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

TOPICS


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

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

Electron-phonon interaction, Feynman diagram \(\rightarrow\) 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-Tc superconductivity

Introduction

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

In 1911, Kammerlingh-Onnes observed 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-Tc superconductivity is observed in many metals, but not in all of them:

\[
\begin{array}{c}
\text{Resistivity} \\
S \left(10^{12} \text{m}^{-1}\right)
\end{array}
\]

\begin{array}{c}
\text{tin} \\
\text{silver}
\end{array}

In 1933, Heissel & Blochendfeld observed the exclusion of magnetic

\[ H \neq 0, \quad T > T_c \]

\[ H \neq 0, \quad T < T_c \]
This phenomenon is directly related to the first one: an ext. magn. field. It does not penetrate the interior of a supercond. substance because the "superconductivity" electrons inside the material produce an additional countaracting 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":

\[ T_c = \frac{\text{const}}{\sqrt{M}} \]

\[ M = \text{isotopic mass of solid} \]
\[ \text{[crystals made from different isotopes of same element]} \]

Exp. suggest that lattice ions play a role in low-Tc 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 occurred in 1956 when Cooper used the existence of the tiny electron-phonon interaction (attractive) to explain the basis of superconductivity in terms of "Cooper pairs".

Note: weakly bound pair, size = 10 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:

\[ \phi_{BCS} = \prod_{\mathbf{k}} (n_{\mathbf{k}} + v_{\mathbf{k}} \hat{a}_{\mathbf{k}}^+ \hat{a}_{\mathbf{k}}^-) |0\rangle \]

where \( n_{\mathbf{k}} \) (\( v_{\mathbf{k}} \)) is the prob. that the s.p. level \( \mathbf{k} \) is unfilled (filled) with a Cooper pair. BCS theory predicts a pairing gap

\[ \Delta = \text{energy gap} \]

"normal" g.s. \[ E_0 \]

\[ \Delta \]

"supercond. g.s. \[ E \]

\[ \frac{E_F}{\Delta} = 10^4 \]

Also, Cooper pair size (lattice spacing) \[ = 10^4 \]

Conduction e\(^-\) density (normal g.s.) \[ = \frac{10^{22}}{\text{cm}^3} \]

Cooper pair density (supercond. g.s.) \[ = \frac{10^{18}}{\text{cm}^3} = 10^4 \]

For mercury:

\[ \Delta(T=0) = 1.1 \times 10^{-3} \text{ eV} \]

Compare to \( E_F = 10 \text{ eV} \).

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

\[ \text{YBa}_2\text{Cu}_3\text{O}_7 \]
Lattice vibrations $\rightarrow$ acoustic sound waves $\rightarrow$ quantize $\rightarrow$ 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 $\delta n^+$ 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 $N$ of the ionic cores, these waves have low frequency $f$ and hence large wavelengths $\lambda = \frac{c}{f}$:

$\lambda$ (acoustic sound waves) $\gg$ lattice spacing $d$

The compressional wave has many characteristics of an
particle (momentum $\hbar k$, energy $E_k$,...) and is therefore often called a "quasi-particle". These quasiparticles are called phonons (Greek: phoné = sound). Similar to real particles, the phonons may "collide" with each other and with conduction electrons.

Because $\lambda \gg d$, the acoustic phonons cannot resolve the metallic lattice structure: as before, it may be replaced by a uniform positive background density, $\rho_0$. 

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 $\delta \rho^+$:

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

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

$$\delta \rho^+(\vec{r}, t) = \rho_0 (-\nabla \cdot \delta \vec{u}(\vec{r}, t)) \quad (FW, 44.5)$$

which also satisfies the above wave eq.

$$\left[ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right] \delta \vec{u}(\vec{r}, t) = 0 \quad (FW, 44.6)$$
The speed of sound, $c$, of the longitudinal waves is determined by the bulk modulus $B$:

$$c = \sqrt{\frac{B}{\rho_0}}$$

with

$$B = -V \frac{\partial P}{\partial V} \text{ pressure entropy} \text{ const}$$

Using the interacting Fermi gas model discussed earlier, one calculates

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

which agrees with exp. within a factor of 2.

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

$$\mathbf{k} = \frac{2\pi}{L} \mathbf{h}, \quad \mathbf{h} = (h_x, h_y, h_z), \quad h_i = \text{integer}$$

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

$$\mathbf{a}(\mathbf{r},t) = \sum \mathbf{e}_k \left[ A_k e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} + \text{H.c.} \right]$$

$\text{H.c.} \quad \text{(long wave!)}$

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

$$L = S d^3r L$$

Lagrange function

$$H = S d^3r H$$

Hamilton function 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 \( \dd{\vec{x}} \). One finds

\[
L (\dd{\vec{x}}, \dd{\frac{\dd{\vec{x}}}{\dd{t}}}, \dd{\frac{\dd{\vec{x}}}{\dd{x}}} : \dd{\dd{\vec{x}}}) = \frac{1}{2} s_0^+ \left( \dd{\frac{\dd{\vec{x}}}{\dd{t}}} \right)^2 - \frac{1}{2} B \left( \nabla \cdot \dd{\vec{x}} \right)^2
\]

(FW 4.4.11b)

The kinetic energy of the continuous mechanical system is described by the density \( s_0^+ \) and the displacement velocity \( \dd{\vec{x}} \), and the bulk modulus \( B \) of the material determines its potential energy.

The displacement vector \( \dd{\vec{x}}(\dd{\vec{r}}, t) \) may be viewed as a classical field (similar to \( E(\dd{\vec{r}}, t) \) in Eq 17).

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

\[
\dd{\vec{p}}(\dd{\vec{r}}, t) = \dd{\frac{\dd{L}}{\dd{\dd{\frac{\dd{\vec{x}}}{\dd{t}}}}} = s_0^+ \dd{\frac{\dd{\vec{x}}}{\dd{t}}} \]

(FW 4.4.12)

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

\[
\mathcal{H}(\dd{\vec{x}}, \dd{\vec{p}}) = \frac{\dd{\vec{p}}^2(\dd{\vec{r}}, t)}{2 s_0^+} + \frac{1}{2} B \left( \nabla \cdot \dd{\vec{x}}(\dd{\vec{r}}, t) \right)^2
\]

The Cartesian components \( \dd{x}_i \) and \( \dd{p}_i \) (\( i = 1, 2, 3 \)) satisfy the following Poisson bracket relations:
\[
\begin{align*}
[\hat{d}_i(\vec{r}, t), \hat{d}_j(\vec{r}', t)]_{\text{PB}} &= 0 = [\hat{\pi}_i(\vec{r}, t), \hat{\pi}_j(\vec{r}', t)]_{\text{PB}}, \\
[\hat{d}_i(\vec{r}, t), \hat{\pi}_j(\vec{r}', t)]_{\text{PB}} &= \delta_{ij} \delta(\vec{r} - \vec{r}')
\end{align*}
\]

**Field quantization → phonons**

Replace the Poisson brackets for the classical quantities by commutators for corresponding operators:

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

\[= \frac{1}{i\hbar} [\hat{d}_i, \hat{\pi}_j]_{\text{QM}}\]

Hence:

\[
\begin{array}{c}
\hat{\pi}(\vec{r}, t), \hat{d}(\vec{r}, t) \\
\text{classical fields}
\end{array} \rightarrow \begin{array}{c}
\hat{\pi}(\vec{r}, t), \hat{d}(\vec{r}, t) \\
\text{quantum fields}
\end{array}
\]

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

\[
\begin{align*}
A^c_{\vec{k}} &\rightarrow \hat{A}^c_{\vec{k}} = \frac{1}{i} \sqrt{\frac{\hbar}{2 \omega_k L^3}} \hat{c}_{\vec{k}}^c \\
A^{\star c}_{\vec{k}} &\rightarrow \hat{A}^{\star c}_{\vec{k}} = i \sqrt{\frac{\hbar}{2 \omega_k L^3}} \hat{c}^c_{\vec{k}}
\end{align*}
\]

\[FW (44.15)\]

\text{rule: the commutation relations for the boson operators are}

\[
[\hat{c}_{\vec{k}}^c, \hat{c}^c_{\vec{k}'}] = 0 = [\hat{c}^c_{\vec{k}}, \hat{c}^c_{\vec{k}'}], \text{ but } [\hat{c}_{\vec{k}}^c, \hat{c}^c_{\vec{k}'}] = \delta_{\vec{k} \vec{k}'}\]
These follow from the comm. relations for \( \hat{\Pi}(\vec{r},t) \) and \\
\( \hat{\tau}(\vec{r},t) \).

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

One finds for the energy of the lattice vibrational waves

\[
\hat{H}_{\text{lattice}} = \hat{H}_{\text{phonon}} = S d^3 r \hat{\Pi} = \sum_{\vec{k}} \hbar \omega_0 \left( \hat{c}^{+}_{\vec{k}} \hat{c}_{\vec{k}} + \frac{1}{2} \right) = \text{phonon field operator}
\]

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: Fettes \& Walecka, p. 393 - 395

One may wonder how realistic our free phonon model is? The approximation used is uniform background, no lattice ions. In a uniform medium, there is no upper limit for wave freq. \( \omega \). But for a real crystal, there is a max. frequency \( \omega_{\text{max}} = \omega_D \) (= 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 \(k_{\text{max}}\):

\[
3N = \sum_{k} \theta(k_{\text{max}} - k) \Rightarrow \frac{L^3}{(2\pi)^3} \int d^3 k \theta(k_{\text{max}} - k)
\]

\[
\Rightarrow 3N = \frac{L^3}{8\pi^3} \int_0^{k_{\text{max}}} k^2 dk \left( \int d^3 k \right) = \frac{L^3}{2\pi^2} \frac{1}{3} k_{\text{max}}^3
\]

Use \(k_{\text{max}} = \frac{\Omega_{\text{max}}}{c} = \frac{\omega_D}{c} \Rightarrow 3N = \frac{L^3}{2\pi^2} \frac{1}{3} \left( \frac{\omega_D}{c} \right)^3.
\]

Solve for \(\omega_D\):

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

\[
\omega_D = \frac{3}{2} \sqrt{18\pi^2 n_0^3} \cdot c \quad (n_0 = \frac{N}{c^3} = \text{number density})
\]

\(n_0 = \frac{N}{c^3} = \text{number density})

with \(c = \sqrt{\frac{B}{M_{\text{io}}}} \quad (B = \text{bulk modulus}, M = \text{ionic mass})
\]

Speed of sound

The Debye freq. \(\omega_D\) defines, in turn, the Debye temperature \(\Theta\) which represents the thermal energy

\[
\hbar \beta \cdot \Theta = \frac{1}{2} \omega_D
\]

\((\hbar = \text{Boltzmann constant})
\)

associated with the max. frequency \(\omega_D\) of lattice vibrations.

The Debye freq. \(\omega_D\) will be of crucial importance for the electron-phonon interaction to be discussed later.
It will provide a frequency cut-off:

\[ \theta (\omega - \omega_d) \]

\[ 0 \to \omega_d \]

Using \( \omega_d \) and \( \theta \) for real crystals in connection with thermodynamics and stat. mech. of the free phonon system, one can explain the specific heat \( C_V \) of metallic crystals:

\[ C_V \overset{\text{def}}{=} (\frac{\partial E}{\partial T})_V \quad \text{spec. heat} \]

\[ E = -T^2 \frac{\partial}{\partial T} \left( \frac{\theta_d}{T} \right)_V \quad \text{energy} \]

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

From these 3 equations one can compute the specific heat in terms of the Debye temp. \( \theta_d \):

\[ C_V = 9 N k_B \left( \frac{\theta_d}{\Theta} \right)^3 \int_0^{\Theta/T} \frac{e^{u \theta_d}}{(e^u - 1)^2} \, du \quad \text{(FW 44.29)} \]

With the limiting cases

| \( C_V = 3 N k_B = \text{const} \) \( (T \to \infty) \) | classical equipartition of energy |
| \( C_V = \frac{12 \pi^4}{5} N k_B \left( \frac{\Theta}{\Theta} \right)^3 \) \( (T \to 0) \) | "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 (+te) were approximated by a uniform background charge $g_0^+$. The Hamiltonian has the structure (Born-Oppenheimer approximation ions at rest):

$$H_{\text{el gas}} = T_{\text{e-}} + V^{(2)}_{\text{e-e}} + V^{(1)}_{\text{e-ion}} + V^{\text{self-energy}}_{\text{ion-ion}}. \quad (1)$$

Let us consider the Coulomb interaction terms involving the ions:

$$V^{(1)}_{\text{e-ion}} = \int d^3r \int d^3r' \frac{e^-(r) \phi_{\text{ion}}(r')}{|r-r'|}. \quad (2)$$

$$V^{\text{self-energy}}_{\text{ion-ion}} = \frac{1}{2} \int d^3r \int d^3r' \frac{\phi_{\text{ion}}(r) \phi_{\text{ion}}(r')}{|r-r'|}. \quad (3)$$

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

$$\phi_{\text{ion}}(r) \rightarrow g_0^+ + \delta g^+(r,t). \quad (4)$$

Insert (4) into (2): uniform background density fluctuation.
\[ V_{\text{ion}} = \int d^3r \int d^3r' \frac{\rho_e(\vec{r}) [1 - \rho_0(\vec{r})]}{|\vec{r} - \vec{r}'|} \]

\[ V_{\text{ion}} = \int d^3r \int d^3r' \frac{\rho_e(\vec{r}) \rho_0^+(\vec{r})}{|\vec{r} - \vec{r}'|} + \int d^3r \int d^3r' \frac{\rho_e(\vec{r}) \delta_g^+(\vec{r})}{|\vec{r} - \vec{r}'|}. \]

\[ = H^0 \text{ e- \& background} = He-phonon \quad \text{(5)} \]

The first term is already included in He-gas, and the second term represents the important electron-phonon interaction.

