BCS

PRELIMINARY NOTES BY L. G. MOLINARI

Measurements of T_c of isotopes of Mercury led independently, in 1950, Emanuel Maxwell and the group of Reynolds to discover the *isotope effect*: $T_c \approx M^{-1/2}$, where M is the ionic mass. The discovery was crucial, showing that phonons are relevant in superconductivity. Soon after John Bardeen published a note [1], and Herbert Fröhlich [2] a paper he was working on.
The interaction of two electrons mediated by a phonon exchange is

$$U^0(k,\omega) = g\frac{v_s^2 k^2}{\omega^2 - v_s^2 k^2}\theta(\omega_D - v_s\, k) \tag{1}$$

with the Debye cutoff. In the narrow energy shell $|\epsilon - \epsilon_F| < \hbar\omega_D$ the interaction is attractive. Since at low T the electronic properties are precisely determined by the particles in the energy shell of width $\sim k_B T$ near the Fermi surface, this feature is important.

... at that time, it appeared that the main problem of the microscopic theory was to show how electron-phonon interactions might yield an energy gap.
That electron-phonon interactions lead to an effective attractive interaction between electrons by exchange of virtual phonons was shown by Fröhlich by use of field-theoretic techniques. His analysis was extended by Pines and myself to include Coulomb interactions. In second order, there is an effective interaction between the quasi-particle excitations of the normal state which is the sum of the attractive phonon-induced interaction and a screened Coulomb interaction ...

The next major step was made by Cooper, who, following up this approach, showed that if there is an effective attractive interaction, a pair of quasi-particles above the Fermi sea will form a bound state no matter how weak the interaction.
If the binding energy is of the order of $k_B T_c$, the size of the pair wave function is of the order of 10^{-5} to 10^{-4} cm. This calculation showed definitely that, in the presence of attractive interactions, the Fermi sea which describes the ground state of the normal metal is unstable against the formation of such bound pairs. However, one could not use this calculation immediately to construct a theory of superconductivity. If all of the electrons within $\approx k_B T_c$ of the Fermi surface form such bound pairs, the spacing between the pairs would be only 10^{-6} cm, a distance much smaller than the size of a pair. Because of the considerable overlap between the pairs, and because of the exclusion principle and required anti-symmetry of the wave functions, they cannot be regarded as moving independently. Thus, the picture proposed earlier by Schafroth (1955), and developed more completely in cooperation with Butler and Blatt of electron pairs as "localized entities (pseudo-molecules) whose center-of-gravity motion is essentially undisturbed", and which at low temperatures undergo an Einstein–Bose condensation is not valid. New methods were required to construct a theory of superconductivity, and this was first accomplished by the joint

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efforts of Cooper, Schrieffer, and myself. (J. Bardeen [4])

In 1954 Max Robert Schafroth made the hypothesis that electrons bind in charged pairs in space, that undergo Bose-Einstein condensation [3].

In 1956, Leon Cooper showed that two electrons with an attractive potential in a shell $(\epsilon_F, \epsilon_F + \hbar\omega_D)$ in momentum space, in presence of electrons that fill the Fermi sphere, can form a bound state [5]. Such Cooper pair has zero total momentum and spin, and a binding energy of the expected size $\Delta \sim k_B T_C$.

In momentum space, the eigenfunctions of $H = \frac{1}{2m}(p_1^2 + p_2^2) + U$ have the form

$$\psi(\mathbf{x_1}\omega_1, \mathbf{x_2}\omega_2) = \frac{1}{V}\sum\nolimits_{\mathbf{k_1}\mathbf{k_2}} c(\mathbf{k_1}, \mathbf{k_2}) e^{i(\mathbf{k_1}\cdot\mathbf{x_1} + \mathbf{k_2}\cdot\mathbf{x_2})}\, \chi_{s,m_s}(\omega_1, \omega_2)$$

with $|\mathbf{k}_i| > k_F$ (the states in the Fermi sphere are unavailable). The function c is symmetric for the exchange of $\mathbf{k_1}$ and $\mathbf{k_2}$ for $s = 0$ (singlet) and antisymmetric for $s = 1$ (triplet).

The center of mass has zero kinetic energy if $\mathbf{k_1} + \mathbf{k_2} = 0$. With this choice that lowers the energy, the eigenvalue equation for $c(\mathbf{k}) = c(\mathbf{k}, -\mathbf{k})$ is

$$\frac{\hbar^2 k^2}{m} c(\mathbf{k}) + \sum\nolimits_{\mathbf{k}'} \langle \mathbf{k}, -\mathbf{k}|U|\mathbf{k}', -\mathbf{k}'\rangle c(\mathbf{k}') = E\, c(\mathbf{k}), \quad |\mathbf{k}'| > k_F$$

The matrix element is supposed to be $-g/V$ if both momenta are in the energy shell $\Gamma = \{\mathbf{k} : \epsilon_F < \epsilon_{\mathbf{k}} < \epsilon_F + \hbar\omega_D\}$. To take advantage only of the attractive part of the interaction, $c(\mathbf{k})$ is chosen to vanish outside Γ.

$$\left(E - \frac{\hbar^2 k^2}{m}\right) c(\mathbf{k}) = -\frac{g}{V} \sum_{\mathbf{k}' \in \Gamma} c(\mathbf{k}')$$

The sum in r.h.s. is a constant $-gC$:

$$c(k) = -g\frac{C}{E - 2\epsilon_k}$$

where $\epsilon_k = \hbar^2 k^2/2m$. A self-consistency condition arises by summing both sides on $\mathbf{k} \in \Gamma$. C cancels and an equation for the energy E of the bound state is obtained:

$$-\frac{1}{g} = \int_\Gamma \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{E - 2\epsilon_k} = \int_\Gamma d\epsilon \frac{\rho(\epsilon)}{E - 2\epsilon}$$

$\rho(\epsilon)$ is the density of states for free electrons per spin component and unit volume. Since $\hbar\omega_D \ll \epsilon_F$, the density is nearly constant in Γ and is taken out

$$-\frac{1}{g\rho(\epsilon_F)} = \int_{\epsilon_F}^{\epsilon_F + \hbar\omega_D} \frac{d\epsilon}{E - 2\epsilon} = -\frac{1}{2}\log\frac{|E - 2\epsilon_F - 2\hbar\omega_D|}{|E - 2\epsilon_F|} = -\frac{1}{2}\log\frac{\Delta + \hbar\omega_D}{\Delta}$$

where Δ is the *binding energy* of the pair: $E = 2\epsilon_F - \Delta$.

It is: $\Delta = (\Delta + 2\hbar\omega_D)\exp(-2/\rho_F g)$. Because of the exponential factor it is $\Delta \ll \hbar\omega_D$. The non-perturbative formula is obtained:

$$\Delta \approx 2\hbar\omega_D \exp\left(-\frac{2}{\rho(\epsilon_F) g}\right) \tag{2}$$

According to the microscopic theory g is the square of the electron-phonon coupling. For the electron gas $\rho(\epsilon_F) = \frac{3}{4}n/\epsilon_F$,where n is the density of electrons and ϵ_F is the Fermi energy[1].

The Cooper pair is destroyed at thermal energy $k_B T_c \approx \Delta \ll k_B T_D$.
The wave-function of the Cooper pair is a spin-singlet (s=0) and, with $\mathbf{r} = \mathbf{x_1} - \mathbf{x_2}$

$$\psi(r) \propto \int_\Gamma \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{2\epsilon_F - \Delta - 2\epsilon_k}$$

The size of a Cooper pair is estimated in momentum space through the integral

$$\langle r^2 \rangle = \frac{\int_\Gamma d\mathbf{k}\, c(k)(-\hbar^2\nabla^2 c)(k)}{\int_\Gamma d\mathbf{k}\, c(k)^2}$$

The square root gives a size much larger than lattice spacing: $r/a_0 \approx (T_F/T_c) \approx 10^4$. This feature makes microscopic details of many (type I) superconductors irrelevant and a mean field description possible.

1. The BCS Hamiltonian

The BCS theory[2] (1957) is a many-electron model, characterized by the attractive interaction that arises in the static limit of the phonon exchange (1) $U^0 = -g\delta(\mathbf{x} - \mathbf{x}')$, which captures the essence [6].

In working out the properties of our simplified model and comparing with experimental results on real metals, we were continually amazed at the excellent agreement obtained. If there was serious discrepancy, it was usually found on rechecking that an error was made in the calculations. Everything fitted together neatly like the pieces of a jigsaw puzzle ... [4].

The theory is here presented in the matrix formulation by Nambu [11].

$$\hat{K} = \int d\mathbf{x} \left[\hat\psi_\uparrow^\dagger k_x \hat\psi_\uparrow + \hat\psi_\downarrow^\dagger k_x \hat\psi_\downarrow - \frac{g}{2}(\hat\psi_\uparrow^\dagger \hat\psi_\downarrow^\dagger \hat\psi_\downarrow \hat\psi_\uparrow + \hat\psi_\downarrow^\dagger \hat\psi_\uparrow^\dagger \hat\psi_\uparrow \hat\psi_\downarrow) \right] \tag{3}$$

where $k_x = \frac{1}{2m}(\mathbf{p} + \frac{e}{c}\mathbf{A})^2 + U(\mathbf{x}) - \mu$ and the Debye cut-off is understood for the attractive interaction.
An integration by parts and an anticommutation bring $\hat\psi_\uparrow^\dagger k_x \hat\psi_\uparrow$ to $-\hat\psi_\uparrow \overline{k}_x \hat\psi_\uparrow^\dagger$ up to a constant[3]. In the quartic interaction the two spin configurations are equivalent:

$$\hat\psi_\uparrow^\dagger \hat\psi_\downarrow^\dagger \hat\psi_\downarrow \hat\psi_\uparrow = \hat\psi_\downarrow^\dagger \hat\psi_\uparrow^\dagger \hat\psi_\uparrow \hat\psi_\downarrow$$

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[1]If z_c is the number of conducting electrons per ion, M_i is the ionic mass, m_e is the electron mass ($m_p/m_e = 1836$), v_F is the Fermi velocity and v_s is the speed of sound, it is

$$\rho(\epsilon_F) g = \frac{z_c}{6}\frac{m_e}{M_i}\left(\frac{v_F}{v_s}\right)^2$$

Al: $v_s = 6320$m/s, $v_F = 2.02 \times 10^6$m/s, $M = 27 m_p$, $z_c = 3$, $\rho_F g = 1.030$.
Sn: $v_s = 3320$m/s, $v_F = 1.90 \times 10^6$m/s, $M = 118 m_p$, $z_c = 4$, $\rho_F g = 1.0078$. These values in the formula give a factor around 0.13.

[2]At the time, Leon Cooper and Robert Schrieffer were respectively post-doc and graduate student of John Bardeen. Read the nice historical account by Hoddeson [13]

[3]The operators k_x and $\overline{k}_x$ differ by the sign of the term linear in $\mathbf{p}$, if any.

