{(\alpha)}_{\vec{k}} + \hat{n}^{(\beta)}_{\vec{k}} | \phi \rangle$$

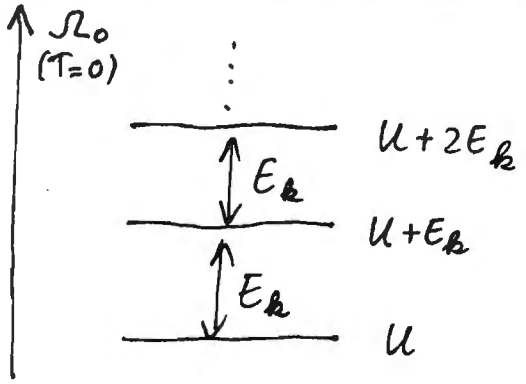
(22)

From this expression we see that the minimum value of the thermodyn. potential is obtained in the quasiparticle vacuum state $|\tilde{0}\rangle \equiv |\phi_0^{BCS}\rangle$ defined by

$$\left.\begin{aligned} \hat{\alpha}_{\vec{k}} |\tilde{0}\rangle = 0 \quad &\Rightarrow \hat{n}^{(\alpha)} |\tilde{0}\rangle = 0 \\ \hat{\beta}_{\vec{k}} |\tilde{0}\rangle = 0 \quad &\Rightarrow \hat{n}^{(\beta)} |\tilde{0}\rangle = 0 \end{aligned}\right\} \quad (23)$$

In the state $|\phi\rangle = |\tilde{0}\rangle$ we have $\Omega_0(T=0) = U$.

The excited states are 1-quasiparticle, 2-quasiparticle, ... excitations. Each of these quasiparticles carries an excitation energy $E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta_k^2} \geq \Delta_k$, hence the name <u>energy gap</u> for <u>Δ_k</u>:



<u>quasiparticle state</u>

$|\phi\rangle = |\tilde{2}\rangle = \hat{\alpha}^+_{\vec{k}} \hat{\beta}^+_{\vec{k}} |\tilde{0}\rangle$

$|\phi\rangle = |\tilde{1}\rangle = \hat{\alpha}^+_{\vec{k}} |\tilde{0}\rangle$ or $\hat{\beta}^+_{\vec{k}} |\tilde{0}\rangle$

$|\phi\rangle = |\tilde{0}\rangle \equiv |\phi_0^{BCS}\rangle$

The normal-ordered product $N(\hat{V})$ in eq. (21) describes quasiparticle interactions, i.e. $\langle \phi | N(\hat{V}) | \phi \rangle$; however it vanishes exactly in the BCS-groundstate (because of Wick's theorem):

$$\langle \tilde{0} | N(\hat{V}) | \tilde{0} \rangle = 0 \quad \underline{\text{(exact!)}}$$

Hence, for excited states $|\phi\rangle \neq |\tilde{0}\rangle$, this term may either be neglected or treated in perturbation theory. If we neglect it, we obtain

$$\hat{K} \approx \hat{K}_0 = U + \hat{H}_1 \quad \text{with}$$

$$U = \text{c-number} = 2 \sum_{\vec{k}} \xi_k v_k^2 + \sum_{\vec{k},\vec{k}'} v_k^2 v_{k'}^2 \langle \vec{k}\,\vec{k}' | \bar{v} | \vec{k}\,\vec{k}' \rangle - \sum_{\vec{k}} u_k v_k \Delta_k$$

$$\hat{H}_1 = \sum_{\vec{k}} E_k \left(\hat{n}^{(\alpha)}_{\vec{k}} + \hat{n}^{(\beta)}_{\vec{k}} \right) \qquad (24)$$

<u>What has Bogolinbov transf. accomplished?</u> The thermodyn. pot. <u>$\hat{K}$</u> of the system is a <u>constant plus a diagonal one-body operator</u>, provided that the interaction among the quasi-particles

$\hat{N}(\hat{V})$ is negligible. It vanishes exactly in the BCS-g.s. (= quasiparticle vacuum $|\tilde{0}\rangle$) and is usually small.
The effective Hamiltonian $\hat{K}_0$ is a 1-body operator in terms of the quasiparticles $(\hat{\alpha}_k, \hat{\beta}_k)$. It contains the attractive electron-phonon equivalent potential "on average" via the matrix elements $\langle \vec{k}\,\vec{k}' | \tilde{v} | \vec{k}\,\vec{k}' \rangle$.