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

\[ V_{\text{ion}} = \frac{1}{2} \int d^3r \int d^3r' \frac{[\rho^+(\vec{r}) + \delta^{g+}(\vec{r})][\rho^+(\vec{r}) + \delta^{g+}(\vec{r})]}{|\vec{r} - \vec{r}'|} = \]

\[ = \frac{1}{2} \int d^3r \int d^3r' \left( \frac{(\rho_0^+)^2}{|\vec{r} - \vec{r}'|} \right) \quad (= H^0, \text{ included in}) \]

\[ = \frac{1}{2} \int d^3r \int d^3r' \left( \frac{\delta^{g+}(\vec{r}) \delta^{g+}(\vec{r}')}{|\vec{r} - \vec{r}'|} \right) \quad \rightarrow \text{neglect terms} \]

\[ \frac{1}{2} \int d^3r \int d^3r' \left( \frac{\delta^{g^+}(\vec{r}) \delta^{g^+}(\vec{r}')}{|\vec{r} - \vec{r}'|} \right) \quad \rightarrow \text{vanishes, see below} \]

\[ \text{(6)} \]

Here, the 2nd term vanishes. To show this we use the def. of the displacement vector, p.t.:

\[ \delta^{g^+}(\vec{r}) = p_0^+ (- \nabla \cdot \vec{a}(\vec{r})) \]

\[ \nabla \cdot \text{2nd term} \propto \int d^3r \delta^{g^+}(\vec{r}) \propto \int d^3r \nabla \cdot \vec{a} = \text{(divergence)} = \]

\[ = \int \nabla \cdot (\vec{a} \cdot d\vec{r}) = 0 \quad \text{(no flow at \infty distance)}. \]
The Coulomb energies involving the ions have the form (eqs 5 and 6):

\[ V_{e-\text{ion}} + V_{e-\text{ion}} \approx H_{e^{-}} + H_{e^{-}\text{phonon}} + H_{e^{-}} \]  

and the quantized lattice vibrations, Hphonon, we arrive at the model Hamiltonian of the system in the form

\[ H_{\text{system}} \approx (T_{e^{-}} + V_{e-e^{-}} + H_{e^{-}} + H_{e^{-}\text{phonon}}) + H_{\text{phonon}} + H_{e^{-}\text{phonon}} \]

\[ = H_{\text{Fermi gas}} \]  

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

\[ H_{\text{system}} = H_{\text{Fermi gas}} + H_{\text{phonon}} + H_{\text{el phonon}} \]

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

\[ H_{\text{Fermi gas}} = \sum \frac{\hbar^2}{2m} \hat{a}_i^+ \hat{a}_i \Rightarrow \text{kin. energy of electrons} \]

\[ + \frac{e^2}{2V} \sum \sum \frac{4\pi}{\hbar^2} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_j \hat{a}_i \]

\[ \Rightarrow \text{electron-electron int. for finite mom. transi} \]

We can depict \( V_{e-e^{-}}^{(2)}(\hat{a}_i \neq 0) \) by a "Feynman-like" graph.
The free phonon Hamiltonian was given in this chapter, p. 11:

\[ \hat{H}_{\text{phonon}} = \sum_{q \leq \omega_0} \hbar \omega_q \left( \hat{c}^+_q \hat{c}_q + \frac{1}{2} \right) \]  \hspace{1cm} (11)

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

\[ \hat{H}_{\text{el-ph}} = \int d^3x \int d^3x' \frac{\hat{\Psi}(\vec{r}) \hat{\Psi}^+(\vec{r}')}{|\vec{r} - \vec{r}'|} \]  \hspace{1cm} (12)

We evaluate the electron density operator from the field creation/annihilation operators:

\[ \hat{\Psi}(\vec{r}) = (-e) \hat{\Psi}^+(\vec{r}) \hat{\Psi}(\vec{r}) = (-e)^2 \left( \sum_{k_1} \hat{a}^+_k \chi_{k_1} \frac{1}{\sqrt{V}} e^{-i \vec{k}_1 \cdot \vec{r}} \chi_{k_1} \right) \]

\[ \left( \sum_{k_2} \hat{a}^+_k \chi_{k_2} \frac{1}{\sqrt{V}} e^{i \vec{k}_2 \cdot \vec{r}} \chi_{k_2} \right) = \]

\[ \frac{(-e)^2}{V} \sum_{k_1, k_2} \sum_{\lambda_1, \lambda_2} \hat{a}^+_k \chi_{k_1} \hat{a}_{k_2} \chi_{k_2} e^{i (\vec{k}_2 - \vec{k}_1) \cdot \vec{r}} \chi_{k_1}^{\lambda_1} \chi_{k_2}^{\lambda_2} \]

Relabel \( \lambda_1 = \lambda \Rightarrow \)

\[ \hat{\Psi}(\vec{r}) = \frac{(-e)^2}{V} \sum_{k_1, k_2} \sum_{\lambda} \hat{a}^+_k \chi_{k_1} \hat{a}_{k_2} \chi_{k_2} e^{i (\vec{k}_2 - \vec{k}_1) \cdot \vec{r}} \chi_{k_1}^{\lambda} \chi_{k_2}^{\lambda} \]  \hspace{1cm} (13)
Now we calculate density fluctuation operator $\delta \hat{d}^+ (\vec{r})$ in (11); from notes on p.7

$$\delta \hat{d}^+ (\vec{r}) = \rho^+ \left( - \nabla \cdot \delta \vec{d} (\vec{r}) \right) = \left( \frac{ie}{\hbar} \right) \left( - \nabla \cdot \delta \vec{d} (\vec{r}) \right)$$

Ion charge number density

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

$$\hat{d} (\vec{r}) = \sum \frac{\hbar}{2 \nu} \gamma \sqrt{\frac{\hbar}{2 \epsilon_0 + 2 \nu e V}} \left[ -i \hat{c}_\beta e^{i \beta \cdot \vec{r}} + i \hat{c}_\beta^+ e^{-i \beta \cdot \vec{r}} \right] \Theta \left( \frac{\nu d}{c} - \frac{1}{c} \right)$$

From the def. of the divergence

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

we obtain for the $x$-component

$$\frac{\partial \hat{d}_x}{\partial x} = \sum \frac{\hbar}{\hbar} \gamma \sqrt{\frac{\hbar}{2 \epsilon_0 + 2 \nu e V}} \left[ -i \hat{c}_\beta \frac{2}{\partial x} (e^{i \beta \cdot \vec{r}}) + i \hat{c}_\beta^+ \frac{2}{\partial x} (e^{-i \beta \cdot \vec{r}}) \right] \Theta \left( \frac{\nu d}{c} - \frac{1}{c} \right)$$

The partial derivatives are

$$\frac{\partial}{\partial x} (e^{\pm i \beta \cdot \vec{r}}) = e^{\pm i \beta \cdot \vec{r}} (\pm i \beta_x)$$

Insert above:

$$\frac{\partial \hat{d}_x}{\partial x} = \sum \frac{\hbar}{\hbar} \gamma \sqrt{\frac{\hbar}{2 \epsilon_0 + 2 \nu e V}} \left[ -i \hat{c}_\beta e^{i \beta \cdot \vec{r}} (\pm i \beta_x) + i \hat{c}_\beta^+ e^{-i \beta \cdot \vec{r}} \right] (-i \beta_x) \Theta \left( \frac{\nu d}{c} - \frac{1}{c} \right)$$

Combine indelimited terms
\[
\frac{\partial \hat{\mathbf{d}}}{\partial x} = \sum \frac{h \varepsilon}{\hbar} \sqrt{\frac{\hbar}{8\pi e^2 \omega V}} \left[ \hat{c}^+ \frac{\hat{q}}{\hbar} e^{i \hat{q} \cdot \hat{r}} + \hat{c} \frac{\hat{q}}{\hbar} e^{-i \hat{q} \cdot \hat{r}} \right] \theta \left( \frac{\omega_0}{c} - \epsilon \right)
\]

Similarly, we calculate the y- and z-components of \( \nabla \cdot \hat{d} \), we get factors \((h y^2 + \hbar z^2)\) such that

\[
\frac{h \varepsilon \frac{y^2}{\hbar}}{\hbar} = \frac{h \varepsilon \frac{y^2}{\hbar} + h \varepsilon \frac{z^2}{\hbar}}{\hbar} = \frac{h \varepsilon}{\hbar} = \hbar \Rightarrow
\]

\[
\nabla \cdot \hat{d} (\hat{r}) = \sum \frac{h \varepsilon}{\hbar} \sqrt{\frac{\hbar}{8\pi e^2 \omega V}} \left[ \hat{c}^+ \frac{\hat{q}_y}{\hbar} e^{i \hat{q}_y \cdot \hat{r}} + \hat{c} \frac{\hat{q}_y}{\hbar} e^{-i \hat{q}_y \cdot \hat{r}} \right] \theta \left( \frac{\omega_0}{c} - \epsilon \right)
\]

From eqns (14) and (16) we find, with \( \hat{r} \rightarrow \hat{r}' \) and \( \hat{\mathbf{q}} \rightarrow \hat{\mathbf{q}}' \):

\[
\partial_+ \hat{g}^+ (\hat{r}') = (-2 e \nu_0) \nabla \cdot \hat{d} (\hat{r}') = (-2 e \nu_0) \sum \frac{h \varepsilon}{\hbar} \sqrt{\frac{\hbar}{8\pi e^2 \omega V}} \left[ \hat{c}^+ \frac{\hat{q}_y}{\hbar} e^{i \hat{q}_y \cdot \hat{r}'} + \hat{c} \frac{\hat{q}_y}{\hbar} e^{-i \hat{q}_y \cdot \hat{r}'} \right] \theta \left( \frac{\omega_0}{c} - \epsilon \right)
\]

The underlined factors can be simplified as follows

\[
(-2 e \nu_0) \sqrt{\frac{\hbar q^2}{8\pi e^2 \omega V}} = (-2 e) \sqrt{\frac{\hbar_0^2 \frac{\varepsilon}{c^2} (\omega g / c)^2}{(M \varepsilon_0) 2 \omega V}} = (-2 e) \sqrt{\frac{\hbar_0 (\omega g / c)^2}{M \cdot 2 V}}
\]

which leads to

\[
\partial_+ \hat{g}^+ (\hat{r}') = (-\frac{2 e}{c}) \sqrt{\frac{\hbar_0}{M}} \sum \frac{\sqrt{2 \omega V}}{2} \left[ \hat{c}^+ \frac{\hat{q}_y}{\hbar} e^{i \hat{q}_y \cdot \hat{r}'} + \hat{c} \frac{\hat{q}_y}{\hbar} e^{-i \hat{q}_y \cdot \hat{r}'} \right] \theta \left( \frac{\omega_0}{c} - \epsilon \right)
\]

\[
\downarrow \text{density} \quad \downarrow \text{ionic mass} \quad \downarrow \text{phonon operator} \quad \downarrow \text{Debye cut-off}
\]