The interaction is simplified as in Hartree-Fock theory, by replacing pairs of creation and destruction operators with their mean values, $\hat\psi^\dagger_\downarrow\hat\psi^\dagger_\uparrow\hat\psi_\uparrow\hat\psi_\downarrow \approx \langle\hat\psi^\dagger_\downarrow\hat\psi^\dagger_\uparrow\rangle\hat\psi_\uparrow\hat\psi_\downarrow + \hat\psi^\dagger_\downarrow\hat\psi^\dagger_\uparrow\langle\hat\psi_\uparrow\hat\psi_\downarrow\rangle$. This is reminiscent of Cooper pairs, and introduces a complex field

$$\boxed{\Delta(x) = -g\langle\,\hat\psi_\uparrow(\mathbf{x})\hat\psi_\downarrow(\mathbf{x})\rangle} \tag{4}$$

It is an order parameter for superconductivity, and will be shown to be proportional to the Ginzburg-Landau field. The thermal average is calculated with the effective Hamiltonian, that no longer conserves the number of electrons

$$\hat K_{\rm BCS} = \int d\mathbf{x}\,\left[-\hat\psi_\uparrow\overline{k}_x\hat\psi^\dagger_\uparrow + \hat\psi^\dagger_\downarrow k_x\hat\psi_\downarrow + \overline{\Delta}\hat\psi_\uparrow\hat\psi_\downarrow + \hat\psi^\dagger_\downarrow\hat\psi^\dagger_\uparrow\Delta\right].$$

The effective Hamiltonian is written in the matrix form:

$$\boxed{\hat K_{\rm BCS} = \int d\mathbf{x}\,\Psi^\dagger(\mathbf{x})(\mathbb{K}_x\Psi)(\mathbf{x})} \tag{5}$$

$$\Psi^\dagger(\mathbf{x}) = \left[\hat\psi^\dagger_\downarrow(\mathbf{x}),\,\hat\psi_\uparrow(\mathbf{x})\right],\quad \mathbb{K}_x = \begin{bmatrix} k_x & \Delta(\mathbf{x}) \\ \overline{\Delta}(\mathbf{x}) & -\overline{k}_x\end{bmatrix},\quad \Psi(\mathbf{x}) = \begin{bmatrix}\hat\psi_\downarrow(\mathbf{x}) \\ \hat\psi^\dagger_\uparrow(\mathbf{x})\end{bmatrix} \tag{6}$$

The components of Ψ and $\Psi^\dagger$ anticommute (note that $(\Psi_r)^\dagger = (\Psi^\dagger)_r$):

$$\{\Psi_r(\mathbf{x}),\Psi^\dagger_s(\mathbf{y})\} = \delta_{rs}\delta_3(\mathbf{x}-\mathbf{y}),\qquad \{\Psi_r,\Psi_s\} = \{\Psi^\dagger_r,\Psi^\dagger_s\} = 0. \tag{7}$$

As the effective Hamiltonian is quadratic in the fields, the model can be solved as a theory of independent particles, with the self-consistent *gap equation* eq.(4). Two equivalent approaches to solution are presented:
• Green functions (Gorkov, 1958 [9] adapted in Nambu's matrix formalism);
• Canonical transformation (de Gennes). The operator $\mathbb{K}_x$ is diagonalized, and canonical operators adapted to the new basis replace the field operators. It generalises the canonical transformation for homogeneous systems by Bogoliubov and Valatin (1958).

2. The Nambu - Gorkov theory

There are advantages in studying the BCS model with the Green function formalism. The imaginary time evolution of operators is $O(\tau) = e^{\tau K/\hbar}Oe^{-\tau K/\hbar}$, where K is the effective hamiltonian (5). The equation of motion of $\Psi(\mathbf{x},\tau)$ is:

$$\begin{aligned}-\hbar\frac{\partial}{\partial\tau}\Psi_r(\mathbf{x},\tau) &= e^{\frac{1}{\hbar}\tau\hat K}[\Psi_r(\mathbf{x}),\hat K]e^{-\frac{1}{\hbar}\tau\hat K}\\ &= e^{\frac{1}{\hbar}\tau\hat K}\int d\mathbf{x}'[\Psi_r(\mathbf{x}),\Psi^\dagger_{s'}(\mathbf{x}')(\mathbb{K}_{s's}\Psi_s)(\mathbf{x}')]e^{-\frac{1}{\hbar}\tau\hat K}\\ &= e^{\frac{1}{\hbar}\tau\hat K}\int d\mathbf{x}'\{\Psi_r(\mathbf{x}),\Psi^\dagger_{s'}(\mathbf{x}')\}(\mathbb{K}_{s's}\Psi_s)(\mathbf{x}')e^{-\frac{1}{\hbar}\tau\hat K}\\ &= (\mathbb{K}_{rs}\Psi_s)(\mathbf{x},\tau)\end{aligned}$$

Let us introduce the thermal Nambu propagator

$$\boxed{-\mathbb{G}(x,x') = \langle\mathcal{T}\Psi(x)\Psi^\dagger(x')\rangle} \tag{8}$$

It is a matrix with components

$$\mathbb{G}(x,x') = -\begin{bmatrix} \langle \mathcal{T}\psi_\downarrow(x)\psi_\downarrow^\dagger(x')\rangle & \langle \mathcal{T}\psi_\downarrow(x)\psi_\uparrow(x')\rangle \\ \langle \mathcal{T}\psi_\uparrow^\dagger(x)\psi_\downarrow^\dagger(x')\rangle & \langle \mathcal{T}\psi_\uparrow^\dagger(x)\psi_\uparrow(x')\rangle \end{bmatrix} = \begin{bmatrix} \mathscr{G}(x,x') & \mathscr{F}(x,x') \\ \mathscr{F}^\dagger(x,x') & -\mathscr{G}(x',x) \end{bmatrix}$$

Note the sign and the exchange of x and x' in one component. The correlators $\mathscr{F}$ and $\mathscr{F}^\dagger$ are named *anomalous* and vanish in the normal phase. In particular:

$$\boxed{\Delta(\mathbf{x}) = -g\mathscr{F}(x,x^+)} \tag{9}$$

The equation of motion of the Nambu propagator,

$$\left[\hbar\frac{\partial}{\partial\tau} + \mathbb{K}_x\right]\mathbb{G}(x,x') = -\hbar\delta_4(x-x')\,\mathbb{I}_2 \tag{10}$$

simplifies in Matsubara (odd) frequency space:

$$\begin{bmatrix} -i\hbar\omega_n + k_x & \Delta(\mathbf{x}) \\ \overline{\Delta}(\mathbf{x}) & -i\hbar\omega_n - \overline{k}_x \end{bmatrix}\mathbb{G}(\mathbf{x},\mathbf{x}';i\omega_n) = -\hbar\delta_3(\mathbf{x}-\mathbf{x}')\,\mathbb{I}_2 \tag{11}$$

$$\mathbb{G}(\mathbf{x},\mathbf{x}',i\omega_n) = \begin{bmatrix} \mathscr{G}(\mathbf{x},\mathbf{x}',i\omega_n) & \mathscr{F}(\mathbf{x},\mathbf{x}',i\omega_n) \\ \mathscr{F}^\dagger(\mathbf{x},\mathbf{x}',i\omega_n) & -\mathscr{G}(\mathbf{x}',\mathbf{x},-i\omega_n) \end{bmatrix} \tag{12}$$

When $\Delta = 0$, eq.(10) is solved by the normal Nambu propagator

$$\mathbb{G}_n(x,x') = \begin{bmatrix} \mathscr{G}_n(x,x') & 0 \\ 0 & -\mathscr{G}_n(x',x) \end{bmatrix}$$

The normal solution is used to transform (10) into a Dyson equation (integration of repeated variables is implicit):

$$\mathbb{G}(x,y) = \mathbb{G}_n(x,y) + \frac{1}{\hbar}\mathbb{G}_n(x,x')\mathbb{D}(\mathbf{x}')\mathbb{G}(x',y), \quad \mathbb{D}(\mathbf{x}) = \begin{bmatrix} 0 & \Delta \\ \overline{\Delta} & 0 \end{bmatrix} \tag{13}$$

In BCS theory the self-energy $\mathbb{D}$ is local and time-independent. The BCS description was found inadeguate for elements like Pb, and a microscopic model with the full phonon-electron interaction was considered. The Dyson equation becomes

$$\mathbb{G}(x,y) = \mathbb{G}_n(x,y) + \mathbb{G}_n(x,x')\mathbb{S}(x',x'')\mathbb{G}(x'',y). \tag{14}$$

where now $\mathbb{S}$ is a bi-local proper self-energy matrix. The 1-phonon exchange diagram $\mathbb{S}(x,y) = -\frac{1}{\hbar}\mathbb{G}(x,y)U^0(x-y)$ is the basis of the strong-coupling theory by Eliashberg (see the handbook by Zakoskin [14]).

The homogeneous solution. In **k**-space the equation of motion (11) for the Nambu propagator is algebraic

$$\begin{bmatrix} i\hbar\omega_n - \xi_k & -\Delta \\ -\overline{\Delta} & i\hbar\omega_n + \xi_k \end{bmatrix}\mathbb{G}(k;i\omega_n) = \hbar\,\mathbb{I}_2$$

with $\xi_k = \epsilon_k - \mu$. The solution is obtained by matrix inversion:

$$\mathbb{G}(k;i\omega_n) = \frac{-\hbar}{\hbar^2\omega_n^2 + \xi_k^2 + |\Delta|^2}\begin{bmatrix} i\hbar\omega_n + \xi_k & \Delta \\ \overline{\Delta} & i\hbar\omega_n - \xi_k \end{bmatrix} \tag{15}$$

The normal and anomalous propagators are obtained:

$$\mathscr{G}(k,i\omega_n) = -\hbar\frac{i\hbar\omega_n + \xi_k}{\hbar^2\omega_n^2 + E_k^2} = \frac{|u_k|^2}{i\omega_n - (E_k/\hbar)} + \frac{|v_k|^2}{i\omega_n + (E_k/\hbar)}$$

$$\mathscr{F}(k,i\omega_n) = -\hbar\frac{\Delta}{\hbar^2\omega_n^2 + E_k^2} = \frac{u_k\overline{v}_k}{i\omega_n - (E_k/\hbar)} - \frac{u_k\overline{v}_k}{i\omega_n + (E_k/\hbar)}$$

