4. TEORIA BCS DELLA SUPERCONDUTTIVITA'

The BCS Hamiltonian

Fröhlich : el-ph interaction can produce an effective attraction between electrons in the range of phonon energies.
Cooper : a weak attraction can only be effective for fermi with $K_{TOT} = 0 \rightarrow +k$ & $-k$, assuming that the attraction is in the $l=0$ singlet state.
BCS Hamiltonian

$$H_{BCS} = \sum_{k\sigma} c^+_{k\sigma} (\varepsilon_k - \mu) c_{k\sigma} - \frac{g}{V} \sum_{\substack{kk' \\ \mu - w_c < \varepsilon_k,\, \varepsilon_{k'} < \mu + w_c}} c^+_{k'\uparrow} c^+_{-k'\downarrow} c_{-k\downarrow} c_{k\uparrow}$$

$g > 0$, V = normalization volume

DOS in 3d $\frac{V}{(2\pi)^3} \rightarrow \sum_k \rightarrow \frac{V}{(2\pi)^3} \int d^3k$

The matrix element of an n particle interaction must be proportional to $V^{-(n-1)}$ in order for the Hamiltonian to be extensive $\propto V$

Energy range of attraction is a width $2w_c$ around μ

NB : The ground state $|\emptyset\rangle$ we used for the Coopers problem (F.L.) cannot be any more the g. state because we have seen this is unstable against the formation of pairs.
Problem : g. state and quasiparticle spectrum of BCS Hamiltonian.
- Solution by BCS
- and by Bogoliubov & Valatin - canonical transformation.

Bogoliubov-Valatin transformation

Suppose the g-state contains bound pairs. Exciting one particle of the pair leaves its partner in an excited state. If one wants to excite only one particle, one must annihilate simultaneously its partner. [Check Rickayzen et al.] *

Ansatz for a canonical transformation or the definition of the operators which create excited states [from c_k, c_{-k}]

$$b_{k\uparrow} = u_k c_{k\uparrow} - v_k c^{+}_{-k\downarrow} \quad ; \quad b_{k\downarrow} = u_k c_{k\downarrow} + v_k c^{+}_{-k\uparrow}$$

and u_k, v_k are variational parameters.

We also assume that phase plays no role in the annihilation process (r-independent phase may be arbitrarily chosen).

These relations may be summarised as

$$\begin{cases} b_{k\sigma} = u_k c_{k\sigma} - \sigma v_k c^{+}_{-k-\sigma} \\ b^{+}_{k\sigma} = u_k c^{+}_{k\sigma} - \sigma c_{-k-\sigma} v_k \end{cases}$$

We want these transformations to be canonical, so that the new operators b, b^{+} are again fermionic operators.

$$[b_{k\sigma}, b_{k'\sigma'}]_{+} = (u_k c_{k\sigma} - \sigma v_k c^{+}_{-k-\sigma})(u_{k'} c_{k'\sigma'} - \sigma' v_{k'} c^{+}_{-k'-\sigma'}) +$$

$$+ (u_{k'} c_{k'\sigma'} - \sigma' v_{k'} c^{+}_{-k'-\sigma'})(u_k c_{k\sigma} - \sigma v_k c^{+}_{-k-\sigma}) =$$

$$= - u_k v_{k'} \sigma' (c_{k\sigma} c^{+}_{-k'-\sigma'} + c^{+}_{-k'-\sigma'} c_{k\sigma}) -$$

$$- u_{k'} v_k \sigma (c^{+}_{-k-\sigma} c_{k'\sigma'} + c_{k'\sigma'} c^{+}_{-k-\sigma})$$

$$+ u_k u_{k'} \underbrace{(c_{k\sigma} c_{k'\sigma'} + c_{k'\sigma'} c_{k\sigma})}^{=0} +$$

$$+ \sigma\sigma' v_k v_{k'} \underbrace{(c^{+}_{-k-\sigma} c^{+}_{-k'-\sigma'} + c^{+}_{-k'-\sigma'} c^{+}_{-k-\sigma})}_{=0} =$$