(17)
We insert eq. (17) for $\delta S^+_k(\vec{r}')$ and eq. (13) for $\delta E(\vec{r})$ into expression (16) for the electron-phonon int:

$$
\hat{H}_{el-ph} = \int d^3r \int d^3r' \frac{1}{|\vec{r} - \vec{r}'|} \delta E(\vec{r}) \delta S^+_k(\vec{r}') =
$$

$$
= \int d^3r \int d^3r' \frac{1}{|\vec{r} - \vec{r}'|} \left[ \left( -\frac{e}{\nu} \right) \sum_\lambda \sum_\alpha \frac{\alpha^{\dagger} \alpha^{\dagger}}{\hbar^2 \nu_\lambda} \right] e^{-i(\vec{q}_\lambda \vec{r} - \omega_\lambda t)}
$$

$$
\times \left( -\frac{2e}{c} \right) \sqrt{\frac{\hbar^2}{M}} \sum_{\lambda \nu} \sqrt{\frac{\hbar^2 \nu_\lambda}{2\nu}} \left[ \hat{c}_\lambda^\dagger e^{i\vec{q}_\lambda \cdot \vec{r}} + \hat{c}_\lambda e^{-i\vec{q}_\lambda \cdot \vec{r}} \right] \theta(\omega_\lambda - \omega_{\nu})
$$

We proceed now like in Chapter 3 (F.W. p.23) or my lecture note (ch.5 p.4) and introduce the new variables:

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

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

$$
\int d^3r \int d^3r' \frac{1}{|\vec{r} - \vec{r}'|} e^{i(\vec{q}_\lambda \cdot \vec{y} + \vec{q}_\nu \cdot \vec{x})} \frac{\sqrt{\hbar^2 \nu_\lambda}}{2\nu} \hat{c}_\lambda^\dagger 
$$

$$
\int d^3x \int d^3y \frac{1}{y} e^{i(\vec{q}_\lambda \cdot \vec{x} + \vec{q}_\nu \cdot \vec{y})} \frac{\sqrt{\hbar^2 \nu_\lambda}}{2\nu} \hat{c}_\lambda =
$$

$$
= \int d^3x \frac{e^{i(\vec{q}_\lambda \cdot \vec{x} + \vec{q}_\nu \cdot \vec{y})}}{\sqrt{2\nu}} \int d^3y \frac{1}{y} e^{i(\vec{q}_\lambda \cdot \vec{x} + \vec{q}_\nu \cdot \vec{y})} =
$$

$$
= V \frac{1}{\sqrt{2\nu}} \frac{1}{\sqrt{2\nu}} = F.T. of Conn. pot
$$

$$
= V \left[ \frac{4\pi}{\hbar^2} \right] \times \frac{4\pi}{\hbar^2}
$$

Inserting (*) into $\hat{H}_{el-ph}$ above and we obtain
\[ H_{el-ph} = \sum_{\hat{k}_1, \hat{k}_2} \sum_{\frac{q}{\Omega}} \left( -\frac{e}{\sqrt{\Omega}} \right) \left( -\frac{2e}{c} \right) \sqrt{\frac{n_0}{m}} \sqrt{\frac{\varepsilon_{\hat{k}_2}}{2V}} \frac{4\pi}{q^2} \sum_{\frac{q}{\Omega}} \right. \\
\left. \theta \left( \frac{\omega_q - \frac{q^2}{2m}}{c} \right) \right] \\
\left[ \delta_{\hat{k}_1, \hat{k}_2 + \frac{q}{\Omega}} \hat{a}^+_{\hat{k}_1, \lambda} \hat{a}^+_{\hat{k}_2, \lambda} \hat{c}_{\frac{q}{\Omega}}^+ + \delta_{\hat{k}_1, \hat{k}_2 + \frac{q}{\Omega}} \hat{a}_{\hat{k}_1, \lambda} \hat{a}_{\hat{k}_2, \lambda} \hat{c}_{\frac{q}{\Omega}}^+ \right] \\
H_{el-ph} = \left( \frac{2e^2}{c} \right) \sqrt{\frac{n_0}{m}} \sum_{\frac{q}{\Omega}} \sum_{\frac{q}{\Omega}} \theta \left( \frac{\omega_q - \frac{q^2}{2m}}{c} \right) \right] \\
\left[ \hat{a}^+_{\hat{k}_1, \lambda} \hat{a}_{\hat{k}_2, \lambda} \hat{c}_{\frac{q}{\Omega}}^+ \right] \\
\text{Finally, replacing the dummy indices } \hat{k}_1, \text{ and } \hat{k}_2 \text{ with } \hat{k}, \text{ we obtain [FW eq. 45.6b]:} \\
H_{el-ph} = \left( \frac{2e^2}{c} \right) \sqrt{\frac{n_0}{m}} \sum_{\frac{q}{\Omega}} \sum_{\frac{q}{\Omega}} \theta \left( \frac{\omega_q - \frac{q^2}{2m}}{c} \right) \right] \\
\left[ \hat{a}^+_{\hat{k}, \lambda} \hat{a}_{\hat{k}, \lambda} \hat{c}_{\frac{q}{\Omega}}^+ \right]

\text{Graphical representation of first term:}

<Diagram>

\[ FW, \text{ Fig. 45.1} \]
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 Coulomb takes the form

\[ U^C(q) = \frac{4\pi e^2}{q^2 + \mu^2} \frac{1}{k(q)} \]

modified Coul. int. \( U^C_0(q) \) 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:

\[
U^C(q) \rightarrow U^C_0(q) + \ldots \rightarrow \sum U^C_0(q)
\]

For details about ring diagram calculations, see FW, chap. 12.

In this approximation, one finds the following results in momentum space:

\[ U^C(r) = \frac{4\pi e^2}{q^2 + \mu^2} \]  

(for \( q \ll \mu \))

which, in coordinate space, is equivalent to a screened Coulomb int.
of range \( r_c = \frac{1}{\alpha} \).

\[ V_r^C(r) \sim \frac{e^{-\alpha r}}{r} \]

One can show that in the expression for Hc+-ph on p. 21, one can replace

\[ \sum \frac{4\pi e^2}{\frac{\Delta^2}{4}} = U_r^c(\frac{\Delta}{4}) \]

"bare"

\[ \sum \frac{4\pi e^2}{\frac{\Delta^2 + \mu^2}{4}} = U_r^c(\frac{\Delta}{4}) \]

"screened"

\[ \implies \sum \frac{4\pi e^2}{\mu^2} = U_r^c(\Delta = 0) \]

"screened" int. at zero momentum transfer

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

\[ \text{We apply now the last approx. to } H_{ec}^+\text{-ph on p. 21, replacing the expression} \]

\[ \frac{2e^2}{c} \sqrt{\frac{n_0}{M}} \sum_{\Delta} \frac{4\pi}{\Delta^2} \rightarrow \frac{2e^2}{c} \sqrt{\frac{n_0}{M}} \sum_{\Delta} \frac{4\pi}{\mu^2} \]

we obtain the coupling constant \( \gamma \) of the electron-photon int:

\[ H_{ec}^+ = \gamma \sum_{\Delta} \sum_{\frac{\alpha}{4}} \sqrt{\frac{\Delta^2}{2\nu}} \theta \left( \frac{\Delta}{2} \right) \left[ \hat{a}^+_{\Delta + \frac{\alpha}{4}, \nu} \hat{a}_{\Delta + \frac{\alpha}{4}, \nu} \phi \right] \]

\[ + \hat{a}^+_{\Delta + \frac{\alpha}{4}, \nu} \hat{a}_{\Delta + \frac{\alpha}{4}, \nu} \phi \]
This diagram theory yields the result (FW 45.8 and 45.9)

\[
\frac{4\pi}{\mu^2} = \frac{\pi^2 a_0}{k_F}
\]

\(a_0 = \text{Bohr radius}\)

and hence the electron-phonon coupling constant \(\gamma\) (see FW 45.12):

\[
\gamma = \frac{2e^2}{c} \sqrt{\frac{n_0}{M}} \frac{\pi^2 a_0}{k_F}
\]

Replacing the speed of sound \(c\) in terms of the bulk modulus \(B\) and ionic mass \(M\) and number density \(n_0\) we get

\[
\frac{1}{c} = \sqrt{\frac{1}{Bn_0}}
\]

resulting in

\[
\gamma = \frac{2e^2}{c} \frac{n_0 \pi^2 a_0}{k_F} \frac{1}{\sqrt{B}} = \frac{2}{\sqrt{B}} \frac{\pi^2 n_0}{M} \frac{a_0}{k_F} \frac{1}{\sqrt{B}}
\]

We see that the electron-phonon coupling constant \(\gamma\) depends on the density of the electron gas \(n_0\), the Fermi momentum \(k_F\) of the electrons, the charge \(e\) of the ionic cores and on the bulk modulus \(B\) of the metal.

Note that \(\gamma\) does not depend on the mass \(M\) of the ionic cores.

However, the phonon frequency spectrum depends on \(M\) because

\[
(\hbar \omega)_{\text{phon}} = \hbar k = c = \hbar k e \frac{1}{\sqrt{Bn_0}}
\]

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

Lit: FW, p. 399-401

One starts from the system Hamiltonian \(\hat{H} = \hat{H}_e + \hat{H}_p + \hat{H}_{ep}\)
To obtain the equivalent e⁻e⁻ interaction from the photon propagator, one follows the same steps as in QED:

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

**Feynman diagram for e⁻e⁻ scattering in QED**

Photon propagator: \( D^{(\phi)}_\mu = -i \frac{g_{\mu\nu}}{q^2} \sim \frac{1}{q^2} = -\frac{1}{q_0^2 + \frac{\vec{q}^2}{4}} \)

where \( q_0 \) is the 4-momentum transfer, given by \( q = p_1' - p_1 \).

In the static limit we have \( q_0 = 0 \) because

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

resulting in

\[
Dr(q_0 = 0, \frac{\vec{q}}{2}) \sim \frac{1}{\frac{\vec{q}^2}{4}}.
\]

**Photon-prop. in static limit \( q_0 = 0 \)**

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

\[
V_{\text{me}}(\vec{q}) \sim e^2 Dr(q_0 = 0, \frac{\vec{q}}{2}) \sim \frac{e^2}{\frac{\vec{q}^2}{4}}.
\]

The inverse F.T. yields

\[
V_{\text{me}}(\vec{r}) = \frac{e^2}{|\vec{r}|}.
\]
Stark e-e interaction for phonon exchange

Feynman diagram

\[ \text{phonon propagator:} \]
\[ D^0(q) = D^0(q_0, \vec{q}) = D^0(q_0, \omega_q = |\vec{q}| \cdot \text{c}) = \left\{ \begin{array}{l}
\frac{\hbar}{9c^2} \frac{\omega^2_q}{q^2 - (\omega^2_q - i\eta)^2} \theta(\omega_0 - \omega_q) \\
\text{FW(46.6)}
\end{array} \right. \]

Static limit \((q_0 = 0)\): \(D^0(q_0 = 0, \vec{q}) = -\frac{\hbar}{9c^2} \theta(\omega_0 - \omega_q) = -\frac{\hbar}{9c^2} \theta(\omega_0 - |\vec{q}| \cdot \text{c})\)

Fourier transform of equivalent electron-electron potential:
\[ U_0(\vec{q}) = \frac{\hbar^2}{c^2} D^0(q_0 = 0, \vec{q}) = -\frac{\hbar^2}{c^2} \theta(\omega_0 - |\vec{q}| \cdot \text{c}) \]

Inverse F.T. yields the equivalent 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 \(\theta(\cdot)\) for a moment. In this case we obtain:

\[ V_{eq}(\vec{r}) \approx (2\pi)^{-3} \int d^3q \ e^{i\vec{q} \cdot \vec{r}} (-\hbar^2) = -\hbar^2 \delta(\vec{r}) \]

(without Debye factor).

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

\[ V_{eq}(\vec{r}) = -\frac{\hbar^2}{\pi^2} f(\vec{r}) \]

\(f(\vec{r})\) = electron-phonon coupling constant, \(FW(45.12)\)
This discovery by Frohlich, 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 (-y^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 \( \Delta \) depends exponentially on the coupling constant \( y^2 \).

That's why perturbation theory fails miserably!!