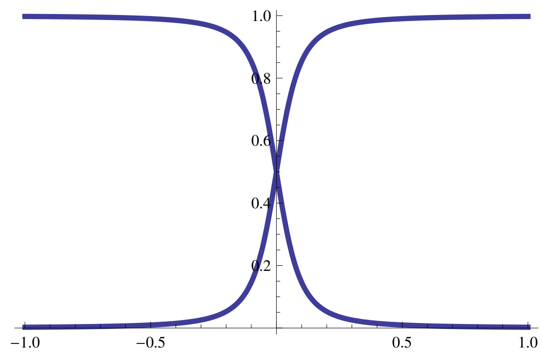

FIGURE 1. The parameters $|u_k|^2$ and $|v_k|^2$ as functions of ξ_k for $|\Delta| = 0.1$.

$$|u_k|^2 = \frac{1}{2}\left(1+\frac{\xi_k}{E_k}\right), \quad |v_k|^2 = \frac{1}{2}\left(1-\frac{\xi_k}{E_k}\right), \quad u_k\overline{v}_k = \frac{\Delta}{2E_k} \tag{16}$$

$$\boxed{E_k = \sqrt{\xi_k^2 + |\Delta|^2}} \tag{17}$$

E_k is the excitation energy of a single electron, with minimum value $|\Delta|$. To break a Cooper pair, two electrons must be excited. Therefore the minimal excitation energy of a superconductor is $2|\Delta|$.
This existence of an energy gap at the Fermi energy is an important result of the BCS theory. It is an energy interval depleted of states (see Fig.2). Its presence explains many properties of superconductors such as:
- *exponential suppression of specific heat* at $T << T_c$;
- *absence of absorption of infrared light* with $\hbar\omega < 2\Delta$;
- *tunneling in n-s or s-s junctions* (Giavaert, 1960). It provides a direct measure of the gap as the jump of the voltage versus tunneling current.
In the normal phase $E_k = |\xi_k|$; then $|u_k| = \theta(\epsilon_k - \mu)$, $|v_k| = \theta(\mu - \epsilon_k)$ and the normal thermal Green function results.

The spectral density of the superconducting phase

$$\rho_s(E) = \sum_{\mathbf{k}} |u_k|^2\delta(E-E_k) + |v_k|^2\delta(E+E_k)$$

(use the approximation $|\Delta| \ll \mu$) clearly shows a sharp energy gap of width 2Δ centred at the chemical potential.

$$\frac{\rho_s(E)}{\rho_0} = \begin{cases} \frac{-E+\sqrt{E^2-\Delta^2}}{\sqrt{E^2-\Delta^2}}\sqrt{1+\frac{E}{\mu}} + \frac{|E|-\sqrt{E^2-\Delta^2}}{\sqrt{E^2-\Delta^2}}\sqrt{1-\frac{E}{\mu}} & -\mu < E < -\Delta \\ 0 & -\Delta < E < \Delta \\ \frac{E-\sqrt{E^2-\Delta^2}}{\sqrt{E^2-\Delta^2}}\sqrt{1-\frac{E}{\mu}} + \frac{E+\sqrt{E^2-\Delta^2}}{\sqrt{E^2-\Delta^2}}\sqrt{1+\frac{E}{\mu}} & \Delta < E < \mu \\ 2\sqrt{1+\frac{E}{\mu}} & \mu < E \end{cases} \tag{18}$$

Near the gap $\rho_s(E) \approx 2\rho_0|E|/\sqrt{E^2-\Delta^2}$.

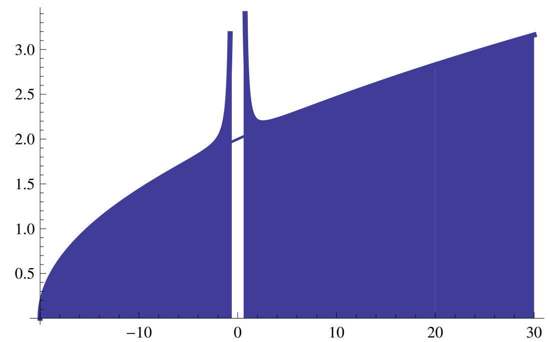

FIGURE 2. The spectral density $\rho_s(E)$, where $E = 0$ at the chemical potential. The thin line is $\rho(E)/\rho(0) = \sqrt{E+\mu}$ of the normal phase; the gap 2Δ is centred on the chemical potential (unrealistic parameters are here used, $\mu = 20$, $\Delta = 0.6$)

The average number of electrons in a state $(\mathbf{k}, \sigma)$ is

$$n_k = \frac{1}{\hbar\beta}\sum_n \mathscr{G}(k, i\omega_n) = \frac{1}{2} - \frac{1}{2}\frac{\xi_k}{E_k}\tanh\left(\frac{\beta \mathrm{E_k}}{2}\right) \tag{19}$$

For $T = 0$ it coincides with v_k^2, that differs from the Fermi distribution in an interval $2\Delta(0)$ centred in $\xi = 0$.

3. THE GAP EQUATION

The gap parameter $\Delta(T)$ is given by the gap equation, where $\mathscr{F}$ is known:

$$\Delta = -\frac{g}{\hbar\beta}\sum_n \int \frac{d\mathbf{k}}{(2\pi)^3}\mathscr{F}(k, i\omega_n)e^{i\omega_n\eta} \tag{20}$$

After the Matsubara sum (20), it is:

$$\frac{1}{g} = \frac{1}{V}\sum_{\mathbf{k}} \frac{1}{2E_k}\tanh\left(\frac{\beta}{2}\mathrm{E_k}\right)\theta(\hbar\omega_{\mathrm{D}} - |\xi_{\mathrm{k}}|)$$

Insertion of the unity $1 = \int d\xi\delta(\xi - \xi_k)$ results in the density of states per unit volume and single spin component of the normal phase, $\rho(\xi) = \frac{1}{V}\sum_{\mathbf{k}}\delta(\xi - \xi_k)$, The sum in $\mathbf{k}$-space is changed to an integral in energy,

$$1 = \frac{g}{2}\int d\xi\, \rho(\xi)\frac{\tanh\left(\frac{1}{2}\beta\sqrt{\xi^2 + |\Delta|^2}\right)}{\sqrt{\xi^2 + |\Delta|^2}}\theta(\hbar\omega_D - |\xi|)$$

The density of states is almost constant in the thin energy shell $|\xi| < \hbar\omega_D$:

$$\boxed{\frac{1}{g\rho(0)} = \int_0^{\hbar\omega_D} d\xi \frac{\tanh\left(\frac{1}{2}\beta\sqrt{\xi^2 + \Delta^2}\right)}{\sqrt{\xi^2 + \Delta^2}} \qquad \textsf{gap equation}} \tag{21}$$

where $\rho(0)$ is the density of states at the Fermi energy, g is the squared coupling constant of the electron-phonon vertex.

• $\mathbf{T=0}$. The gap equation becomes:

$$\frac{1}{g\rho_0} = \int_0^{\hbar\omega_D} d\xi \, \frac{1}{\sqrt{\xi^2+\Delta_0^2}}$$

with solution similar to Cooper's result for the binding energy of a pair:

$$\Delta_0 = \frac{\hbar\omega_D}{\sinh\frac{1}{g\rho(0)}} \approx 2\hbar\omega_D \exp\left(-\frac{1}{g\rho_0}\right) \tag{22}$$

The first correction is exponentially small:

$$\Delta(T) = \Delta_0 - \sqrt{2\pi k_B T \Delta_0}\, \exp(-\frac{\Delta_0}{k_B T}) \tag{23}$$

• $\mathbf{T=T_c}$. At the critical temperature the order parameter Δ is zero, and the gap equation is an equation for T_c:

$$\begin{aligned}\frac{1}{g\rho_0} &= \int_0^{\hbar\omega_D} \frac{d\xi}{\xi} \tanh\left(\tfrac12 \beta_c\xi\right) = \int_0^{x_c} \frac{dx}{x} \tanh x \\ &= \tanh\left(x_c\right)\log(x_c) - \int_0^{x_c} dx\, \frac{\log x}{\cosh^2 x} \\ &\approx \log x_c - \int_0^{\infty} dx \frac{\log x}{\cosh^2 x} \\ &= \log x_c + \log(\frac{4}{\pi}e^C), \qquad x_c = \frac{\hbar\omega_D}{2k_BT_c} = \frac{T_D}{2T_c}\end{aligned}$$

The approximations are justified by $T_D/T_c \gg 1$. With $C \approx 0.5772..$, the result is

$$\boxed{k_BT_c \;=\; 1.134\; \hbar\omega_D \;\exp\left(-\frac{1}{g\rho_0}\right)} \tag{24}$$

The following universal ratio is obtained:

$$\boxed{\frac{2\Delta_0}{k_BT_c} = 2\pi e^{-C} \approx 3.52}$$

	$2\Delta_0/k_BT_c$
Al	3.53
Sn	3.63
Hg	3.95
La	3.72
Pb	3.95
Nb	3.65

From: L. P. Levy, Magnétisme et supraconductivité, EDP Sciences 1997.

Near T_c the order parameter is (see Remark 6.1)

$$\Delta(T) = \pi k_BT_c\sqrt{\frac{8}{7\zeta(3)}}\,\sqrt{1-\frac{T}{T_c}} \tag{25}$$

Proof. Let us start from the very beginning: $\Delta = -g\mathscr{F}(\mathbf{x}\tau,\mathbf{x}\tau^+)$. For the homogeneous system it is:

$$\Delta = 2g\rho_0\frac{1}{\beta}\sum_{\omega_n}\int_0^{\hbar\omega_D} d\xi \frac{\Delta}{\hbar^2\omega_n^2+\xi^2+\Delta^2}$$

near T_c the gap parameter is small, then we expand:

$$\frac{1}{g} = 2\rho_0\frac{1}{\beta}\sum_{\omega_n}\int_0^{\hbar\omega_D} d\xi \left[\frac{1}{\hbar^2\omega_n^2+\xi^2} - \frac{\Delta^2}{(\hbar^2\omega_n^2+\xi^2)^2}+\dots\right]$$

The Matsubara sums are evaluated in the first integral with temperature β:

$$\frac{1}{g\rho_0} = \int_0^{\frac{1}{2}\beta\hbar\omega_D} \frac{dx}{x}\tanh x - 2\frac{\Delta^2}{\beta}\sum_{\omega_n}\int_0^{\hbar\omega_D} d\xi \frac{1}{(\hbar^2\omega_n^2+\xi^2)^2}$$

In the second integral Δ is small and we can set the Matsubara frequencies at $T = T_c$. With $\xi = \hbar|\omega_n|x$ the second term is

$$-2\frac{\Delta^2}{\beta_c}\sum_{\omega_n}\frac{1}{(\hbar|\omega_n|)^3}\int_0^{\omega_D/|\omega_n|}\frac{dx}{(1+x^2)^2}$$