Discussion of BCS gap equation (19)

From eq. (19), p. 119,

$$\Delta_k = \frac{1}{2} \sum_{\vec{k}'} \langle \vec{k}-\vec{k} | v | \vec{k}'-\vec{k}' \rangle \frac{\Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}}$$

(Δ_k: gap; v: el-ph.; $\Delta_{k'}$: gap)

we notice immediately that there is always a "trivial solution"

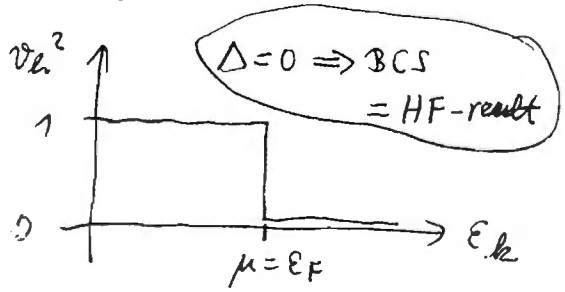
$$\Delta_k = 0 \,, \quad \forall k$$ (i.e. vanishing pairing gap Δ)

Inserting this into eq. (18a) on p. 119:

$$v_k^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta_k^2}}\right) = \frac{1}{2}\left(1 - \frac{\xi_k}{|\xi_k|}\right) = \frac{1}{2}\left(1 - \frac{(\varepsilon_k - \mu)}{|\varepsilon_k - \mu|}\right) =$$

($\sqrt{\xi_k^2 + \Delta_k^2} \to 0$; $\frac{(\varepsilon_k-\mu)}{|\varepsilon_k-\mu|} = \pm 1$)

$$= \Theta(\mu - \varepsilon_k)$$, i.e. we obtain the HF g.s. distribution:



We see that in this case ($\Delta = 0$), the chemical potential $\mu \equiv \varepsilon_F$!

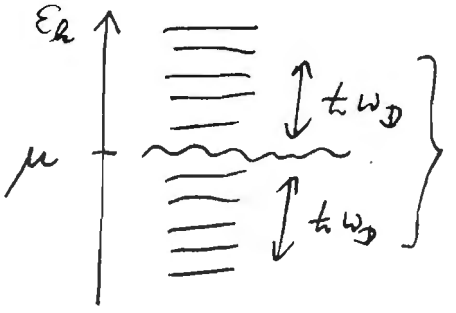
In general, the BCS-gap eq. needs to be solved numerically for a given 2-body residual interaction v.

However, one can solve the eq. analytically if one assumes an attractive interaction with constant matrix elements near the Fermi surface, i.e.

$$\langle \vec{k}-\vec{k} | v | \vec{k}'-\vec{k}' \rangle \approx \frac{g}{L^3} \; \theta(\hbar\omega_D - |\varepsilon_k - \mu|)\,\theta(\hbar\omega_D - |\varepsilon_{k'} - \mu|)$$

(v: el-ph.; g: ↓ constant strength; $\hbar\omega_D$: ↓ Debye-energy = mean phonon energy)

This means:



θ-functions contributes in this energy region

Inserting the above approx. for $\langle .. | v | .. \rangle$ into the gap eq. one finds

$$\Delta_k = \frac{1}{2} \frac{g}{L^3} \theta(\hbar\omega_D - |\varepsilon_k - \mu|) \sum_{\vec{k}'} \frac{\Delta_{k'}\, \theta(\hbar\omega_D - |\varepsilon_{k'} - \mu|)}{\sqrt{|\varepsilon_{k'} - \mu|^2 + \Delta_{k'}^2}} \qquad (*)$$

with the solution (see FW):

$$\boxed{\Delta_k = \underset{\text{↑ const.}}{\Delta} \cdot \theta(\hbar\omega_D - |\varepsilon_k - \mu|)} \qquad (**)$$

and the constant gap Δ is determined from [insert $(**)$ into $(*)$]:

$$1 = \frac{g}{2L^3} \sum_k \theta(\hbar\omega_D - |\varepsilon_k - \mu|) \frac{1}{\sqrt{\Delta^2 + (\varepsilon_k - \mu)^2}}$$

Replacing $\sum_k \to \int d^3k$, one finds (FW 37.49):

Supercond. state

$$\Delta = 2(\hbar\omega_D)\exp\left(-\frac{1}{N(0)g}\right)$$

$N(0)$ = density of states near Fermi surface ($\uparrow$ or $\downarrow$)

- Δ: gap parameter
- $\hbar\omega_D$: Debey energy
- g: constant strength of electron-phonon int.