Note: because of page remembering, the next page is page 107a.
Cooper's model assumptions (1956)

1) The model considers \( n \) electrons only which interact via a \( n \)-body potential \( \mathcal{V} \). \( \lambda \) = coupling constant. The electrons are treated as distinguishable particles because of opposite spin, using a simple product HF, i.e. no antisymmetry:

\[
H_0 = -\frac{\hbar^2}{2m} \nabla_x^2 \quad \text{and} \quad H_0 \varphi_n(\vec{x}_1, \vec{x}_2) = E_n \varphi_n(\vec{x}_1, \vec{x}_2)
\]

with

\[
\varphi_n(\vec{x}_1, \vec{x}_2) = \varphi_{n_1, n_2}(\vec{x}_1, \vec{x}_2) = \frac{e^{i\vec{k}_1 \cdot \vec{x}_1}}{L^{3/2}} \frac{e^{i\vec{k}_2 \cdot \vec{x}_2}}{L^{3/2}}
\]

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, \( \mathcal{V} \), 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

\[ \hat{P} = \hat{p}_1 + \hat{p}_2 = \text{total pair momentum} \]

\[ 2 \hat{b} = \hat{b}_1 - \hat{b}_2 = \text{rel. momentum of pair} \]

\[ \hat{R} = \frac{m_1 \hat{x}_1 + m_2 \hat{x}_2}{2m} = \frac{1}{2} (\hat{x}_1 + \hat{x}_2) = \text{c.m. coordinate} \]

\[ \hat{x} = \hat{x}_1 - \hat{x}_2 = \text{relative coordinate} \]

Inverting these relations, one finds

\[ \hat{b}_1 = \hat{b} + \frac{\hat{P}}{2}, \quad \hat{b}_2 = -\hat{b} + \frac{\hat{P}}{2}, \quad \hat{x}_1 = \hat{R} + \frac{\hat{x}}{2}, \quad \hat{x}_2 = \hat{R} - \frac{\hat{x}}{2} \]

Using these relations, we can express the W.F for 2 free electrons in the form

\[ \Psi_{n}(\hat{x}_1, \hat{x}_2) \equiv \Psi_{\hat{b}_1, \hat{b}_2}(\hat{x}_1, \hat{x}_2) \rightarrow \Psi_{\hat{b}, \hat{x}}(\hat{R}, \hat{x}) = \frac{e^{i(\hat{P} \cdot \hat{R} - \frac{\hat{x}^2}{2})}}{L^{3/2}} \]

The energy of the free pair can be written as

\[ E_{n=0} \equiv E_{\hat{b}_1, \hat{b}_2} = \frac{\hbar^2}{2m} (\hat{b}_1^2 + \hat{b}_2^2) = \frac{\hbar^2 \hat{b}^2}{m} + \frac{\hbar^2 \hat{p}^2}{4m} \]

Consider now 2 interacting electrons:

\[ \left[ H_0 + \lambda V(\hat{x}_1, \hat{x}_2) \right] \Psi(\hat{x}_1, \hat{x}_2) = E \Psi(\hat{x}_1, \hat{x}_2) \]

\[ \lambda \text{ is a coupling constant} \ (\lambda > 0 \text{ repulsive, } \lambda < 0 \text{ attractive}) \]

or in bra-ket notation:

\[ (\hat{H}_0 + \lambda \hat{V}) \left| \Psi \right\rangle = E \left| \Psi \right\rangle \]

\[ \Rightarrow (E - \hat{H}_0) \left| \Psi \right\rangle = \lambda \hat{V} \left| \Psi \right\rangle , \text{ take inverse of operator:} \]

\[ \left| \Psi \right\rangle = (E - \hat{H}_0)^{-1} \lambda \hat{V} \left| \Psi \right\rangle \]
Insert completeness relation

\[ \sum_n |\psi_n \rangle \langle \psi_n| = 1 \], where \( H_0 |\psi_n \rangle = E_n |\psi_n \rangle \]

\[ |\psi \rangle = \sum_n (E - H_0)^{-1} |\psi_n \rangle \langle \psi_n| A |\psi \rangle \]

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

\[ |\psi \rangle = |\psi_0 \rangle \langle \psi_0| A |\psi \rangle + \sum_{n \neq 0} |\psi_n \rangle \langle \psi_n| A |\psi \rangle \]  \hfill (1)

We show now that

\[ \langle \psi_0| A |\psi \rangle = E - E_0 \]  \hfill (2)

Proof:

\[ (H_0 + A)|\psi \rangle = E|\psi \rangle \]

\[ \langle \psi_0| (H_0 + A)|\psi \rangle = E \langle \psi_0| \psi \rangle \]

\[ E_0 \langle \psi_0| \psi \rangle + \langle \psi_0| A |\psi \rangle = E \langle \psi_0| \psi \rangle \]

\[ \Rightarrow \langle \psi_0| A |\psi \rangle = (E - E_0) \langle \psi_0| \psi \rangle = E - E_0 \quad \text{q.e.d.} \]

Note: \((2) \rightarrow (1) \) yields

\[ |\psi \rangle = |\psi_0 \rangle + \sum_{n \neq 0} \frac{|\psi_n \rangle \langle \psi_n| A |\psi \rangle}{E - E_n} \]  \hfill (3)

We separate now relative and total momenta for the

3 different types of WFs, \( |\psi_0 \rangle \), \( |\psi_{n \neq 0} \rangle \) and \( |\psi \rangle \):
\[ |\psi_n \rangle = |\Psi_{p_1, p_2} \rangle = |\Psi_{p_1, p_2}^{(E)}(x) \rangle = e^{i \frac{\vec{p} \cdot \vec{r}}{L}} \frac{e^{i \frac{\vec{p} \cdot \vec{x}}{L}}}{L^{3/2}} \]

\[ |\psi_{n+0} \rangle = |\Psi_{p_1, p_2}^{(E)}(x) \rangle = e^{i \frac{\vec{p} \cdot \vec{r}}{L}} \frac{e^{i \frac{\vec{p} \cdot \vec{x}}{L}}}{L^{3/2}} \]

\[ |\psi \rangle = \psi_E(x) = e^{i \frac{\vec{p} \cdot \vec{r}}{L}} \frac{\psi_{p_1}^{(E)}(x)}{L^{3/2}} \]

**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 ground state of the 2 interacting electrons. The notation \( \psi_{p_1, p_2}(x) \)

means that the interacting pair has energy \( E \) and that the interaction \( \lambda V \) it loses the total momentum \( \vec{p} \).

Now calculate the matrix element in (3):

\[ \langle \phi_{n+0} | \lambda V | \psi \rangle = \int d^3x \int d^3R \frac{e^{-i \frac{\vec{p} \cdot \vec{r}}{L}}}{L^3} \frac{e^{-i \frac{\vec{p} \cdot \vec{x}}{L}}}{L^3} \lambda V(x) \psi_{p_1, p_2}^{(E)}(x) \]

\[ \cdot e^{i \frac{\vec{p} \cdot \vec{r}}{L}} \frac{\psi_{p_1, p_2}^{(E)}(x)}{L^{3/2}} \]

\[ = \int d^3x \frac{e^{-i \frac{\vec{p} \cdot \vec{x}}{L}}}{L^3} \lambda V(x) \psi_{p_1, p_2}^{(E)}(x) \left( \int d^3R \frac{1}{L^{3/2}} \right) = 1 \]

\[ = \frac{\lambda}{L^3} \int d^3x e^{-i \frac{\vec{p} \cdot \vec{x}}{L}} V(x) \psi_{p_1, p_2}^{(E)}(x) \psi_{p_1, p_2}^{(E)}(x) \]

\[ \Rightarrow \langle \phi_{n+0} | \lambda V | \psi \rangle = \frac{\lambda}{L^3} \langle \vec{r} | V | \psi_{p_1, p_2}^{(E)}(x) \rangle \]

\[ \langle \phi_{n+0} | \lambda V | \psi \rangle = \frac{\lambda}{L^3} \langle \vec{x} | V | \psi_{p_1, p_2}^{(E)}(x) \rangle \]

\[ \boxed{\langle \phi_{n+0} | \lambda V | \psi \rangle = \frac{\lambda}{L^3} \langle \vec{r} | V | \psi_{p_1, p_2}^{(E)}(x) \rangle} \] (4)
Insert the matrix element $\langle 4 \rangle$ and the expressions for $|\psi_0\rangle$ and $|\psi\rangle$ into

$$eq. \ (3): \ |\psi\rangle = |\psi_0\rangle + \sum_{k \neq 0} \frac{|\psi_n\rangle \langle \psi_n | 2\ell V |\psi\rangle}{E - E_n}$$

$$\mathcal{L} e^{-\frac{x^2}{\mathcal{L}^2}} \psi_0^{(E)}(x) = \mathcal{L} e^{-\frac{x^2}{\mathcal{L}^2}} e^{it\cdot x} + \mathcal{L} e^{-\frac{x^2}{\mathcal{L}^2}} e^{-it\cdot x}\right\}$$

\[\sum_{k \neq 0} \frac{e^{it\cdot x}}{E - E_{k_1, k_2}} \frac{2}{\mathcal{L}^3} \langle \hat{\ell} \cdot V | \psi_0^{(E)} \rangle\]

\[\text{Note: Pauli blocking!}\]

$$\psi_0^{(E)}(x) = e^{it\cdot x} + \frac{1}{\mathcal{L}^3} \sum_{|\mathcal{L} + \frac{\mathcal{L}}{2}| > k_F} \sum_{|\mathcal{L} - \frac{\mathcal{L}}{2}| > k_F} \frac{e^{it\cdot x} \langle \hat{\ell} \cdot V | \psi_0^{(E)} \rangle}{E - E_{k_1, k_2}}$$

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

$$E - E_{k_1, k_2} = \left(\frac{\mathcal{L}^2 \vec{k}^2}{m} + \frac{\mathcal{L}^2 \vec{p}^2}{4m}\right) - \left(\frac{\mathcal{L}^2 \vec{r}^2}{m} + \frac{\mathcal{L}^2 \vec{p}^2}{4m}\right) = \frac{t^2}{m} (\vec{k}^2 - \vec{r}^2)$$

where the quantity $\vec{k}^2$ parametrizes the unknown Cooper pair energy with interaction $\ell V$.

Replace the sum by an integral: $\frac{1}{\mathcal{L}^3} \sum \rightarrow \int d^3x$.

We observe the "Pauli blocking" of the 2 overlapping regions from the integration region!
Using the shorthand notation $\nu(x) = \frac{m}{4\pi^2} V(x)$, we finally arrive at the famous "Bethe-Goldstone" eqn:

\[ \psi_{\nu, k}(x) = e^{ik \cdot x} + \frac{m}{(2\pi)^3} \int \frac{d^3 t}{2\pi^2} e^{i t \cdot \tilde{T}} \frac{1}{k^2 - t^2} \langle \tilde{T} | \nu | \psi_{\nu, \tilde{T}} \rangle \tag{6} \]

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

We observe that the Bethe-Goldstone eqn. contains the same state vector $| \psi_{\nu, \tilde{T}} \rangle$ on both sides (underlined); hence, it must be solved by iteration:

\[ | \psi_{\nu, k}^{(E)} \rangle = | \tilde{T} \rangle + 2 \left( \frac{m}{2\pi^2} \right) \int \frac{d^3 t}{2\pi^2} | \tilde{T} \rangle \frac{1}{k^2 - t^2} \langle \tilde{T} | \nu | \psi_{\nu, \tilde{T}}^{(E)} \rangle \]

We now write on the RHS:

\[ | \psi_{\nu, k}^{(E)} \rangle = 1 | \tilde{T} \rangle + 2 \left( \frac{m}{2\pi^2} \right) \int \frac{d^3 t}{2\pi^2} | \tilde{T} \rangle \frac{1}{k^2 - t^2} \langle \tilde{T} | \nu | \psi_{\nu, \tilde{T}}^{(E)} \rangle \]

\[ | \psi_{\nu, k}^{(E)} \rangle = 1 | \tilde{T} \rangle + 2 \left( \frac{m}{2\pi^2} \right) \int \frac{d^3 t}{2\pi^2} | \tilde{T} \rangle \frac{1}{k^2 - t^2} \langle \tilde{T} | \nu | \psi_{\nu, \tilde{T}}^{(E)} \rangle + 0(k^2) \approx 0 \]

and we neglect terms of order $k^2$ and higher because the coupling constant $\lambda$ is assumed to be small.