The upper limit is put ∞ with small error (because of the weight in front of the integral, and because of the decay of the function as $1/x^4$. It becomes:

$$-2\frac{\Delta^2}{\pi^3(k_BT_c)^2}2\sum_{n=0}^{\infty}\frac{1}{(2n+1)^3}\frac{\pi}{4} = -\frac{\Delta^2}{(\pi k_BT)^2}\frac{7}{8}\zeta(3)$$

The equation for $1/g$ now is:

$$\frac{1}{g\rho_0} = \int_0^{\frac{1}{2}\beta\hbar\omega_D}\frac{dx}{x}\tanh x - \frac{\Delta^2}{(\pi k_BT)^2}\frac{7}{8}\zeta(3) \tag{26}$$

The first integral, at $\beta = \beta_c$ is precisely $1/g\rho_0$ Then:

$$\int_{\frac{1}{2}\beta\hbar\omega_D}^{\frac{1}{2}\beta_c\hbar\omega_D}\frac{dx}{x}\tanh x = -\frac{\Delta^2}{(\pi k_BT)^2}\frac{7}{8}\zeta(3)$$

The function $\tanh x$ is 1 for large x. The integral is now $\log(T/T_c)$. Write $T = T_c - (T_c - T_T)$ in the log and expand for small $T_c - T$:

$$1 - \frac{T}{T_c} = \frac{\Delta^2}{(\pi k_BT_c)^2}\frac{7}{8}\zeta(3)$$

The result is obtained. □

4. Thermodynamics

If $K_\lambda = K_0 + \lambda V$, then $\frac{d}{d\lambda}Z_\lambda = \frac{d}{d\lambda}\mathrm{tr}(e^{-\beta K_\lambda}) = -\beta Z_\lambda\langle V\rangle_\lambda$. Integration gives the difference of thermodynamic potentials $\Omega_1 - \Omega_0 = \int_0^1 d\lambda\langle V\rangle_\lambda$, where the thermal average is evaluated with K_λ.

In BCS we have $K_s = K_n - g\int d\mathbf{x}(\psi_\downarrow^\dagger\psi_\uparrow^\dagger\psi_\uparrow\psi_\downarrow)$. The formula gives:

$$\begin{aligned}\Omega_s - \Omega_n &= -\int_0^g dg'\int d\mathbf{x}\langle\psi_\downarrow^\dagger\psi_\uparrow^\dagger\psi_\uparrow\psi_\downarrow\rangle_{g'}\\ &\approx -\int_0^g dg'\int d\mathbf{x}\langle\psi_\downarrow^\dagger\psi_\uparrow^\dagger\rangle_{g'}\langle\psi_\uparrow\psi_\downarrow\rangle_{g'} = -\int_0^g\frac{dg'}{g'^2}\int d\mathbf{x}|\Delta'(\mathbf{x})|^2\end{aligned}$$

For a homogeneous system:

$$\frac{\Omega_s - \Omega_n}{V} = -\int_0^g\frac{dg'}{g'^2}\Delta'^2$$

Differentiation of the gap equation gives:

$$-\frac{dg'}{g'^2} = d\Delta'\rho_0\frac{\partial}{\partial\Delta'}\int_0^{\hbar\omega_D}d\xi\frac{\mathrm{th}(\frac{\beta}{2}\sqrt{\xi^2+\Delta'^2}}{\sqrt{\xi^2+\Delta'^2}}$$

Now change to variable $\Delta' = \Delta(g')$ and integrate by parts:

$$\frac{\Omega_s - \Omega_n}{V} = \rho_0 \int_0^\Delta d\Delta' \Delta'^2 \frac{\partial}{\partial \Delta'} \int_0^{\hbar\omega_D} d\xi \frac{\text{th}(\frac{\beta}{2}\sqrt{\xi^2+\Delta'^2}}{\sqrt{\xi^2+\Delta'^2}}$$
$$= \rho_0 \Delta^2 \int_0^{\hbar\omega_D} d\xi \frac{\text{th}(\frac{\beta}{2}\sqrt{\xi^2+\Delta'^2}}{\sqrt{\xi^2+\Delta'^2}} - 2\rho_0 \int_0^\Delta d\Delta'\Delta' \int_0^{\hbar\omega_D} d\xi \frac{\text{th}(\frac{\beta}{2}\sqrt{\xi^2+\Delta'^2}}{\sqrt{\xi^2+\Delta'^2}}$$
$$= \frac{\Delta^2}{g} - 2\rho_0 \int_0^{\hbar\omega_D} d\xi \int_0^\Delta d\Delta'\Delta' \frac{\text{th}(\frac{\beta}{2}\sqrt{\xi^2+\Delta'^2}}{\sqrt{\xi^2+\Delta'^2}}$$

change variable to $x = \dfrac{\beta}{2}\sqrt{\xi^2+\Delta'^2}$

$$= \frac{\Delta^2}{g} - 4\frac{\rho_0}{\beta}\int_0^{\hbar\omega_D} d\xi \int_{\frac{\beta}{2}\xi}^{\frac{\beta}{2}\sqrt{\xi^2+\Delta^2}} dx\, \text{th}x$$
$$= \frac{\Delta^2}{g} - \frac{4\rho_0}{\beta}\int_0^{\hbar\omega_D} d\xi \left[\log\cosh(\frac{\beta}{2}\sqrt{\xi^2+\Delta^2}) - \log\cosh(\frac{\beta}{2}\xi)\right]$$
$$= \frac{\Delta^2}{g} - 2\rho_0 \int_0^{\hbar\omega_D} d\xi \left[\sqrt{\xi^2+\Delta^2} - \xi\right] - \frac{4\rho_0}{\beta}\int_0^{\hbar\omega_D} d\xi \left[\log(1+e^{-\beta\sqrt{\xi^2+\Delta^2}}) - \log(1+e^{-\beta\xi})\right]$$

In the last integral the function is exponentially small for $\xi > \frac{\beta}{2}\hbar\omega_D$ and the upper limit can be set $+\infty$.

$$\int_0^\infty d\xi \log(1+e^{-\beta\xi}) = \frac{1}{\beta}\sum_{\ell=1}^\infty \frac{(-1)^{\ell+1}}{\ell}\int_0^\infty dx e^{-\ell x} = \frac{1}{\beta}\sum_{\ell=1}^\infty \frac{(-1)^{\ell+1}}{\ell^2} = \frac{1}{\beta}\frac{\pi^2}{12}$$
$$\int_0^{\hbar\omega_D} d\xi\sqrt{\xi^2+\Delta^2} = \Delta^2\int_0^{\bar\theta} d\theta\,\text{ch}^2(\theta) = \frac{\Delta^2}{2}\left[\bar\theta + \text{sh}(\bar\theta)\text{ch}(\bar\theta)\right]$$

where $\text{sh}\bar\theta = \frac{\hbar\omega_D}{\Delta} \gg 1$ is solved by $\bar\theta = \log(\frac{2\hbar\omega_c}{\Delta}) + \frac{1}{4}(\frac{\Delta}{\hbar\omega_D})^2 + \ldots$. Then:

$$\int_0^{\hbar\omega_D} d\xi\sqrt{\xi^2+\Delta^2} = \frac{\Delta^2}{2}\left[(\frac{\hbar\omega_D}{\Delta})^2 + \frac{1}{2} + \log(\frac{2\hbar\omega_D}{\Delta}) + \frac{1}{8}(\frac{\Delta}{\hbar\omega_D})^2 + \ldots\right]$$

We omit terms of order $(\Delta/\hbar\omega_D)^2$

$$\frac{\Omega_s - \Omega_n}{V} = \frac{\Delta^2}{g} - \rho_0\Delta^2\left[\log(\frac{2\hbar\omega_D}{\Delta}) + (\frac{\hbar\omega_D}{\Delta})^2 + \frac{1}{2} + \ldots\right] + \rho_0(\hbar\omega_D)^2$$
$$+ \frac{\pi^2}{3}\frac{\rho_0}{\beta^2} - \frac{4\rho_0}{\beta}\int_0^\infty d\xi\log(1+e^{-\beta\sqrt{\xi^2+\Delta^2}})$$
$$= \frac{\Delta^2}{g} - \rho_0\Delta^2\log(\frac{2\hbar\omega_D}{\Delta}) - \frac{\Delta^2}{2}\rho_0 + \frac{\pi^2}{3}\frac{\rho_0}{\beta^2} - \frac{4\rho_0}{\beta}\int_0^\infty d\xi\log(1+e^{-\beta\sqrt{\xi^2+\Delta^2}}) + \ldots$$

Simplify with eq.(22) for Δ_0: $\log(\frac{2\hbar\omega_D}{\Delta}) = \log\frac{\Delta_0}{\Delta} + \frac{1}{g\rho_0}$. Then:

$$\frac{\Omega_s - \Omega_n}{V} = -\rho_0\Delta^2\left[\log\frac{\Delta_0}{\Delta} + \frac{1}{2}\right] + \frac{\pi^2}{3}\frac{\rho_0}{\beta^2} - \frac{4\rho_0}{\beta}\int_0^\infty d\xi\log(1+e^{-\beta\sqrt{\xi^2+\Delta^2}}) \tag{27}$$

The thermodynamics is discussed in two limit cases: T near 0 and near T_c.

• $T \ll T_c$, where $\Delta(T) = \Delta_0 \left[1 - \sqrt{2\pi k_B T/\Delta_0} e^{-\Delta_0/k_B T} + ...\right] \equiv \Delta_0(1-\delta)$.
The expansion in small δ is made, with leading terms

$$\frac{\Omega_s - \Omega_n}{V} = -\frac{1}{2}\rho_0\Delta_0^2 + \frac{\pi^2}{3}\rho_0(k_B T)^2 - 4\rho_0 k_B T \int_0^\infty d\xi e^{-\beta\sqrt{\xi^2+\Delta_0^2}} + ...$$

The integral is dominated by the small $x \ll 1$ region:

$$\int_0^\infty d\xi e^{-\beta\sqrt{\xi^2+\Delta_0^2}} = \Delta_0 \int_0^\infty dx e^{-\beta\Delta_0\sqrt{1+x^2}} \approx \Delta_0 e^{-\beta\Delta_0} \int_0^\infty dx e^{-\frac{1}{2}\beta\Delta_0 x^2}$$
$$= \sqrt{k_B T \Delta_0} e^{-\beta\Delta_0} \sqrt{\frac{\pi}{2}}$$

Then:

$$\frac{\Omega_s - \Omega_n}{V} = -\frac{1}{2}\rho_0\Delta_0^2 + \frac{\pi^2}{3}\rho_0(k_B T)^2 - \rho_0\sqrt{2\pi\Delta_0}(k_B T)^{3/2} e^{-\beta\Delta_0} \quad (28)$$