Like in Cooper's model we see that Δ is a highly nonanalytic fctn of the pairing strength g, and a perturb. theory treatment would not work because

$$\Delta = 2(\hbar\omega_D)\left[1 + \left(-\frac{1}{N(0)g}\right) + \frac{1}{2}\left(-\frac{1}{N(0)g}\right)^2 + \frac{1}{3!}\left(-\frac{1}{N(0)g}\right)^3 + \dots\right]$$

and with $N(0)g \approx 0.2 - 0.3$ (FW p. 333) we get, using $1/N(0)g \approx 4$:

$$\Delta = 2(\hbar\omega_D)\left[1 - 4 + 8 - 10.7 + \dots\right],$$

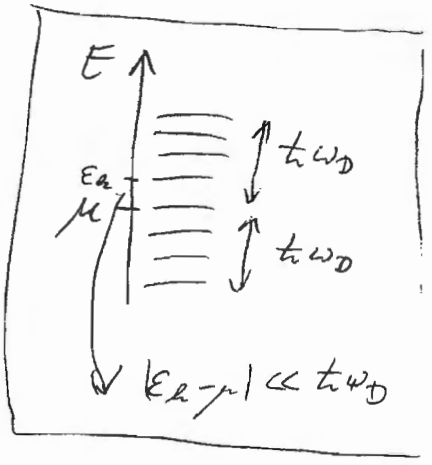
whereas $\Delta_{exact} = 2(\hbar\omega_D)\, e^{-4} = 2(\hbar\omega_D) \times 0.018$

The occupation prob. v_k^2 in supercond. state

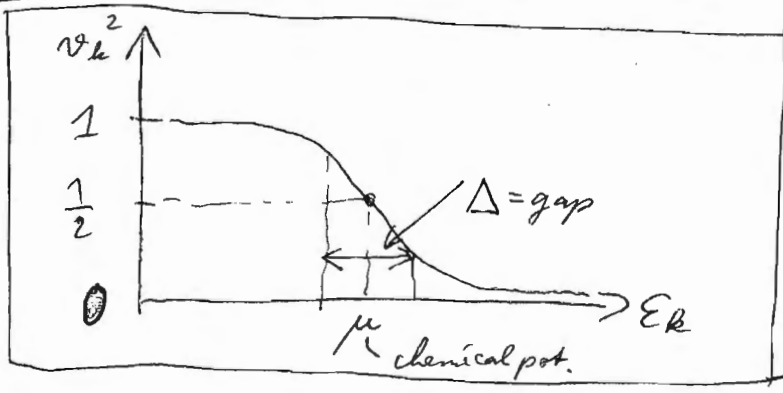
From the expression (18) for v_k^2,

$$v_k^2 = \frac{1}{2}\left(1 - \frac{(\varepsilon_k - \mu)}{\sqrt{(\varepsilon_k - \mu)^2 + \Delta_k^2}}\right)$$

we find in the limit of a constant pairing gap $\Delta_k = \Delta \times \theta(\hbar\omega_D - |\varepsilon_k - \mu|) \to \Delta$, which is true for $|\varepsilon_k - \mu| \ll \hbar\omega_D$:



$$v_k^2 = \frac{1}{2}\left(1 - \frac{(\varepsilon_k - \mu)}{\sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}}\right)$$



see FW1 fig. 37.1

We see that the Fermi energy is no longer sharply defined; it has been smeared out in energy over a range corresponding to the Debey energy $\hbar\omega_D$.