From eq. (2) we have: $| E - E_0 \rangle = \langle \psi_0 | \nu | \psi \rangle$

Inserting eqns (4) and (5) for the special case $\nu = 0$, i.e. $\tilde{T} = \tilde{T}$:

\[ (E - E_0)^{(5)} = \frac{\hbar^2}{m} (k^2 - h^2) = \langle \psi_0 | \nu | \psi \rangle^{(5)} \approx \frac{2}{\xi^3} \langle \tilde{T} | \nu | \psi_{\nu, \tilde{T}}^{(E)} \rangle \]

or

\[ (k^2 - h^2) = \frac{1}{\xi^3} \left( \frac{m}{2\hbar^2} \right)^2 \langle \tilde{T} | \nu | \psi_{\nu, \tilde{T}}^{(E)} \rangle \tag{?} \]
Inserting the Bethe-Goldstone eqn. (in first iteration RHs)

\[ \psi^{(E)}_{\mathbf{p}, \mathbf{h}} = \psi_{\mathbf{h}} + \Delta \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \mathbf{k} \left\langle \psi_{\mathbf{k}} | \mathbf{v} | \mathbf{h} \right\rangle \frac{1}{K^2 - t^2} \left\langle \mathbf{v} | \mathbf{v} | \mathbf{h} \right\rangle + \ldots \]

Into eq. (7) yields

\[ (K^2 - t^2) = \frac{2}{c^2} \left[ \left\langle \psi_{\mathbf{k}} | \mathbf{v} | \mathbf{h} \right\rangle + \Delta \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \left\langle \psi_{\mathbf{k}} | \mathbf{v} | \mathbf{h} \right\rangle \frac{1}{K^2 - t^2} \right] \]

Using \( \left\langle \mathbf{v} | \mathbf{v} | \mathbf{h} \right\rangle = \left\langle \psi_{\mathbf{h}} | \mathbf{v} | \mathbf{h} \right\rangle^* \), the last eq. can be rewritten

\[ (K^2 - t^2) = \frac{2}{c^2} \left\langle \psi_{\mathbf{h}} | \mathbf{v} | \mathbf{h} \right\rangle + \Delta \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{1}{K^2 - t^2} \left( \frac{2}{c^2} \left\langle \psi_{\mathbf{h}} | \mathbf{v} | \mathbf{h} \right\rangle \right)^2 \]

This equation determines the energy shift of the electron pair due to the interaction \( \Delta \mathbf{v} \).

\[ \Delta E_{\text{pair}} = E - E_0 = \left( \frac{t^2 K^2}{m} + \frac{t^2 P^2}{4m} \right) - \left( \frac{t^2 K^2}{m} + \frac{t^2 P^2}{4m} \right) \]

\[ = \frac{t^2}{m} (K^2 - t^2) \]

The diagram illustrates the energy shift for free electrons and Cooper pairs.
Equation (8) for the energy shift \((k^2 - \hbar^2)\) cannot be solved analytically without further approximations. However, one can solve (8) graphically if one generalizes the interaction \(V(x)\) to a "non-local separable" potential of the form

\[
V(x) \rightarrow V(x, x') = u(x) v(x') u(x')^* = u(x) u(x')^*.
\]

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

\[\Rightarrow \langle \hat{\mathbf{p}} | \mathbf{v} | \hat{\mathbf{t}} \rangle \equiv \int d^3x \varphi_\mathbf{p}^*(x) V(x) \varphi_\mathbf{p}^*(x) \rightarrow \]

\[
\int d^3x \int d^3x' \varphi_\mathbf{p}^*(x) V(x, x') \varphi_\mathbf{p}^*(x') = \int d^3x \varphi_\mathbf{p}^*(x) = u(x) u(x')^*
\]

\[
= \int d^3x e^{-i\hat{\mathbf{p}} \cdot \hat{x}} u(x) \int d^3x' e^{i\hat{\mathbf{p}} \cdot \hat{x}'} u(x')^* = u^*(t)
\]

Hence:

\[
\langle \hat{\mathbf{p}} | \mathbf{v} | \hat{\mathbf{t}} \rangle = u(x) u^*(t)
\]

for non-local separable potential \(V(x)\)

Insert (11) into (8):

\[
(k^2 - \hbar^2) = \frac{2}{\gamma^3} |u(h)|^2 + \lambda \int \frac{d^3x}{2\pi} \frac{1}{k^2 - \hbar^2} \left\{ \frac{2}{\gamma^3} |u(h)|^2 \right\} |u(\tau)|^2
\]

\[
= \left( k^2 - \hbar^2 \right)
\]

because from (8):

\[
k^2 - \hbar^2 = \frac{2}{\gamma^3} \langle \hat{\mathbf{p}}^2/\hbar^2 \rangle + O(\lambda^2) = \frac{2}{\gamma^3} |u(h)|^2 + O(\lambda^2)
\]

Divide eq. (12) by

\[
\lambda \cdot (k^2 - \hbar^2) \Rightarrow
\]
\[ \frac{1}{2} = \frac{1}{c^3} \frac{|u(k)|^2}{(k^2 - k_f^2)} + \int \frac{d^3t}{(2\pi)^3} \frac{|u(t)|^2}{k^2 - t^2} \equiv f(k^2) \quad (13) \]

The first term of \( f(k^2) \) has a pole at \( k^2 = k_f^2 \).

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

\[ \int \frac{d^3t}{(2\pi)^3} \frac{|u(t)|^2}{k^2 - t^2} = \int_{t_{\text{min}}}^{\infty} \frac{t^2 dt}{(2\pi)^3} \frac{|u(t)|^2}{k^2 - t^2} \int d\mathbf{t} \quad (14) \]

where \( t_{\text{min}} \) is obtained from the expression for \( \Gamma \), see p. 107:

\[ \Gamma = |\sqrt{t + \frac{2}{c^2}}| > k_F \]

2. Pole at \( k^2 = k_{\text{min}}^2 \), with \( t_{\text{min}} = \frac{k_F^2 - \frac{p^2}{c^2}}{4} \),

hence \( k^2 = k_F^2 - \frac{p^2}{4} \) for second pole.
Adding both terms together, we get the following "graphical solution".

We observe: For a repulsive residual int. \((\lambda > 0)\), there is only one solution
\[ k^2 = k_0^2 \], i.e. \( E - E_0 = 0 \),
but for an attractive interaction, there are two solutions:

a) \( k^2 = k_0^2 \), i.e. \( E = E_0 \)
b) \( k^2 = k_c^2 < k_0^2 \), i.e. \( E < E_0 \)

Let's study the "Cooper pair" solution with \( k^2 = k_c^2 \) in more detail.

The 1st term in \( f(k^2) \) is negligible near \( k^2 = k_0^2 \) (see graphs) and we have, for \( \lambda < 0 \):
\[
\frac{1}{\lambda} = \int \frac{d^3 \mathbf{r}}{(2\pi)^3} \frac{|u(\mathbf{r})|^2}{k^2 - \epsilon} \quad \text{will} \quad \lambda = \frac{1}{\lambda} \geq \pm \frac{\hbar^2 k_c^2}{m}
\]
Thus: \[
\frac{1}{\lambda} = \frac{1}{\lambda} \cdot \left( \frac{\hbar^2}{m} \right) \int_{t_{\text{min}}}^{\infty} \frac{t^2 dt}{(2\pi)^3} \frac{|u(t)|^2}{t^2 - k^2}.
\]

Consider now the special case.

\[ \vec{\rho} = \text{total pair mom.} = 0 \]

\[ 2 t_{\text{min}} = \frac{\hbar}{\Delta} \rightarrow \frac{\hbar^2}{4} = \Delta \]

\[ \Rightarrow t_{\text{min}} = \frac{\hbar}{\sqrt{2}} \]

Assume that \(|u(t)|^2\) contributes mostly near \(t_{\text{min}} = \frac{\hbar}{\sqrt{2}}\):

\[ |u(t)|^2 \approx |u(\frac{\hbar}{\sqrt{2}})|^2 \]

and take it outside the integral:

\[
\frac{1}{\lambda} = \frac{4\pi}{8\pi^3} \frac{|u(\hbar/\sqrt{2})|^2}{\hbar} \int_{\hbar}^{\infty} \frac{t^2 dt}{t^2 - k^2} = \frac{|u(\hbar/\sqrt{2})|^2}{\hbar} \int_{\hbar}^{\infty} \frac{t^2 dt}{t^2 - k^2}
\]

Inserting an approximate solution for the integral, one finds:

\[
\frac{1}{\lambda} = \frac{|u(\hbar/\sqrt{2})|^2}{2\pi^2} \left[ \frac{1}{2} \frac{\hbar}{\lambda} \ln \left( \frac{\hbar^2}{\lambda^2 - k^2} \right) \right] \quad \text{(for } \vec{\rho} = 0)\]

Solving for \(-\ln(\ldots)\), we obtain:

\[
- \frac{4\pi^2}{\hbar} = -\ln \left( \frac{\hbar^2}{\lambda^2 - k^2} \right) = \ln \left( \frac{\lambda^2 - k^2}{\hbar^2} \right).
\]

Exponentiating yields:

\[
\exp \left( - \frac{4\pi^2}{\hbar} \frac{1}{\lambda^2 |u(\hbar/\sqrt{2})|^2} \right) = \frac{\hbar^2 - k^2}{\hbar^2} = \frac{\frac{1}{2} \hbar^2 - \frac{1}{2} \frac{k^2}{m}}{\frac{1}{2} \hbar^2 - \frac{1}{2} \frac{k^2}{m}} = \frac{2(\epsilon_{\hbar} - \epsilon_k)}{2\epsilon_{\hbar}}
\]

Defining the "pairing gap \(\Delta\)" via

\[ \Delta \overset{\text{def}}{=} 2(\epsilon_{\hbar} - \epsilon_k) \quad (15a) \]

results in the expression:

\[ \Delta = \left( 2 \epsilon_{\hbar} \right) \exp \left( - \frac{4\pi^2}{\hbar} \frac{1}{\lambda^2 |u(\hbar/\sqrt{2})|^2} \right) \quad (15b) \]

Pairing gap \(\Delta\) is Fermi energy \(\epsilon_{\hbar}\) (empty state) F.T. of nonlocal not.
Finally, we express the energy shift of the Cooper pair in terms of $\Delta$:

$$
\Delta E_{\text{pair}} = E - E_0 = \frac{t_n^2}{m} (k^2 - \hbar^2) = 2 (\varepsilon_k - \varepsilon_{k_F}) = 2 (\varepsilon_{k_F} - \varepsilon_k) + 2 (\varepsilon_{k_F} - \varepsilon_k) \Rightarrow 
$$

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

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

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

Eq. (15b) shows that the pairing gap $\Delta$ depends exponentially on the electron-phonon interaction coupling constant $\lambda = -121$:

$$
\Delta = \exp \left( -\frac{1}{121} \ldots \right) \quad (18)
$$

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

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

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

$$
\frac{1}{\lambda} = \int \frac{d^3p}{(2\pi)^3} \frac{|t(k)|^2}{k^2 - t^2}, \quad \text{with } \Gamma = \left| \frac{p}{2} \pm \frac{t}{2} \right| > k_F.
$$

The phase space for this integral is maximized if $\vec{p} = 0$:

a) finite $\vec{p}$

$$
\Gamma \quad \frac{\partial \Gamma}{\vec{p} = 0} \quad \Gamma
$$

(shaded area $= \pi$)

b) $\vec{p} = 0$

$$
\Gamma \quad \frac{\partial \Gamma}{\vec{p} = 0} \quad \Gamma
$$

(shaded area $= \pi$)
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

\[ V_{\text{el-phon}}(\mathbf{r}, \mathbf{r}') = -\frac{\hbar^2}{m^*} \nabla^2 \delta(\mathbf{r} - \mathbf{r}') \]

is very weak (\(\hbar^2/m^*\) 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 \(\Delta\), even for an arbitrarily weak residual interaction:

\[ \Delta = (2 \varepsilon_{\text{F}}) \exp \left( -\frac{4\pi}{\varepsilon_{\text{F}} \lambda_{\text{F}} \sqrt{n(\varepsilon_{\text{F}})^2}} \right), \]

where \(\lambda_{\text{F}} = \frac{\hbar}{m^*}\).