Only the first term is non-zero for $T = 0$: it is the energy stored in the Cooper pairs per unit volume.
Since $N_s = N_n$ it is $\Delta\Omega/V = f_s - f_n$ (difference of free energies per unit volume), i.e. the (negative) condensation energy per unit volume. For $T \ll T_c$:

$$\frac{H_c(T)^2}{8\pi} = \frac{1}{2}\rho_0\Delta_0^2 \left[1 - \frac{2\pi^2}{3}\left(\frac{k_B T_c}{\Delta_0}\right)^2 \frac{T^2}{T_c^2} + ...\right]$$

It follows that $H_c(0) = \Delta_0\sqrt{4\pi\rho_0}$ and

$$\frac{H_c(T)}{H_c(0)} = 1 - \frac{\pi^2}{3}\left(\frac{k_B T_c}{\Delta_0}\right)^2 \frac{T^2}{T_c^2} + ... = 1 - \frac{e^{2C}}{3}\frac{T^2}{T_c^2} + ...$$

The universal ratio was used. The number is 1.06 and modifies the empirical law by K. Onnes. The difference of entropies per unit volume is (the largest terms are kept; note that $k_B T < \Delta_0$ in this limit):

$$s_s - s_n = -\frac{\partial}{\partial T}\frac{\Omega_s - \Omega_n}{V}$$
$$\approx -\frac{2\pi^2}{3}\rho_0 k_B T + 2\rho_0\sqrt{2\pi\Delta_0}(k_B T)^{3/2}\frac{\Delta_0}{k_B T^2} e^{-\Delta_0/k_B T}$$

The specific heats per unit volume can be obtained separately:

$$c_n = T\frac{\partial s_n}{\partial T} = \frac{2\pi^2}{3}\rho_0 k_B^2 T$$
$$c_s = 2\rho_0\sqrt{2\pi}k_B^2 T (\frac{\Delta_0}{k_B T})^{5/2} e^{-\beta\Delta_0}$$

• $T \approx T_c$. It is not easy to use the formula (27). We go back to:

$$\frac{\Omega_s - \Omega_n}{V} = \int_0^\Delta d\Delta' \Delta'^2 \frac{d}{d\Delta'}\frac{1}{g'}$$

The derivative is done easily with (26):

$$\frac{\Omega_s - \Omega_n}{V} = \int_0^\Delta d\Delta' \Delta'^2 \left[-\rho_0 \frac{2\Delta'}{(\pi k_B T_c)^2}\frac{7}{8}\zeta(3)\right] = -\frac{7}{16}\rho_0\zeta(3)\frac{\Delta^4}{(\pi k_B T_c)^2}$$

Insertion of the expression (25) for $\Delta(T)$ near T_c gives:

$$\frac{\Omega_s-\Omega_n}{V}=-\frac{1}{2}\rho_0(\pi k_BT_c)^2\frac{8}{7\zeta(3)}\left(1-\frac{T}{T_c}\right)^2=-\frac{H_c(T)^2}{8\pi} \tag{29}$$

With the value of $H_c(0)=\sqrt{4\pi\rho_0}\Delta_0$ found at $T=0$ we obtain, near T_c:

$$\frac{H_c(T)}{H_c(0)}=\frac{\pi k_BT_c}{\Delta_0}\sqrt{\frac{8}{7\zeta(3)}}\left(1-\frac{T}{T_c}\right)\approx 1.74\left(1-\frac{T}{T_c}\right)$$

The first fraction is the universal ratio e^C. The empirical law near T_c gives instead a factor 2.
The difference of the entropy densities

$$s_s-s_n=-\rho_0\frac{8\pi^2}{7\zeta(3)}k_B^2T_c\left(1-\frac{T}{T_c}\right)$$

gives the difference of specific heats at T_c:

$$c_s-c_n=T_c\frac{\partial}{\partial T}(c_s-c_n)=\rho_0\frac{8\pi^2}{7\zeta(3)}k_B^2T_c$$

With $c_n=\frac{2}{3}\pi^2\rho_0k_B^2T$ the ratio for the jump of specific heats at T_c is obtained:

$$\frac{c_s-c_n}{c_n}=\frac{12}{7\zeta(3)}=1.43 \tag{30}$$

Some experimental values are: 1.60 (Sn), 1.45 (Al), 2.71 (Pb).

5. The Meissner effect

In linear response, the current density in presence of a vector field is

$$J_i(x)=-\frac{e^2}{mc}n(\mathbf{x})A_i(x)-\frac{1}{\hbar c}\int dx'\mathscr{D}^R_{ij}(x,x')A_j(x')$$

The retarded correlator $i\mathscr{D}^R_{ij}(x,x')=\theta(t-t')\langle[\delta j_i(x),\delta j_j(x')]\rangle$ is evaluated through the T-ordered one $-\mathscr{D}_{ij}(\mathbf{x}\tau,\mathbf{y}\tau')=\langle\mathsf{T}j_i(\mathbf{x}\tau)j_j(\mathbf{y}\tau')\rangle_{conn}$.
The charged current operator (in absence of $\mathbf{A}$) is:

$$j_i(\mathbf{x})=-\frac{i\hbar e}{2m}\sum_\mu\left[\psi^\dagger_\mu\frac{\partial\psi_\mu}{\partial x_i}(\mathbf{x})-\frac{\partial\psi^\dagger_\mu}{\partial x_i}\psi_\mu(\mathbf{x})\right]$$

$$\begin{aligned}-\mathscr{D}_{ij}(\mathbf{x}\tau,\mathbf{y}\tau')&=\langle\mathsf{T}\delta j_i(\mathbf{x}\tau)\delta j_j(\mathbf{y}\tau')\rangle\\&=\left(-i\frac{e\hbar}{2m}\right)^2\left[\frac{\partial}{\partial x_1^i}-\frac{\partial}{\partial x_2^i}\right]\left[\frac{\partial}{\partial x_3^j}-\frac{\partial}{\partial x_4^j}\right]\mathscr{D}(\mathbf{x_1}\tau,\mathbf{x_2}\tau,\mathbf{x_3}\tau',\mathbf{x_4}\tau')\end{aligned}$$

$$\begin{aligned}\mathscr{D}(\mathbf{x_1}\tau,\mathbf{x_2}\tau,\mathbf{x_3}\tau',\mathbf{x_4}\tau')&=\sum_{\mu\nu}\langle\mathsf{T}\psi^\dagger_\mu(\mathbf{x}_1,\tau)\psi_\mu(\mathbf{x}_2,\tau)\psi^\dagger_\nu(\mathbf{x}_3,\tau')\psi_\mu(\mathbf{x}_4,\tau')\rangle_{conn}\\&=\sum_{\mu\nu}[\mathscr{G}_{\mu\nu}(\mathbf{x}_2\tau,\mathbf{x}_3\tau')\mathscr{G}_{\nu\mu}(\mathbf{x}_4\tau',\mathbf{x}_1\tau)-\mathscr{F}^\dagger_{\mu\nu}(\mathbf{x}_1\tau,\mathbf{x}_3\tau')\mathscr{F}_{\mu\nu}(\mathbf{x}_2\tau,\mathbf{x}_4\tau')]\end{aligned}$$

The last line is the Hartree Fock approximation.
For an homogeneous system, the Fourier expansions are inserted so that derivatives

are done explicitly. Then the expressions of the BCS correlators are used. After long algebra:

$$\mathscr{D}_{ij}(q,i\nu) = \left(\frac{e\hbar}{2m}\right)^2 \int \frac{d\mathbf{k}}{(2\pi)^3}(q_i+2k_i)(q_j+2k_j)$$
$$\Big\{ -(u_k u_{k+q} + v_k v_{k+q})^2 (n_{k+q} - n_k)\left[\frac{\hbar}{i\hbar\nu - E_{k+q} + E_k} - \frac{\hbar}{i\hbar\nu + E_{k+q} - E_k}\right]$$
$$+ (u_k v_{k+q} - u_k v_{k+q})^2 (1 - n_{k+q} - n_k)\left[\frac{\hbar}{i\hbar\nu - E_{k+q} - E_k} + \frac{\hbar}{i\hbar\nu + E_{k+q} + E_k}\right]\Big\}$$

The replacement $i\nu \to \nu + i\eta$ yields the retarded function. The static limit is:

$$\mathscr{D}^R_{ij}(q,0) = \left(\frac{e\hbar}{2m}\right)^2 2\hbar \int \frac{d\mathbf{k}}{(2\pi)^3}(q_i+2k_i)(q_j+2k_j)(u_k u_{k+q} + v_k v_{k+q})^2 \frac{n_{k+q} - n_k}{E_{k+q} - E_k}$$

Now take the long-scale limit, $q \to 0$:

$$\begin{aligned}\mathscr{D}^R_{ij}(0,0) &= \left(\frac{e\hbar}{2m}\right)^2 8\hbar \int \frac{d\mathbf{k}}{(2\pi)^3} k_i k_j (u_k^2 + v_k^2)^2 \frac{\partial n(E_k)}{\partial E_k} \\ &= \delta_{ij}\, \frac{2}{3}\frac{e^2\hbar^3}{m^2} \int \frac{d\mathbf{k}}{(2\pi)^3} k^2 \frac{\partial n(E_k)}{\partial E_k} \\ &= \delta_{ij}\, \frac{1}{3}\frac{e^2\hbar}{m\pi^2} \int dk\, k^4 \frac{\partial n(E)}{\partial E}\end{aligned}$$

where $E = \sqrt{(\epsilon_k - \mu)^2 + \Delta^2}$. For small q the static supercurrent is:

$$J_i(q) = -\frac{e^2 n}{mc} A_i(q) - \frac{1}{\hbar c}\mathscr{D}^R_{ij}(0,0) A_j(q)$$

Dedine the super-electron density in the BCS theory:

$$n_S(T) = n + \frac{\hbar^2}{3\pi^2 m}\int_0^\infty dk\, k^4 \frac{\partial}{\partial E}\frac{1}{e^{\beta E}+1} \tag{31}$$

For low q one obtains the relation by London

$$\mathbf{J}(q) = -\frac{e^2}{mc} n_S(T) \mathbf{A}(q)$$

that implies the Meissner effect, with screening length

$$\delta^2(T) = \frac{4\pi e^2 n_S(T)}{mc^2}$$

The temperature limit behaviours of the density n_S are:

$$\frac{n_S(T)}{n} = \begin{cases} 1 - \sqrt{\frac{2\pi\Delta_0}{k_B T}}\exp(-\frac{\Delta_0}{k_B T}) & T \to 0 \\ 1 - \frac{T}{T_c} & T \to T_c^- \end{cases} \tag{32}$$

Near $T = 0$ the effective number of Cooper pairs is $\approx \rho_0 \Delta_0$. However all electrons participate to the supercurrent (like in superfluidity: all bosons are superfluid, but only a fraction makes the condensate).
For T near T_c Fetter and Walecka have an extra factor 2.