Energy difference: Supercond. g.s. – normal g.s.

nomenclature: $E_s \hat{=}$ supercond. g.s. energy
$E_n \hat{=}$ normal g.s. energy

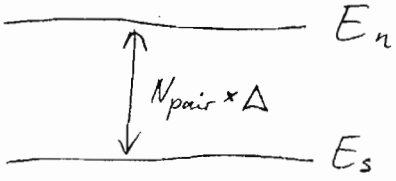
We have seen that the thermod. pot. at $T=0$ is for the g.s.

$$\Omega(T=0) \overset{\text{p.114}}{=} E_{gs} - \mu N = U \quad \Rightarrow E_{gs} = U + \mu N$$
(see eq. (22))

Hence, we can express the energy difference as follows:

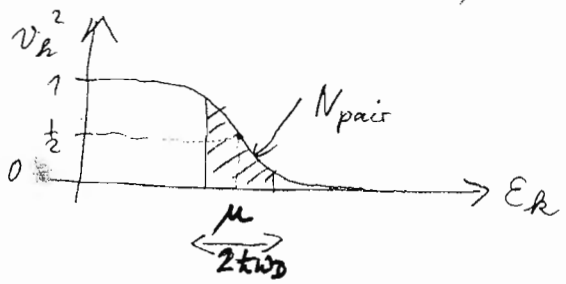
$$E_s - E_n = (U_s - U_n) + \underbrace{(\mu_s - \mu_n)N}_{\approx 0 \text{ (little change in Fermi energy)}} \approx U_s - U_n$$

Inserting the values for v_k^2 etc. for the superconducting and normal state into eq. (24) for U, we find after some considerable algebra the following simple expression:



$$\boxed{E_s - E_n = -(N_{pair} \times \Delta) < 0}$$

where Δ is the binding energy of one Cooper pair and N_{pair} is the number of Cooper pairs within an energy shell of thickness $\hbar\omega_D$ around the "Fermi surface" μ:



A few remarks about BCS theory at finite T

Ref: Fetter & Walecka §51 (uses Green's functions)

One finds the following interesting results:

pairing gap as function of T

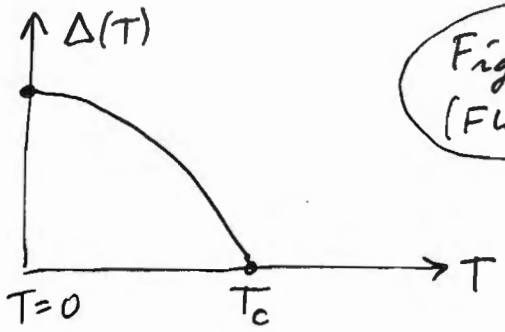


Fig. 51.1 (FW p. 449)

relation: pairing gap Δ (T=0) and T_c

BCS theory at finite T predicts (FW, eq. 51.43)

$$k_B T_c \approx 1.13\, \hbar\omega_D \exp\left[-\frac{1}{N(0)\cdot g}\right] \qquad (1)$$

Recall expression for Δ (T=0), p. 124:

$$\Delta(T=0) = 2\,\hbar\omega_D \exp\left[-\frac{1}{N(0)\cdot g}\right] \qquad (2)$$

Take ratio of (1) and (2):

$$\frac{\Delta\,(T=0)}{k_B T_c} = \frac{2}{1.13} \approx 1.76 \Rightarrow$$

$$\Delta\,(T=0) \approx 1.76\,(k_B T_c)$$

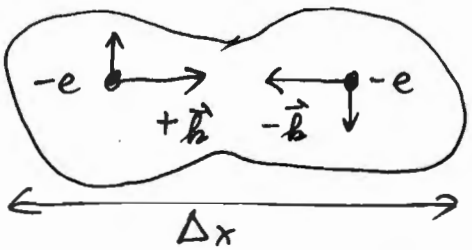
Δ → gap; T_c → critical temp.

FW, eq. (51.44)

What causes superconductivity?

Rigorous theory: Fetter & Walecka, § 52

Phenomenology: Eisberg & Resnick, Quantum Physics, 2nd ed., p. 487 – 488



The Cooper pair looks like a particle with charge $q = -2e$ and total momentum $\vec{P} = \vec{0}$. The pair is weakly bound and, hence, its spatial extent Δx is large $\sim 10^4$ Å.

metal at $T=0$

no ext. field

metal at $T=0$

$\vec{E} \neq 0$

$\dot{\vec{P}} = \vec{F} = -2e\vec{E}$

$\vec{P}(t) = (-2e\vec{E})t$

If we add an ext. $\vec{E}$-field, all Cooper pairs have exactly the same pair momentum $\vec{P}(t)$ → highly correlated motion ↛ no "random-motion scattering with lattice imperfections ↛ zero electrical resistance.

Pairing in atomic nuclei (brief discussion)

→ see PowerPoint slides on Website!