The reason is, ultimately, the "Pauli blocking" of electrons in the medium, as manifested by the integration region \(\Gamma\).
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 Coulomb) electron gas with uniform ionic background 
charge, see FW eq. (3.19), and an additional attractive 
"residual" two-body electron-phonon potential:

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

with

$$\hat{H}_{\text{el-gas}} = \sum_{i,j} \frac{e^2}{2m} \hat{\mathbf{r}}_i \cdot \hat{\mathbf{r}}_j + \frac{e^2}{2\varepsilon} \sum_{i,j} \sum_{\delta=0} \left( \frac{4\pi}{\Omega} \right)^2 \delta(\mathbf{r}_i - \mathbf{r}_j)$$  \hspace{1cm} (2)

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

$$V^{(2)}_{\text{el-ph}} = \frac{1}{2} \sum_{i,j} V(\mathbf{x}_i, \mathbf{x}_j) = \text{Frolich, 1950}$$  \hspace{1cm} (FW 46.9)  \hspace{1cm} (3)

We will transform this to occup. # next 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

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

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

$$\hat{H}_{\text{el-gas}}^{\text{HF}} = \sum_{\alpha} \left< \beta | \hat{h}_{\text{HF}} | \alpha \right> \hat{a}_{\alpha}^+ \hat{a}_{\alpha} = \sum_{\alpha} e_{\alpha}^0 \hat{a}_{\alpha}^+ \hat{a}_{\alpha}$$

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

$$e_{\alpha}^0 = \left< \alpha | \hat{h}_{\text{HF}} | \alpha \right> = \left< \alpha | \hat{t} | \alpha \right> + \sum_{\beta=1}^{N} \left< \alpha | \hat{v}^{(2)}_{\text{HF},e-e} | \beta \alpha \right>$$

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:

$$\Phi_{\alpha}^{\text{HF}}(\vec{x}) = \left< \vec{x} | \alpha \right> \Rightarrow \left< \vec{x} | \hat{a}_{\alpha}^+ \right> = \Phi_{\alpha}^{\text{HF}}(\vec{x}) = L^{-3/2} e^{i \vec{p} \cdot \vec{x}} q_{\lambda}$$

This leads to

$$\hat{H}_{\text{el-gas}}^{\text{HF}} = \sum_{\xi, \lambda} e_{\xi, \lambda}^0 \hat{a}_{\xi, \lambda}^+ \hat{a}_{\xi, \lambda}$$

and one obtains for the HF s.p. energies the full expression (see FW p. 127):
\[ \varepsilon_0 = \frac{t^2 k^2}{2m} + n V(h=0) - \left( \frac{1}{2\pi} \right)^3 \int d^3 k' V(h-h') \Theta(h-h') \] (78)

where \( V(h) \) is the Fourier transform of the bare screened repulsive Coulomb potential between the electrons.

The 2-body residual interaction (attraction in el-\( \text{ph} \)) has the form

\[ V_{eg_{el-\text{ph}}}^{(2)} = -\frac{1}{2} \sum_{\{\lambda_4, \lambda_5\}} \left\{ \begin{array}{c}
\langle \hat{a}_{\lambda_4} \hat{a}_{\lambda_5} | v | \hat{\phi}_{\lambda_3} \phi_{\lambda_2} \rangle \\
\hat{a}_{\lambda_3} \phi_{\lambda_2} \end{array} \right\} = \delta_{\lambda_3 \lambda_1} \delta_{\lambda_2 \lambda_4} \langle \hat{a}_{\lambda_3} \phi_{\lambda_2} | v | \hat{\phi}_{\lambda_1} \rangle \] (8)

\[ \hat{a}_{\lambda_3}^{+} \hat{a}_{\lambda_2}^{+} \hat{a}_{\lambda_4} \hat{a}_{\lambda_5} \]

where the 2-body post. matrix element \( \langle \cdot | v | \cdot \rangle \) 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 \( \Omega \) (see FW p. 34):

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

thermodyn. int. temp. entropy chem. potential

This is the starting point of the BCS theory at finite \( T \), see FW p. 51.

We will here study the \( T=0 \) case only.

\[ \Rightarrow \Omega(T=0, V, \mu) = E - \mu N \]

\[ \hat{\Omega} = \text{thermodyn. post. op.} = \hat{\chi} - \mu \hat{N} \]

(9b)

\[ \text{c-number} \]

\[ \text{operator} \]
Bardeen, Cooper, and Schrieffer ("BCS") start from a model g.s. \( |\Phi_{\text{BCS}}\rangle \) which is based on Cooper's model:

The BCS g.s. contains "Cooper pairs" of electrons with opposite momenta \( \hbar \langle \hat{v} \rangle - \hbar \langle \hat{u} \rangle \), i.e. pair momentum \( \mathbf{P} = 0 \), and opposite spins (reduces "Pauli repulsion" of pairs):

\[
|\Phi_{\text{BCS}}\rangle = \prod_{l=1}^{\infty} \left( u_{\mathbf{k}} + v_{\mathbf{k}} \hat{a}_{\mathbf{k}\uparrow} \hat{a}_{\mathbf{-k}\downarrow} \right) |0\rangle
\]

From the normal condition \( \langle \Phi_{\text{BCS}} | \Phi_{\text{BCS}} \rangle = 1 \) one finds

\[
u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1
\]

i.e. \( u_{\mathbf{k}}^2 \) is the prob. that the s.p. level \( \mathbf{k} \) is unfilled, and \( v_{\mathbf{k}}^2 \) is the prob. that it is filled with a Cooper pair. We will see later that the BCS theory predicts:

\[\nu_{\mathbf{k}}^2 \]

\[\mathbf{BCS} \quad T=0\]

\[1\]

\[\frac{1}{2}\]

\[0\]

\[\mu = \text{chem. pot.}\]

\[\mathbf{k}\]

\[i.e. \text{there is no longer a sharp Fermi surface (particles are scattered by residual int. into unoccupied states above } \mu, \text{ even at } T=0).\]

\[\theta(\epsilon_F-\epsilon_k) \]

\[\mathbf{HF} \quad T=0\]

\[1\]

\[0\]

\[\epsilon_F\]

\[\mathbf{HF}\]

\[\text{compared to HF g.s.}\]
It turns out that because of approximations in the g.s., the particle # is no longer conserved in the BCS theory, in fact one finds for the particle # fluctuation, see FV, problem 10.6, p. 337:

\[
S(N) = \frac{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2}{\langle \hat{N} \rangle^2} = \frac{\sum \left( u_k^2 v_k^2 \right)}{\left( \sum v_k^2 \right)^2} \neq 0
\]  

where

\[
\langle \hat{N} \rangle = \langle \phi_0^{\text{BCS}} | \hat{N} | \phi_0^{\text{BCS}} \rangle = \langle \phi_0^{\text{BCS}} | \sum \hat{a}_{\lambda \lambda}^{\dagger} \hat{a}_{\lambda \lambda} | \phi_0^{\text{BCS}} \rangle
\]

and

\[
\langle \hat{N}^2 \rangle = \langle \phi_0^{\text{BCS}} | \hat{N} \hat{N} | \phi_0^{\text{BCS}} \rangle = \langle \phi_0^{\text{BCS}} | \sum \hat{a}_{\lambda \lambda}^{\dagger} \hat{a}_{\lambda \lambda} \hat{a}_{\lambda' \lambda'}^{\dagger} \hat{a}_{\lambda' \lambda'} | \phi_0^{\text{BCS}} \rangle
\]

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

\[
\langle \phi_0^{\text{BCS}} | \hat{N} | \phi_0^{\text{BCS}} \rangle = \frac{1}{N} \quad \text{actual particle #}
\]

The thermodynamic potential at zero temp. is therefore given by

\[
\Omega(T=0, V, \mu) = E - \mu N
\]

\[
\langle \phi_0^{\text{BCS}} | \hat{K} | \phi_0^{\text{BCS}} \rangle = \langle \phi_0^{\text{BCS}} | \hat{H} - \mu \hat{N} | \phi_0^{\text{BCS}} \rangle
\]

Bardeen, Cooper, and Schrieffer (1957) used a variational approach (like in HF theory) to obtain \( u_k \), \( v_k \), energy gap, and
J. S. energy. One varies the thermodynamic potential with respect to the quantities \( u_h, v_h \) which determine the BCS ground state:

\[
\begin{align*}
\delta \left[ \langle \phi_0^{BCS} | \hat{K} | \phi_0^{BCS} \rangle \right] &= 0 \\
&\quad \text{with } (u_h^2 + v_h^2 = 1)
\end{align*}
\]

\[
\Rightarrow \text{result: } u_h, v_h, \Delta_h, E_g^{BCS}
\]

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

\[
\hat{K} = \sum \left( E_h^0 - \mu \right) \hat{a}_h^{\dagger} \hat{a}_h + V_{el-el-ph} \quad \text{HF s.p. chem. energies, pot.}
\]

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**

<table>
<thead>
<tr>
<th># or ( \epsilon )</th>
<th>( \hat{a}_h^{\dagger} \hat{a}_h )</th>
<th>( \hat{c}_i \rightarrow (\hat{a}_i, \hat{h}_i) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \hat{E}_F ) or ( \epsilon_F )</td>
<td>$\ldots$</td>
<td>$\phi_0^{HF} = \hat{c}_1^{\dagger} \hat{c}_2^{\dagger} \ldots \hat{c}_F^{\dagger}</td>
</tr>
<tr>
<td>See lecture notes ch. 3, p. 2-3: Canonical transf. from original operators to p-h operators</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: particle creation = hole destruction
The HF g.s. is the vacuum with respect to the "particle-hole quasiparticle":
\[
\hat{\alpha}\ket{\phi_0^\text{HF}} = 0, \quad \hat{\beta}\ket{\phi_0^\text{HF}} = 0 \quad (\text{FW 7.40})
\]

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

\[
\hat{C}_h^\uparrow = \Theta(k - k_F) \hat{A}_h^\uparrow + \Theta(k_F - k) \hat{B}_h^\uparrow
\]

The Bogoliubov transform is a generalization of this transform:

\[
\hat{A}_h^\uparrow = \nu_h \hat{A}_h^\uparrow + \nu_h \hat{B}_h^\uparrow
\]

\[
\hat{B}_h^\uparrow = \nu_h \hat{A}_h^\uparrow + \nu_h \hat{B}_h^\uparrow
\]

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

The inverse of the above transform yields the quasiparticle operators \( \hat{\alpha}_h \) and \( \hat{\beta}_h \):
\[ \hat{\mathcal{\Psi}}^+ = \hat{u}_h \hat{\hat{a}}^\dagger_{h\uparrow} - \hat{v}_h \hat{\hat{a}}_{h\downarrow} \]  

\[ \Rightarrow \quad \text{quasiparticle} = \hat{u}_h \hat{\hat{a}}_{h\uparrow} - \hat{v}_h \hat{\hat{a}}_{h\downarrow} \]

So, the quasiparticle is a linear superposition of particle and hole with prob. amplitudes \( \hat{u}_h \) and \( -\hat{v}_h \).

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

\[ \text{Cooper pair} = \hat{\hat{a}}^\dagger_{h\downarrow} \hat{\hat{a}}_{h\uparrow} = \uparrow \quad \downarrow \]

Note that the quasiparticle always appears as a superposition of the original state \( |h\rangle \) and the time-reversed state \( |-h\rangle \)

\[ |h\rangle = |+h, \uparrow\rangle \quad \Rightarrow \quad |-h\rangle = \hat{T} |h\rangle = |-h, \uparrow\rangle = |+h, \downarrow\rangle \]

Time-reversal op.

Simple "classical" reasoning: under \( \hat{T} \) we have \( \vec{r} \rightarrow -\vec{r}, \quad t \rightarrow -t \)

\[ \hat{p} = m \frac{d\vec{r}}{dt} \Rightarrow m (-\frac{d\vec{r}}{dt}) = -\hat{p} \quad \text{and} \quad \hat{L} = \vec{r} \times \hat{p} \Rightarrow -\vec{r} \times (-\hat{p}) = -\hat{L}, \]

and the spin has to transform in the same way as the orbital \( \hat{L} \).