6. The Ginzburg - Landau limit of BCS

The Ginzburg-Landau theory was derived from the microscopic BCS model by Gorkov in 1959 [10]. Near the transition line $H = H_c(T)$, the function Δ is small, and the Dyson equation (13) for $\mathbb{G}(\mathbf{x},\mathbf{y};i\omega_n)$ can be solved by iteration (Born series):

$$\mathbb{G} = \mathbb{G}_n + \frac{1}{\hbar}\mathbb{G}_n\mathbb{D}\mathbb{G}_n + \frac{1}{\hbar^2}\mathbb{G}_n\mathbb{D}\mathbb{G}_n\mathbb{D}\mathbb{G}_n + \frac{1}{\hbar^3}\mathbb{G}_n\mathbb{D}\mathbb{G}_n\mathbb{D}\mathbb{G}_n\mathbb{D}\mathbb{G}_n + \dots$$

The truncation to third order in $\mathbb{D}$ evaluates the correlators $\mathscr{F}(\mathbf{x},\mathbf{y},i\omega_n)$ and $\mathscr{G}(\mathbf{x},\mathbf{y},i\omega_n)$ in terms of the normal Green function and the gap function Δ:

$$\begin{aligned}(33)\quad \mathscr{G}(1,2,i\omega_n) &= \mathscr{G}_n(1,2,i\omega_n)\\ &- \frac{1}{\hbar^2}\mathscr{G}_n(1,3,i\omega_n)\Delta(3)\mathscr{G}_n(4,3,-i\omega_n)\overline{\Delta}(4)\mathscr{G}_n(4,2,i\omega_n)\end{aligned}$$

$$\begin{aligned}(34)\quad \mathscr{F}(1,2,i\omega_n) &= -\frac{1}{\hbar}\mathscr{G}_n(1,3,i\omega_n)\Delta(3)\mathscr{G}_n(2,3,-i\omega_n)\\ &+ \frac{1}{\hbar^3}\mathscr{G}_n(1,3,i\omega_n)\Delta(3)\mathscr{G}_n(4,3,-i\omega_n)\overline{\Delta}(4)\mathscr{G}_n(4,5,i\omega_n)\Delta(5)\mathscr{G}_n(2,5,-i\omega_n);\end{aligned}$$

(space variables $3,4,5$ are integrated). The expansion (33) is used to evaluate the super-current, and yields the second G.L. equation. Eq.(34) with $2 = 1^+$ and summation of Matsubara frequencies, is a cubic equation for the gap function $\Delta(1)$, and yields the first G.L. equation for the order parameter $\psi \propto \Delta$:

$$\frac{1}{g}\Delta(1) = \int d2\, Q(1,2)\Delta(2) + \int d234\, R(1,2,3,4)\Delta(2)\overline{\Delta}(3)\Delta(4) \qquad (35)$$

with weight functions

$$Q(1,2) = \frac{1}{\hbar^2\beta}\sum_n \mathscr{G}_n(1,2,i\omega_n)\mathscr{G}_n(1,2,-i\omega_n)$$

$$R(1,2,3,4) = -\frac{1}{\hbar^4\beta}\sum_n \mathscr{G}_n(1,2,i\omega_n)\mathscr{G}_n(3,2,-i\omega_n)\mathscr{G}_n(3,4,i\omega_n)\mathscr{G}_n(1,4,-i\omega_n)$$

The Green function oscillate rapidly on a scale $r \gg k_F^{-1}$, that measures the average distance of electrons. For simplicity we restrict to the case of zero magnetic field (see Fetter-Walecka for the case with magnetic field).

$$\mathscr{G}_n(\mathbf{x},\mathbf{y},i\omega_n) = \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{i\omega_n - \xi_k/\hbar} = -\frac{m}{2i\pi^2}\frac{1}{r}\int_{\mathbb{R}} xdx\frac{e^{ik_F xr}}{x^2 - z^2}$$

where $r = |\mathbf{x}-\mathbf{y}|$ and $z^2 = \frac{2m}{\hbar^2 k_F^2}(\mu + i\hbar\omega_n) \approx 1 + i\hbar\omega_n/\mu$ for $T \ll T_F$. For $\mu \gg \hbar\omega_n$ it is $z = \pm 1 \pm \frac{i}{2}\hbar\omega_n/\mu$. The integral is evaluated with the residue theorem, by closing the path in Im $x > 0$. The encircled pole is $x = \mathrm{sign}(\omega_n) + i|\omega_n|/\mu$.

$$\mathscr{G}_n(\mathbf{x},\mathbf{y},i\omega_n) = -\frac{m}{2\pi\hbar r}\exp\left[ik_F r\,\mathrm{sign}(\omega_n) - r\frac{|\omega_n|}{v_F}\right] \qquad (36)$$

As a consequence Q has an exponential decay

$$\begin{aligned} Q(|\mathbf{x}-\mathbf{y}|) =& \frac{1}{\hbar^2\beta}\sum_n \mathscr{G}_n(\mathbf{x},\mathbf{y},i\omega_n)\mathscr{G}_n(\mathbf{x},\mathbf{y},-i\omega_n) \\ =& \frac{m^2}{4\pi^2\hbar^4\beta r^2}\sum_{n\, odd} e^{-2r\frac{|\omega_n|}{v_F}} = \frac{m^2}{4\pi^2\hbar^4\beta r^2}\left[\sinh\frac{2\pi r}{\hbar\beta v_F}\right]^{-1} \end{aligned}$$

The order parameter of GL theory decays on the scale of the coherence length ξ, that diverges near T_c. In BCS the order parameter is expected to decay similarly. The following expansions are justified:

$$\begin{aligned} \int d\mathbf{y} Q(|\mathbf{y}-\mathbf{x}|)\Delta(\mathbf{y}) &= \int d\mathbf{y} Q(y)\Delta(\mathbf{y}+\mathbf{x}) \\ &= \int d\mathbf{y} Q(y)\left[1 + y_j\frac{\partial}{\partial x_j} + \frac{1}{2}y_j y_k\frac{\partial^2}{\partial x_j\partial x_k} + ...\right]\Delta(\mathbf{x}) \\ &= \Delta(\mathbf{x})\int d\mathbf{y} Q(y) + \frac{1}{6}\nabla^2\Delta(\mathbf{x})\int d\mathbf{y} y^2 Q(y) + \dots \end{aligned}$$

$$\begin{aligned} \int d\mathbf{y}\, Q(y) =& \frac{1}{\beta}\sum_n\int d\mathbf{y}\int\frac{d\mathbf{k}d\mathbf{q}}{(2\pi)^6}e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{y}}\frac{1}{i\hbar\omega_n-\xi_k}\frac{1}{-i\hbar\omega_n-\xi_q} \\ =& \frac{1}{\beta}\sum_n\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{\hbar^2\omega_n^2+\xi_k^2} \approx \rho_0\int_0^{\beta\hbar\omega_D}\frac{d\xi}{\xi}\tanh\frac{\xi}{2} \\ =& \rho_0\log\frac{T_c}{T} + \frac{1}{g} \approx \rho_0\frac{T_c-T}{T_c} + \frac{1}{g}. \\ \int d\mathbf{y} y^2 Q(y) =& \frac{m^2\beta^2 v_F^3}{8\pi^4\hbar}\int_0^\infty dy\frac{y^2}{\sinh y} = \frac{m^2\beta^2 v_F^3}{8\pi^4\hbar}\frac{7\zeta(3)}{2} = \frac{7\zeta(3)}{8}\rho_0\left[\frac{\hbar v_F}{\pi k_B T_c}\right]^2 \end{aligned}$$

$$\rho_0 = \frac{mk_F}{2\pi^2\hbar^2}$$

The same approximation applies to the term with kernel R, which is itself a correction: $\int d\mathbf{x}_{123}R(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\Delta(\mathbf{x}_1)\overline{\Delta}(\mathbf{x}_2)\Delta(\mathbf{x}_3) \approx R\,\Delta(\mathbf{x})|\Delta(\mathbf{x})|^2$

$$\begin{aligned} R &= \int d(234)\, R(1,2,3,4) \\ &= -\frac{1}{\hbar^4\beta}\sum_n\int d(234)\mathscr{G}_n(1,2,i\omega_n)\mathscr{G}_n(3,2,-i\omega_n)\mathscr{G}_n(3,4,i\omega_n)\mathscr{G}_n(1,4,-i\omega_n) \\ &= -\frac{1}{\beta}\int\frac{d\mathbf{k}}{(2\pi)^3}\sum_n\frac{1}{(\hbar^2\omega_n^2+\xi_k^2)^2} \approx -\frac{1}{\beta}\rho_0\sum_n\frac{1}{(\hbar|\omega_n|)^3}\int_{\mathbb{R}}\frac{dx}{(1+x^2)^2} \\ &= -\frac{7\zeta(3)}{8(\pi k_B T_c)^2}\rho_0 \end{aligned}$$

Remark 6.1. *For a homogeneous system, the order parameter Δ does not depend on position. Eq.*(35) *is:* $\frac{\Delta}{g} = \Delta\int d\mathbf{y}Q(y) + \Delta^3 R$ *i.e.*

$$0 = \rho_0\frac{T_c-T}{T_c} - \Delta^2\,\frac{7\zeta(3)}{8\pi^2}\rho_0\beta_c^2$$

The equation gives the expression (25) *of $\Delta(T)$ close to the transition.*

Equation (35) for Δ is:

$$0 = C\nabla^2\Delta(\mathbf{x}) + A\Delta(\mathbf{x}) + R\Delta(\mathbf{x})^3$$

with $C = \frac{1}{6}\int d\mathbf{y}y^2 Q(y)$, $A = \int d\mathbf{y}Q(y) - \frac{1}{g}$. If we assume that $\Delta(\mathbf{x}) = Kf(\mathbf{x})$:

$$0 = -\frac{C}{A}\nabla^2 f - f - K^2\frac{R}{A}f^3$$

It becomes the 1st GL equation $0 = -\xi^2\nabla^2 f - f + f^3$ with the identifications

$$\xi = \sqrt{\frac{7\zeta(3)}{48\pi^2}}\frac{\hbar v_F}{k_B T_c}\sqrt{\frac{T_c}{T_c - T}}, \quad \Delta(\mathbf{x}) = k_B T_c\sqrt{\frac{8\pi^2}{7\zeta(3)}}\sqrt{1 - \frac{T}{T_c}}f(\mathbf{x}) \tag{37}$$

The expression for $|a|$ is obtained from ξ:

$$|a| = \frac{\hbar^2}{2m^*\xi^2} = \left(\frac{2m}{m^\star}\right)\frac{6}{7\zeta(3)}\frac{(\pi k_B T_c)^2}{\epsilon_F}\left(1 - \frac{T}{T_c}\right)$$

The expression for b is obtained from $H_c(T)$ near the transition, eq.(29), where GL holds:

$$b = \frac{4\pi a^2}{H_c(T)^2} = \left(\frac{2m}{m^\star}\right)^2\frac{6}{7\zeta(3)}\frac{(\pi k_B T_c)^2}{n\epsilon_F}$$

where we used $\rho_0\epsilon_F = (3/4)n$, where n is the uniform density of electrons. The ratio for the bulk density is:

$$\psi_\infty^2 = \frac{|a|}{b} = \left(\frac{m^\star}{2m}\right)n\left(1 - \frac{T}{T_c}\right)$$

If we identify $\psi_\infty^2 = n_S$ and compare with (32) near T_c, we conclude that $m^\star = 2m$.

7. The Bogoliubov - de Gennes equations

The matrix operator $\mathbb{K}_x$ acts on the Hilbert space $\mathrm{L}^2(\mathbb{R}^3)\times\mathbb{C}^2$ and is self-adjoint. It has real eigenvalues, and the eigenvectors form an orthonormal basis. The eigenvalue equation

$$\boxed{\begin{bmatrix} k_x & \Delta(\mathbf{x}) \\ \overline{\Delta}(\mathbf{x}) & -\overline{k}_x \end{bmatrix}\begin{bmatrix} u_a(\mathbf{x}) \\ v_a(\mathbf{x}) \end{bmatrix} = E_a\begin{bmatrix} u_a(\mathbf{x}) \\ v_a(\mathbf{x}) \end{bmatrix}} \tag{38}$$

gives the pair of *Bogoliubov - de Gennes equations*:

$$(ku_a)(\mathbf{x}) + \Delta(\mathbf{x})v_a(\mathbf{x}) = E_a u_a(\mathbf{x})$$
$$(\overline{k}v_a)(\mathbf{x}) - \overline{\Delta}(\mathbf{x})u_a(\mathbf{x}) = -E_a v_a(\mathbf{x})$$

If $(u_a,\, v_a)$ solves them with eigenvalue $E_a > 0$, then $(-\overline{v}_a,\, \overline{u}_a)$ is a solution with eigenvalue $-E_a$. The equations (38) with eigenvalues $\pm E_a$ may be written jointly:

$$\mathbb{K}_x\begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix}\begin{bmatrix} E_a & 0 \\ 0 & -E_a \end{bmatrix} \tag{39}$$

The ortho-normalization and completeness of the doublets in Hilbert space may be expressed in matrix form:

$$\int d\mathbf{x} \begin{bmatrix} \overline{u}_b(\mathbf{x}) & \overline{v}_b(\mathbf{x}) \\ -v_b(\mathbf{x}) & u_b(\mathbf{x}) \end{bmatrix} \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} = \delta_{ab}\, \mathbb{I}_2 \tag{40}$$

$$\sum_{E_a>0} \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} \begin{bmatrix} \overline{u}_a(\mathbf{y}) & \overline{v}_a(\mathbf{y}) \\ -v_a(\mathbf{y}) & u_a(\mathbf{y}) \end{bmatrix} = \delta(\mathbf{x}-\mathbf{y})\, \mathbb{I}_2 \tag{41}$$

Diagonalization of the many-body Hamiltonian. The matrix relation (39) suggests that the many-body Hamiltonian is diagonalized by the following transformation to new operators:

$$\begin{bmatrix} \hat\psi_\downarrow(\mathbf{x}) \\ \hat\psi^\dagger_\uparrow(\mathbf{x}) \end{bmatrix} = \sum_a \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} \begin{bmatrix} \hat\alpha_a \\ \hat\beta^\dagger_a \end{bmatrix} \tag{42}$$

This and the adjoint are, in detail:

$$\hat\psi_\downarrow(\mathbf{x}) = \sum_a (u_a(\mathbf{x})\hat\alpha_a - \overline{v}_a(\mathbf{x})\hat\beta^\dagger_a), \quad \hat\psi^\dagger_\downarrow(\mathbf{x}) = \sum_a (\overline{u}_a(\mathbf{x})\hat\alpha^\dagger_a - v_a(\mathbf{x})\hat\beta_a) \tag{43}$$

$$\hat\psi_\uparrow(\mathbf{x}) = \sum_a (\overline{v}_a(\mathbf{x})\hat\alpha^\dagger_a + u_a(\mathbf{x})\hat\beta_a), \quad \hat\psi^\dagger_\uparrow(\mathbf{x}) = \sum_a (v_a(\mathbf{x})\hat\alpha_a + \overline{u}_a(\mathbf{x})\hat\beta^\dagger_a) \tag{44}$$

Inversion is done with the aid of (40):

$$\begin{bmatrix} \hat\alpha_a \\ \hat\beta^\dagger_a \end{bmatrix} = \int d\mathbf{x} \begin{bmatrix} \overline{u}_a(\mathbf{x}) & \overline{v}_a(\mathbf{x}) \\ -v_a(\mathbf{x}) & u_a(\mathbf{x}) \end{bmatrix} \begin{bmatrix} \hat\psi_\downarrow(\mathbf{x}) \\ \hat\psi^\dagger_\uparrow(\mathbf{x}) \end{bmatrix} \tag{45}$$

The adjoint operators are also obtained. The transformation is canonical i.e. the new operators have canonical anticommutation relations:

$$\{\hat\alpha_a, \hat\alpha^\dagger_b\} = \delta_{ab}, \qquad \{\hat\beta_a, \hat\beta^\dagger_b\} = \delta_{ab} \tag{46}$$

and all other anticommutators vanish. By eq.(39)

$$(\mathbb{K}_x\Psi)(\mathbf{x}) = \sum_a \begin{bmatrix} u_a(\mathbf{x}) & -\overline{v}_a(\mathbf{x}) \\ v_a(\mathbf{x}) & \overline{u}_a(\mathbf{x}) \end{bmatrix} \begin{bmatrix} E_a & 0 \\ 0 & -E_a \end{bmatrix} \begin{bmatrix} \hat\alpha_a \\ \hat\beta^\dagger_a \end{bmatrix}$$

Evaluation of $\hat K_{BCS} = \int d\mathbf{x}\, \Psi^\dagger \mathbb{K}\Psi$ and (40) give a diagonal operator for quasiparticles (*bogolons*):

$$\boxed{\hat K_{BCS} = U_0 + \sum_a E_a(\hat\alpha^\dagger_a\hat\alpha_a + \hat\beta^\dagger_a\hat\beta_a)} \tag{47}$$

where $U_0 = -\sum_a E_a$. The ground state is defined by

$$\hat\alpha_a|BCS\rangle = 0 \qquad \hat\beta_a|BCS\rangle = 0, \quad \forall a$$

The gap equation. The change of basis (43) simplifies the gap equation, with thermal average with the diagonal operator (47)

$$\begin{aligned} \Delta(\mathbf{x}) &= -g\sum_{ab} u_a(\mathbf{x})\overline{v}_b(\mathbf{x})\langle\hat\alpha^\dagger_a\hat\alpha_b\rangle - \overline{v}_a(\mathbf{x})u_b(\mathbf{x})\langle\hat\beta_a\hat\beta^\dagger_b\rangle \\ &= g\sum_a u_a(\mathbf{x})\overline{v}_a(\mathbf{x})[1-2n(E_a)] \end{aligned}$$

where $n(E_a) = (e^{\beta E_a} + 1)^{-1}$ is the Fermi-Dirac occupation number of the state with energy E_a. Then:

$$\boxed{\Delta(\mathbf{x}) = g \sum_a u_a(\mathbf{x}) \overline{v}_a(\mathbf{x}) \tanh\left(\frac{\beta}{2} E_a\right)} \tag{48}$$

The equation must be solved self-consistently with the Bogoliubov - de Gennes equations for u_a and v_a. As the gap function depends on temperature, the amplitudes u_a, v_a as well as the energies E_a depend on T.

Exercise 7.1. Show that $\Omega = -\frac{2}{\beta}\sum_a \log\left(2\cosh\frac{1}{2}\beta E_a\right)$.

Exercise 7.2. Show that the average density of electrons is:

$$n(\mathbf{x}) = \sum_a |u_a(\mathbf{x})|^2 n_a + |v_a(\mathbf{x})|^2 (1 - n_a). \tag{49}$$

Homogeneous systems. In homogeneous problems there is no external field and Δ is constant. An analytic solution is found in momentum space. We seek for a solution of the Bogoliubov - de Gennes equations of the form

$$\begin{bmatrix} u_k(\mathbf{x}) \\ v_k(\mathbf{x}) \end{bmatrix} = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} \begin{bmatrix} u_k \\ v_k \end{bmatrix} \tag{50}$$

The eigenvalue equation is algebraic:

$$\begin{bmatrix} \xi_k & \Delta \\ \overline{\Delta} & -\xi_k \end{bmatrix} \begin{bmatrix} u_k \\ v_k \end{bmatrix} = E_k \begin{bmatrix} u_k \\ v_k \end{bmatrix}$$

where $\xi_k = \epsilon_k - \mu$ is the single-particle energy of the normal phase, measured with respect to the chemical potential. The homogeneous system admits a nontrivial solution if

$$\boxed{E_k = \sqrt{\xi_k^2 + |\Delta|^2}} \tag{51}$$

(the positive root is selected for stability). The **energy gap** $|\Delta|$ separating the Fermi surface $\xi = 0$ from the lowest excitation, profoundly modifies the properties of the electron gas at low temperatures.