We define

\[ \hat{u}_h \hat{\hat{a}}_{h\uparrow} - \hat{v}_h \hat{\hat{a}}_{h\downarrow} = \hat{\beta}_{-h} \]

Referring to

\[ \hat{\beta}_{-h} = \frac{1}{2} \left( \hat{\beta}^+ \hat{\beta}^- + \hat{\beta}^- \hat{\beta}^+ \right) \]

resulting in

\[ \hat{\beta}_{-h} = \frac{1}{2} \left( \hat{\beta}^+ \hat{\beta}^- + \hat{\beta}^- \hat{\beta}^+ \right) = \hat{T} (\hat{\beta}^+ \hat{\beta}^-) = \hat{T} (\hat{u}_h \hat{\hat{a}}_{h\uparrow}^\dagger - \hat{v}_h \hat{\hat{a}}_{h\downarrow}^\dagger) = \]

\[ = \hat{u}_h \hat{\hat{a}}_{h\downarrow}^\dagger - \hat{v}_h \hat{\hat{a}}_{h\uparrow}^\dagger \]

[Ring & Schmuk 1981, p. 234]
Choosing the usual "BCS plane convention"

\[ U_h = v_h = \text{real and} \]
\[ U^-_h = U_h > 0, \quad v^-_h = -v_h < 0 \]

one obtains for the "quasiparticle creation" operator

\[ \hat{\beta}^+ - h = U_h \hat{a}^+_{- h} + v_h \hat{a}^+_{h} \tag{FW 37.1} \]

One straightforwardly proves that the transform

\[ \left( \hat{a}^+_{h \uparrow}, \hat{a}^-_{h \downarrow} \right) \rightarrow \left( \hat{\alpha}^+_{h \uparrow}, \hat{\beta}^+_{h \downarrow} \right) \]

is canonical, i.e. same anticommutation relations

\[ \{ \hat{\beta}^+_{h \uparrow}, \hat{\beta}^+_{h \downarrow} \} = 0, \{ \hat{\alpha}^+_{h \uparrow}, \hat{\alpha}^+_{h \downarrow} \} = 0 \]

\[ \text{all other } \{, \} = 0 \tag{FW 37.2} \]

provided that \[ U_h^2 + v_h^2 = 1 \tag{37.4} \]

In analogy to the HF g.s., Bogoliubov assumes the BCS-g.s. to be the quasiparticle vacuum with respect to the \( \hat{\alpha}^+_{h \uparrow}, \hat{\beta}^+_{h \downarrow} \):

\[ \hat{\alpha}^+_{h \uparrow} | \phi^{\text{BCS}}_0 \rangle = 0 \equiv \hat{\alpha}^+_{h \uparrow} | \tilde{0} \rangle = 0 \rightarrow \text{quasiparticle vacuum} \tag{FW 37.8} \]

\[ \hat{\beta}^+_{h \downarrow} | \phi^{\text{BCS}}_0 \rangle = 0 \equiv \hat{\beta}^+_{h \downarrow} | \tilde{0} \rangle = 0 \]

The BCS-g.s. can be constructed in analogy to HF case, eq. 1:

\[ | \tilde{0} \rangle \equiv | \phi^{\text{BCS}}_0 \rangle = \hat{\beta}^+_1 \hat{\beta}^+_2 \ldots \hat{\beta}^+_n | 0 \rangle \quad \text{(all R"{o}mpf & Schuck p. 249)} \]
One can prove (difficult!) that the state is identical to the original BCS state vector
\[
|\phi_{BCS}\rangle = \prod_{k=1}^{\infty} (\nu_k + \nu_k^* \hat{a}_{k+}^\dagger \hat{a}_{k-}^\dagger) |\text{vacuum}\rangle
\]

Our goal is to compute
\[
\Omega (T=0) = E - \mu N = \langle \phi_{BCS} | \hat{H} - \mu N | \phi_{BCS} \rangle = \langle \tilde{\phi} | \hat{H} - \mu N | \tilde{\phi} \rangle
\]

Inserting the structure of \( \hat{H} \), we find from eqns (16) and (8):
\[
\hat{K} = \hat{H} - \mu N = \sum_{\bar{\ell}} \left( \epsilon_{\ell}^* - \mu \right) \hat{a}_{\bar{\ell}}^+ \hat{a}_{\bar{\ell}} + \frac{1}{2} \sum_{\bar{\ell}_1 \ldots \bar{\ell}_4} \delta_{\bar{\ell}_1 \bar{\ell}_2} s_{\bar{\ell}_3 \bar{\ell}_4}
\]

The calculation of \( \langle \tilde{\phi} | \hat{K} | \tilde{\phi} \rangle \) is greatly simplified by using Wick's theorem, because all normal-ordered expectation values
\[
\langle \tilde{\phi} | N_{\alpha_\beta} (...) | \tilde{\phi} \rangle = 0
\]

Look at the first term in \( \hat{K} \) above; it involves the calculation of
\[
\hat{A} = \sum_{\ell} \left( \epsilon_{\ell}^* - \mu \right) \hat{a}_{\ell}^+ \hat{a}_{\ell}
\]

Since we sum over all \( \bar{\ell} \) (+ and -), we can change \( \bar{\ell} \rightarrow -\bar{\ell} \) in the second part:
\[ T_\tau = \sum_{k \delta} (\varepsilon_{k+\delta} - \mu) \left[ \hat{\alpha}_{k+\delta}^+ \hat{\alpha}_{k}^+ \right] \]  

Using Wick's theorem for operators of the form

\[ \hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu} = T (\hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu}) = N (\hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu}) + \hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu} \]  

where \( T, N \) and \( \underline{\cdots} \) are with respect to the quasiparticles \( \alpha, \beta \) which annihilate \( |0\rangle \).

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

\[ \hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu} = \langle 0 | \hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu} | 0 \rangle = \langle \phi_{\beta}^{(0)} | q_{\beta}^{(0)} \rangle \]

Let us evaluate the contraction

\[ \hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu}^+ = \langle 0 | \hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu}^+ | 0 \rangle = \text{c.m.} (37.5) = \]

\[ = \langle 0 | (v_k \hat{\alpha}_{\tau}^+ + v_\nu \hat{\beta}_{\tau}^-) (v_k \hat{\alpha}_{\nu}^+ + v_\nu \hat{\beta}_{\nu}^-) | 0 \rangle = \]

\[ = \langle 0 | v_k v_k' \hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu}^+ + v_k v_\nu \hat{\beta}_{\tau}^- \hat{\alpha}_{\nu}^+ + v_\nu v_k \hat{\alpha}_{\tau}^+ \hat{\beta}_{\nu}^- + \]

\[ + v_\nu v_\nu \hat{\beta}_{\tau}^- \hat{\beta}_{\nu}^- | 0 \rangle = \]

\[ = v_k v_\nu \langle 0 | \hat{\beta}_{\tau}^- \hat{\beta}_{\nu}^- \rangle = v_k v_\nu \delta_{\tau,\nu} = v_k^2 \delta_{\tau,\nu} \]

\[ = (\delta_{\tau,\nu} - \hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu}^+ \right|_0 \]

\[ \text{i.e.} \quad \hat{\alpha}_{\tau}^+ \hat{\alpha}_{\nu}^+ = v_k^2 \delta_{\tau,\nu} \]  

(5) (see FN 37.9)
Similarly one finds the other contraction

\[
\hat{a}_1^+ \hat{a}_1^- \hat{a}_2^+ \hat{a}_2^- = v_2^2 \delta_{12} \delta_{12} (\text{same})
\]  
(6)  
(see FW 37.10)

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

\[
\hat{T}_1 = \frac{1}{\hbar} \sum \left( \epsilon_0 - \mu \right) \left[ N(\hat{a}_1^+ \hat{a}_2^- \hat{a}_2^+ \hat{a}_1^-) + N(\hat{a}_2^+ \hat{a}_1^- \hat{a}_1^+ \hat{a}_2^+) + 2v_2^2 \right]
\]  
(7)

The \(N\)-products with respect to \(\hat{a}_1, \hat{a}_2\) can be calculated, if desired, see FW 67.11).

The potential operator term \(\hat{V} = V_{\text{eg.d-phe}}\) in (2) involves terms of the form (see [1] with \(1/\hbar\), ch. 4, p. 12):

\[
\hat{a}_1^+ \hat{a}_2^+ \hat{a}_4^+ \hat{a}_3^- = W_{\text{dir}} = T \left( a_1^+ a_2^+ a_4 a_3 \right) =
\]

\[
N(a_1^+ a_2^+ a_4 a_3) + N(a_1^+ a_2^+ a_4 a_3) + N(a_1^+ a_2^+ a_4 a_3) +
\]

\[
+ N(a_1^+ a_2^+ a_4 a_3) + N(a_1^+ a_2^+ a_4 a_3) + N(a_1^+ a_2^+ a_4 a_3) +
\]

\[
+ N(a_1^+ a_2^+ a_4 a_3) + N(a_1^+ a_2^+ a_4 a_3) + N(a_1^+ a_2^+ a_4 a_3) +
\]

\[
+ N(a_1^+ a_2^+ a_4 a_3)
\]  
(8)

One encounters a few new contractions in the pot. term, in particular the pairing tensor amplitudes (\(\rightarrow\) homework) of the form.
\[ F_k^{(1)} = \hat{\alpha}_k^+ \hat{\alpha}_{-k}^+ = \langle \bar{\alpha} \ket \cdots \ket \bar{\alpha} \] 
\[ F_k^{(2)} = \hat{\alpha}_{-k}^- \hat{\alpha}_k^+ = \langle \bar{\alpha} \ket \cdots \ket \bar{\alpha} \] 

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

\[ \hat{\mathcal{K}} = \hat{\mathcal{U}} + \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2 + N(\hat{\mathcal{V}}) \]  

with (FW 37.26)

\[ \hat{\mathcal{U}} = \text{``c-numbers'' = } 2 \sum_{k} \frac{\mathcal{V}_k \mathcal{v}_k^2}{2} + \sum_{k,k'} \frac{\mathcal{v}_k^2 \mathcal{v}_{k'}^2}{2} \langle \bar{\mathcal{q}}_{k,k'} \ket \bar{\mathcal{q}}_{k,k'} \rangle \]

\[ - \sum_{k} \mathcal{v}_k \mathcal{v}_k \Delta_k \]

\[ \hat{\mathcal{H}}_1 = \sum_{k} \left( \frac{\mathcal{v}_k^2}{2} \hat{\mathcal{a}}_k^+ \hat{\mathcal{a}}_k^+ + \frac{\mathcal{v}_k^2}{2} \hat{\mathcal{\dot{a}}}_k^+ \hat{\mathcal{\dot{a}}}_k^+ \right) \left[ (\mathcal{v}_k^2 - \mathcal{v}_k^2) s_k + 2 \mathcal{v}_k \mathcal{v}_k \Delta_k \right] \]  
\[ \text{quasiparticle numbers operator} \]

\[ \hat{\mathcal{H}}_2 = \sum_{k} \left( \frac{\mathcal{v}_k^2}{2} \hat{\mathcal{a}}_k^+ \hat{\mathcal{a}}_k^+ + \frac{\mathcal{v}_k^2}{2} \hat{\mathcal{\dot{a}}}_k^+ \hat{\mathcal{\dot{a}}}_k^+ \right) \left[ 2 \mathcal{v}_k \mathcal{v}_k \Delta_k - (\mathcal{v}_k^2 - \mathcal{v}_k^2) \Delta_k \right] \]  
\[ \text{creates/destroys two quasiparticles} \]

\[ N(\hat{\mathcal{V}}) = \text{normal-ordered product of } \hat{\mathcal{V}}, \text{ no contractions,} \]
\[ \text{contains up to } 4 \text{ quasiparticle creation/annihilation operators} \]

In these terms, we have used the full abbreviations
\[ \varepsilon_h = (\varepsilon_h^0 - \mu) \] s.p. energy with respect to clinical potential \( \mu \)

\[\varepsilon_h = \varepsilon_h^0 - \sum \frac{\langle \hat{\varepsilon} \hat{\varepsilon}' | V | \hat{\varepsilon} \hat{\varepsilon}' \rangle}{\hat{\varepsilon}^2} \] s.p. HF energy modification due to electron-phonon attractive part.

\[ \Delta_h = \sum \frac{\langle \hat{\varepsilon}_h - \hat{\varepsilon}_2 | V | \hat{\varepsilon}_h - \hat{\varepsilon}_2 \rangle}{\hat{\varepsilon}_2^2} \] energy gap

So far, we have transformed \( \hat{\varepsilon} \) in terms of quasiparticle operators \( \hat{\varepsilon}_h, \beta \). The canonical transform has not yet been specified (except for the constraint \( \varepsilon_2^2 + \varepsilon_h^2 = 1 \)).