The amplitudes solve the normalization condition $|u_k|^2 + |v_k|^2 = 1$ and the eigenvalue condition $\xi_k u_k + \Delta\, v_k = E_k u_k$. The latter gives $|\Delta||v_k| = (E_k - \xi_k)|u_k|$, with solutions

$$|u_k|^2 = \frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right), \quad |v_k|^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right) \tag{52}$$

In the normal phase $E_k = |\xi_k|$; then: $|u_k| = \theta(\epsilon_k - \mu)$ and $|v_k| = \theta(\mu - \epsilon_k)$.
The equation $\xi_k u_k + \Delta\, v_k = E_k u_k$ gives $\Delta|v_k|^2 = (E_k - \xi_k) u_k \overline{v}_k$ i.e. the useful relation:

$$u_k \overline{v}_k = \frac{\Delta}{2E_k} \tag{53}$$

The expansion of the field operators in the two canonical basis,

$$\begin{bmatrix} \hat\psi_\downarrow(\mathbf{x}) \\ \hat\psi^\dagger_\uparrow(\mathbf{x}) \end{bmatrix} = \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} \begin{bmatrix} \hat a_{\mathbf{k},\downarrow} \\ \hat a^\dagger_{-\mathbf{k},\uparrow} \end{bmatrix} = \sum_{\mathbf{k}} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} \begin{bmatrix} u_k & -\overline{v}_k \\ v_k & \overline{u}_k \end{bmatrix} \begin{bmatrix} \hat\alpha_{\mathbf{k}} \\ \hat\beta^\dagger_{-\mathbf{k}} \end{bmatrix}$$

implies the Bogoliubov - Valatin transformation:

$$\begin{bmatrix} \hat a_{\mathbf{k},\downarrow} \\ \hat a^\dagger_{-\mathbf{k},\uparrow} \end{bmatrix} = \begin{bmatrix} u_k & -\overline{v}_k \\ v_k & \overline{u}_k \end{bmatrix} \begin{bmatrix} \hat\alpha_{\mathbf{k}} \\ \hat\beta^\dagger_{-\mathbf{k}} \end{bmatrix} \tag{54}$$

and the Hermitian conjugate. Inversion gives:

$$\hat\alpha_{\mathbf{k}} = \bar u_k \hat a_{\mathbf{k},\downarrow} + \bar v_k \hat a^\dagger_{-\mathbf{k},\uparrow}, \qquad \hat\alpha^\dagger_{\mathbf{k}} = u_k \hat a^\dagger_{\mathbf{k},\downarrow} + v_k \hat a_{-\mathbf{k},\uparrow} \tag{55}$$

$$\hat\beta_{\mathbf{k}} = -\bar v_k \hat a^\dagger_{-\mathbf{k},\downarrow} + \bar u_k \hat a_{\mathbf{k},\uparrow}, \qquad \hat\beta^\dagger_{\mathbf{k}} = -v_k \hat a_{-\mathbf{k},\downarrow} + u_k \hat a^\dagger_{\mathbf{k},\uparrow} \tag{56}$$

The operators $\hat\alpha_{\mathbf{k}}$ and $\hat\beta_{\mathbf{k}}$ annihilate, for all vectors $\mathbf{k}$, the state

$$\boxed{|BCS\rangle = \prod\nolimits_{\mathbf{k}} (\bar u_k + \bar v_k a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow})|0\rangle} \tag{57}$$

which reads as a sea of Cooper pairs[4]. In the normal phase ($\Delta = 0$) it coincides with the filled Fermi sphere.
Creation operators break Cooper pairs and create excited states (bogolons) consisting of Cooper pairs and unpaired electrons. For example:

$$\hat\alpha^\dagger_{\mathbf{k}}|BCS\rangle = \prod_{\mathbf{q}\neq\mathbf{k}} (\bar u_q + \bar v_q \hat a^\dagger_{-\mathbf{q}\uparrow} \hat a^\dagger_{\mathbf{q}\downarrow}) \hat a^\dagger_{\mathbf{k}\downarrow}|0\rangle$$

$$\hat\beta^\dagger_{-\mathbf{k}}|BCS\rangle = \prod_{\mathbf{q}\neq\mathbf{k}} (\bar u_q + \bar v_q \hat a^\dagger_{-\mathbf{q}\uparrow} \hat a^\dagger_{\mathbf{q}\downarrow}) \hat a^\dagger_{\mathbf{k}\uparrow}|0\rangle$$

$$\hat\alpha^\dagger_{\mathbf{k}}\beta^\dagger_{-\mathbf{k}}|BCS\rangle = \bar u_k \prod_{\mathbf{q}\neq\mathbf{k}} (\bar u_q + \bar v_q \hat a^\dagger_{-\mathbf{q}\uparrow} \hat a^\dagger_{\mathbf{q}\downarrow}) \hat a^\dagger_{\mathbf{k}\downarrow} \hat a^\dagger_{\mathbf{k}\uparrow}|0\rangle$$

Exercise 7.3. Show that the thermal occupation numbers are

$$\langle \hat a^\dagger_{\mathbf{k}\uparrow} \hat a_{\mathbf{k}\uparrow}\rangle = \frac{1}{2}\left[1 - \frac{\xi_k}{E_k}\tanh(\tfrac{1}{2}\beta E_k)\right]$$

Note that $\langle BCS|\hat a^\dagger_{\mathbf{k}\uparrow}\hat a_{\mathbf{k}\uparrow}|BCS\rangle = |v_k|^2$ (the thermal average at $T = 0$).

Exercise 7.4. The Nambu-Gorkov propagators can be represented as expansions in the Bogoliubov - de Gennes eigenstates. Show that:

$$\mathscr{G}(\mathbf{x},\mathbf{x}',i\omega_n) = \sum_a \frac{u_a(\mathbf{x})\overline{u}_a(\mathbf{x}')}{i\omega_n - E_a/\hbar} + \frac{\overline{v}_a(\mathbf{x})v_a(\mathbf{x}')}{i\omega_n + E_a/\hbar} \tag{58}$$

$$\mathscr{F}(\mathbf{x},\mathbf{x}',i\omega_n) = \sum_a -\frac{u_a(\mathbf{x})\overline{v}_a(\mathbf{x}')}{i\omega_n - E_a/\hbar} + \frac{\overline{v}_a(\mathbf{x})u_a(\mathbf{x}')}{i\omega_n + E_a/\hbar} \tag{59}$$

[4] In [6] Bardeen, Cooper and Schrieffer (1957) introduced the state with variational parameters u_k and v_k with $|u_k|^2+|v_k|^2 = 1$ for normalization. Minimization of $\langle BCS|\hat K_{\rm eff}|BCS\rangle$ with respect to the parameters yields the same results presented here. Bogoliubov and Valatin independently simplified the theory by their canonical transformation [7, 8].

and recover the gap equation (48) by evaluating the Matsubara sum

$$\Delta(\mathbf{x}) = -g\frac{1}{\hbar\beta}\sum_n \mathscr{F}(\mathbf{x},\mathbf{x},i\omega_n)e^{i\omega_n\eta}$$

8. Appendix: the Hartree approximation

To gain some understanding of the Hartree approximation in BCS, let $\hat{K} = \hat{K}_0 + \hat{K}_1$, where K_0 is the one-particle term, and $\hat{K}_1$ is the quartic term (see also [14]). The thermal average of field operators in interaction picture is

$$\langle\mathcal{T}\hat{\psi}(x_1)\hat{\psi}(x_2)\dots\rangle_K = \frac{\langle\mathcal{T}\mathscr{U}_I(\hbar\beta,0)\hat{\psi}(x_1)\hat{\psi}(x_2)\dots\rangle_{K_0}}{\langle\mathscr{U}_I(\hbar\beta,0)\rangle_{K_0}}. \tag{60}$$

where $x = (\mathbf{x},\tau)$ and

$$\mathscr{U}_I(\hbar\beta,0) = \mathsf{T}\exp\left(-\frac{1}{\hbar}\int\int_0^{\hbar\beta} dx\left[-g\,(\hat{\psi}^\dagger_\downarrow\hat{\psi}^\dagger_\uparrow)(x^+)(\hat{\psi}_\uparrow\hat{\psi}_\downarrow)(x)\right]\right)$$

The four-fermion interaction may be splitted with the introduction of an auxiliary complex field $\Phi(x)$.

Consider the following multidimensional integral with complex variables:

$$\int\prod_j\frac{d^2z_j}{\pi}e^{-\sum_k(|z_k|^2+\bar{\alpha}_k z_k+\bar{z}_k\beta_k)} = e^{\sum_k\bar{\alpha}_k\beta_k}$$

In the extension to a continuum, the label k is replaced by a variable x that may be multi-dimensional. The result is known as the Hubbard-Stratonovich transform:

$$\frac{1}{Z_\Phi}\int\mathscr{D}^2\Phi e^{-\int dx\{|\Phi(x)|^2+\overline{\alpha(x)}\Phi(x)+\overline{\Phi(x)}\beta(x)\}} = e^{\int dx\overline{\alpha(x)}\beta(x)} \tag{61}$$

$$Z_\Phi = \int\mathscr{D}^2\Phi e^{-\int dx|\Phi(x)|^2}$$

The formula is usually used in the reverse direction: at the cost of an integral with auxiliary field, the product of the fields α and $\bar{\beta}$ is decoupled.

We obtain a Gaussian functional integral, where all pairs of operators commute because of T-ordering:

$$\mathscr{U}_I(\hbar\beta,0) = \frac{1}{Z_\Phi}\int\mathscr{D}^2\Phi\mathsf{T}\exp\left[-\frac{1}{\hbar g}|\Phi(x)|^2 - \frac{1}{\hbar}(\overline{\Phi}\hat{\psi}_\uparrow\hat{\psi}_\downarrow + \hat{\psi}^\dagger_\downarrow\hat{\psi}^\dagger_\uparrow\Phi)(x)\right]$$

$$Z_\Phi = \int\mathscr{D}^2\Phi\ \exp\left[-\frac{1}{\hbar g}\int dx|\Phi(x)|^2\right]$$

The BCS partition function is $Z = Z_0\langle\mathscr{U}_I(\hbar\beta,0)\rangle_{K_0}$, with $Z_0 = \mathrm{tr}\,(e^{-\beta K_0})$ and

$$\langle\mathscr{U}_I(\hbar\beta,0)\rangle_{K_0} = \frac{1}{Z_\Phi}\int\mathscr{D}\Phi\left\langle\mathsf{T}e^{-\frac{1}{\hbar}S[\Phi,\overline{\Phi}]}\right\rangle_{K_0} \tag{62}$$

A variation $\delta\bar{\Phi}$ of the field gives, to first order

$$\langle\mathsf{T}e^{-\frac{1}{\hbar}S[\Phi,\bar{\Phi}+\delta\bar{\Phi}]}\rangle_{K_0} = \left\langle\mathsf{T}e^{-\frac{1}{\hbar}S[\Phi,\bar{\Phi}]}\left[1+\int dx\delta\bar{\Phi}(x)\left[\frac{1}{g}\Phi(x)+\hat{\psi}_\uparrow(x)\hat{\psi}_\downarrow(x)\right]+\dots\right]\right\rangle_{K_0}$$

Since the measure is invariant, this gives a Ward identity:

$$0 = \frac{1}{Z_\Phi}\int\mathscr{D}\Phi\left\langle\mathsf{T}e^{-\frac{1}{\hbar}S[\Phi,\bar{\Phi}]}\left[\Phi(x)+g\hat{\psi}_\uparrow(x)\hat{\psi}_\downarrow(x)\right]\right\rangle_{K_0}$$

Now comes the approximation: the main contribution to the functional integral comes from the auxiliary field Φ that maximises the Boltzmann weight $\langle \mathsf{T} e^{-S/\hbar} \rangle$. The extremum $\Delta(x)$ makes the first variation to vanish

$$\left\langle \mathsf{T} e^{-\frac{1}{\hbar} S[\Delta,\bar{\Delta}]} \left[\Delta(x) + g\hat{\psi}_{\uparrow}(x)\hat{\psi}_{\downarrow}(x) \right] \right\rangle_{K_0} = 0 \tag{63}$$

This is the *gap equation* (4) for $\Delta(\mathbf{x})$ (time-dependence cancels because of equal times).

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