We will choose \( u_h \) and \( v_h \) such that

\[ H_2 = 0 \Rightarrow 2 u_h v_h \varepsilon_h - (u_h^2 - v_h^2) \Delta_h = 0 \]

\[ \Rightarrow u_h, v_h \]

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

The thermodynamic potential operator becomes

\[ \hat{K} \rightarrow U + \hat{H}_F + N(\hat{\varepsilon}) \] (10b)

Note that eqns (10a, b) are still exact. We have made no approximations to \( \hat{K} \).
From the normal condition \( u_h^2 + v_h^2 = 1 \) and from eq. (18a) one finds after some algebra (FW1 p.330/331):

\[
\nu_h^2 = \frac{1}{2} \left( 1 - \frac{E_h}{E_h'} \right) \quad \text{with} \quad E_h := \sqrt{E_h^2 + \Delta_h^2} \quad (18a)
\]

We examine now the "energy gap" \( \Delta_h \) defined on p. 118:

\[
\Delta_h = \sum_{\vec{k}'} \langle \vec{k} - \vec{k}' | v | \vec{k}' - \vec{k} \rangle u_h^* v_h' \quad (18b)
\]

Solving eq. (10a) for \( u_h^* v_h' \) results in

\[
2 \ u_h^* v_h' \bar{E}_h' = (u_h^2 - v_h^2) \Delta_h' \\

\nu_h^* v_h' = \frac{1}{2} \left( \frac{u_h^4 - v_h^2}{\bar{E}_h'} \right) \Delta_h' \quad \text{insert} \quad u_h^2 = 1 - v_h^2 \\

\nu_h^* v_h' = \frac{1}{2} \left( \frac{1 - 2 v_h^2}{\bar{E}_h'} \right) \Delta_h' \quad (18a) \quad \frac{1}{2} \left( 1 - \frac{E_h'}{E_h' + \Delta_h'^2} \right) \Delta_h' \\

\nu_h^* v_h' = \frac{1}{2} \left( \frac{1 - 2 v_h^2}{\bar{E}_h'} \right) \Delta_h' \quad (18a) \quad \frac{1}{2} \left( \frac{\Delta_h'}{\bar{E}_h' + \Delta_h'^2} \right) \Delta_h' \quad (18c)
\]

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

\[
\Delta_h = \frac{1}{2} \sum_{\vec{k}'} \langle \vec{k} - \vec{k}' | v | \vec{k}' - \vec{k} \rangle \frac{\Delta_h'}{\sqrt{\bar{E}_h'^2 + \Delta_h'^2}} \quad (19)
\]

Note that if we replace \( \sum_{\vec{k}'} \rightarrow \pi \delta \bar{E}_h' \), (19) becomes a non-linear integral equation which is difficult to solve:

\[
\Delta_h = \frac{1}{2} \pi \delta \bar{E}_h' \ldots \frac{\Delta_h'}{\sqrt{\bar{E}_h'^2 + \Delta_h'^2}}
\]
Using the relations for $u_\beta$ and $v_\beta$, we can simplify $H_1$:

\[
\hat{H}_1 = \sum_{\beta \in \mathcal{B}} \left( \hat{\alpha}_\beta^+ \hat{\alpha}_\beta + \hat{\beta}_\beta^+ \hat{\beta}_\beta \right) \left[ \frac{u_\beta^2 - v_\beta^2}{E_\beta} \hat{\epsilon}_\beta + 2 u_\beta v_\beta \Delta \beta \right] = \frac{\hat{\epsilon}_\beta}{E_\beta} \frac{E_\beta}{\Delta \beta} = \frac{E_\beta^2}{E_\beta} = E_\beta
\]

\[
\hat{H}_1 = \sum_{\beta \in \mathcal{B}} E_\beta \left( \hat{\alpha}_\beta^+ \hat{\alpha}_\beta + \hat{\beta}_\beta^+ \hat{\beta}_\beta \right) \Rightarrow \hat{H}_1 = \sum_{\beta \in \mathcal{B}} E_\beta \left( \hat{\alpha}_\beta^+ \hat{\alpha}_\beta + \hat{\beta}_\beta^+ \hat{\beta}_\beta \right) \Rightarrow \hat{H}_1 = \sum_{\beta \in \mathcal{B}} E_\beta \left( \hat{\alpha}_\beta^+ \hat{\alpha}_\beta + \hat{\beta}_\beta^+ \hat{\beta}_\beta \right)
\]

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

\[
\hat{K} = \hat{K}_0 + N(\hat{\epsilon}) \quad \text{with} \quad \hat{K}_0 = U + \hat{H}_1 = U + \sum_{\beta \in \mathcal{B}} E_\beta \left( \hat{\alpha}_\beta^+ \hat{\alpha}_\beta + \hat{\beta}_\beta^+ \hat{\beta}_\beta \right)
\]

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

\[
\mathcal{L}_0 (T=0) = \langle \phi | \hat{K}_0 | \phi \rangle = U + \sum_{\beta \in \mathcal{B}} E_\beta \langle \phi | \hat{\alpha}_\beta^+ \hat{\alpha}_\beta + \hat{\beta}_\beta^+ \hat{\beta}_\beta | \phi \rangle
\]

From this expression we see that the minimum value of the thermodynamic potential is obtained in the quasiparticle vacuum state $\ket{\bar{\phi}} = \ket{\phi_0 \bar{\phi}_0}$ defined by

\[
\hat{\alpha}_\beta \ket{\bar{\phi}} = 0 \Rightarrow \hat{\alpha}_\beta^+ \ket{\bar{\phi}} = 0
\]

\[
\hat{\beta}_\beta \ket{\bar{\phi}} = 0 \Rightarrow \hat{\beta}_\beta^+ \ket{\bar{\phi}} = 0
\]

In the state $\ket{\phi} = \ket{\bar{\phi}}$ we have $\mathcal{L}_0 (T=0) = U$. 

\[
(23)
\]
The excited states are 1- quasiparticle, 2- quasiparticle,...
excitations. Each of these quasiparticles carries an
excitation energy, \( E_{\kappa} = \sqrt{(E_{\kappa} - \mu)^2 + \Delta_{\kappa}^2} \geq \Delta_{\kappa} \), hence the
name energy gap for \( \Delta_{\kappa} \):

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

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

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

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

\[
U = c\text{-number } = 2 \sum_{\kappa} \frac{\xi_\kappa v_\kappa^2}{E_\kappa} + \sum_{\kappa, \kappa'} v_\kappa v_{\kappa'}^* \langle \hat{h}_{\kappa} \hat{h}_{\kappa'} | \tilde{0} \rangle \tilde{0} \rangle - \sum_{\kappa} \frac{\xi_\kappa v_\kappa^2}{E_\kappa}
\]

\[
\hat{H}_1 = \sum_{\kappa} \frac{E_\kappa}{\hbar} \left( \hat{h}_{\kappa}^{(w)} + \hat{h}_{\kappa}^{(b)} \right)
\]

What has Bogoliubov transf. accomplished? The thermodyn. pot.
\( \hat{K} \) of the system is a constant plus a diagonal one-body operator,
provided that the interaction among the quasi-particle
\( N(V) \) is negligible. It vanishes exactly in the BCS-g.s. (\( = \) quasiparticle vacuum \( \left| 0 \right> \)) and is usually small.

The effective Hamiltonian \( \hat{H}_0 \) is a 1-body operator in terms of the quasiparticles \( (2\hbar \beta \gamma) \). It contains the attractive electron-phonon equivalent potential "on average" via the matrix element \( \left< \hat{h} \hat{h}^\dagger | V | \hat{h}^\dagger \hat{h} \right> \).

**Discussion of BCS gap equation (19)**

From eq. (19), p. 119,

\[
\Delta_k = \frac{1}{2} \sum \left< \hat{h} - \hat{h}^\dagger | V | \hat{h}^\dagger - \hat{h} \right> \frac{\Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}}
\]

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

\[
\Delta_k = 0, \quad \forall k \quad \text{(i.e.: vanishing pairing gap \( \Delta \))}
\]

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

\[
\nu_{2k} = \frac{1}{2} \left( 1 - \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta_k^2}} \right) = \frac{1}{2} \left( 1 - \frac{\xi_k}{|\xi_k|} \right) = \frac{1}{2} \left( 1 - \frac{(\epsilon_k - \mu)}{|\epsilon_k - \mu|} \right) = \pm 1
\]

= \( \Theta(\mu - \epsilon_k) \), i.e. we obtain the HF g.s. distribution: \( \Delta = 0 \Rightarrow \text{BCS} \)

We see that in this case \( \Delta = 0 \), the chemical potential \( \mu = \epsilon_F \).
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.

\[
\langle \hat{\mathbf{h}} - \hat{\mathbf{h}}' | v | \hat{\mathbf{h}}' - \hat{\mathbf{h}} \rangle \approx \frac{2}{\varepsilon_0} \Theta \left( \varepsilon_0 - 1 \varepsilon_k - \mu \right) \Theta \left( \varepsilon_0 - 1 \varepsilon_k' - \mu \right)
\]

\( \varepsilon_0 \rightarrow \) constant shift

Debye-energy = mean phonon energy

This means:

\[
\varepsilon_k \uparrow \quad \Theta \left( \varepsilon_0 - 1 \varepsilon_k - \mu \right) \quad \Theta \left( \varepsilon_0 - 1 \varepsilon_k' - \mu \right) \quad \Theta \text{-functions contribute in this energy region}
\]

Importantly, the above approx. for \( \langle \mathbf{v} \rangle \rightarrow \) into the gap eq. one finds

\[
\Delta \varepsilon = \frac{1}{2} \frac{9}{2 \varepsilon_0} \sum \Theta \left( \varepsilon_0 - 1 \varepsilon_k - \mu \right) \frac{\Delta \varepsilon'}{\sqrt{\varepsilon_k'^2 + \Delta \varepsilon'^2}}
\]

with the solution (see FW):

\[
\Delta \varepsilon = \Delta \cdot \Theta \left( \varepsilon_0 - 1 \varepsilon_k - \mu \right)
\]

and the constant gap \( \Delta \) is determined from [and \((***) \rightarrow (*)\)]:

\[
1 = \frac{9}{2 \varepsilon_0} \sum \Theta \left( \varepsilon_0 - 1 \varepsilon_k - \mu \right) \frac{1}{\sqrt{\Delta^2 + (\varepsilon_k - \mu)^2}}
\]

Replacing \( \sum \rightarrow S \varepsilon d^3 \varepsilon \), one finds (FW 37.49):
We see that the Fermi energy is no longer sharply defined; it has been smeared out in energy over a range corresponding to the Debye energy $\Theta_D$.

**Energy difference: supercond. g.s. - normal g.s.**

**Nomenclature:**
- $E_s$ = supercond. g.s. energy
- $E_n$ = normal g.s. energy

We have seen that the Fermi potential at $T=0$ is for the g.s.

\[
\Omega(T=0) = E - \mu N = U \Rightarrow E = U + \mu N
\]

See eq. (22)

Hence, we can express the energy difference as follows:

\[
E_s - E_n = (U_s - U_n) + (\mu_s - \mu_n) N \approx U_s - U_n
\]

$\approx 0$ (little change in Fermi energy)

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

\[
E_s - E_n = -(N_{\text{pair}} \times \Delta) < 0
\]

where $\Delta$ is the binding energy of one Cooper pair and $N_{\text{pair}}$ is the number of Cooper pairs within an energy shell of thickness $\Delta$ around the "Fermi surface" $\mu$.
A few remarks about BCS theory at finite $T$

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

One finds the following interesting result:

**Fig. 51.1**

(FW p. 449)

![Graph showing pairing gap as a function of $T$.](image)

Relation: pairing gap $\Delta(T = 0)$ and $T_c$

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

$$\hbar T_c \approx 1.13 \, \text{t} \, \omega, \exp \left[ -\frac{1}{N(0) g} \right] \quad (1)$$

Recall expression for $\Delta(T = 0)$, p. 124:

$$\Delta(T = 0) = 2 \, \text{t} \, \omega_d \exp \left[ -\frac{1}{N(0) g} \right] \quad (2)$$

Take ratio of (1) and (2):

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

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

FW, eq. (51.44)
What causes superconductivity?

**Rigorous Theory:** Fetter & Walecka, § 52

**Phenomenology:** E. Berg & Resnick, Quantum Physics, 2nd ed., p. 487 - 488

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

If we add an ext. $E$-field, all Cooper pairs have exactly the same pair momentum $\vec{P}(t)$ → highly correlated motion

→ no "random-moion scattering with lattice imperfections → zero electrical resistance.

Pairing in atomic nuclei (brief discussion)

→ see PowerPoint slides on Website?