$$= -u_k v_{k'} \sigma' \overbrace{[c_{k\sigma}\, c^+_{k'-\sigma'}]}^{\delta_{k,-k'}\delta_{\sigma,-\sigma'}} - u_{k'} v_k \sigma \overbrace{[c^+_{k-\sigma}\, c_{k'\sigma'}]}^{\delta_{-k,k'}\delta_{-\sigma,\sigma'}} =$$

$$= -u_k v_{-k}(-\sigma) - u_{-k} v_k(+\sigma) = 0$$

and analogously for

$$[b^+_{k\sigma}, b^+_{k'\sigma'}]_+ = 0$$

Then

$$[b_{k\sigma}, b^+_{k'\sigma'}]_+ = (u_k c_{k\sigma} - \sigma v_k c^+_{-k-\sigma})(u_{k'} c^+_{k'\sigma'} - \sigma' v_{k'} c_{-k'-\sigma'}) +$$

$$+ (u_{k'} c^+_{k'\sigma'} - \sigma' v_{k'} c_{-k'-\sigma'})(u_k c_{k\sigma} - \sigma v_k c^+_{-k-\sigma}) =$$

$$= u_k u_{k'} (\overbrace{c_{k\sigma} c^+_{k'\sigma'} + c^+_{k'\sigma'} c_{k\sigma}}^{\delta_{kk'}\delta_{\sigma\sigma'}}) +$$

$$+ v_k v_{k'} \sigma\sigma' (\underbrace{c^+_{-k-\sigma} c_{-k'-\sigma'} + c_{-k'-\sigma'} c^+_{-k-\sigma}}_{\delta_{kk'}\delta_{\sigma\sigma'}}) =$$

$$= (u_k^2 + v_k^2)\,\delta_{kk'}\delta_{\sigma\sigma'}$$

and this leads to the condition

$$u_k^2 + v_k^2 = 1$$

Inverse transform:

- multiply first eq. by u_k
- multiply second eq. by σv_k and change $k\sigma$ with $-k, -\sigma$

$$\begin{cases} u_k b_{k\sigma} = u_k^2 c_{k\sigma} - \sigma \cancel{u_k v_k} c^+_{-k-\sigma} \\ \sigma v_k b^+_{-k-\sigma} = \sigma \cancel{v_k u_k} c^+_{-k-\sigma} - \sigma^2 v_k^2 c_{k\sigma} \end{cases}$$

$$\Sigma \rightarrow \quad u_k b_{k\sigma} + \sigma v_k b^+_{-k-\sigma} = u_k^2 c_{k\sigma} + \sigma^2 v_k^2 c_{k\sigma}$$

$$\begin{cases} c_{k\sigma} = u_k b_{k\sigma} + \sigma v_k b^+_{-k-\sigma} \\ c^+_{k\sigma} = u_k b^+_{k\sigma} + \sigma v_k b_{-k-\sigma} \end{cases}$$

Then we transform the Hamiltonian

$$c^+_{k\sigma} c_{k\sigma} = (u_k b^+_{k\sigma} + \sigma v_k b_{-k-\sigma})(u_k b_{k\sigma} + \sigma v_k b^+_{-k-\sigma}) =$$

$$= u_k^2 b^+_{k\sigma} b_{k\sigma} + v_k^2 \underbrace{b_{-k-\sigma} b^+_{-k-\sigma}}_{(1 - b^+_{-k-\sigma} b_{-k-\sigma})} + \sigma u_k v_k (b^+_{k\sigma} b^+_{-k-\sigma} + b_{-k-\sigma} b_{k\sigma})$$

$$H_0 = 2\sum_k (\varepsilon_k - \mu) v_k^2 + \sum_k (\varepsilon_k - \mu)(u_k^2 - v_k^2) \sum_\sigma b^+_{k\sigma} b_{k\sigma} +$$

$$+ 2\sum_k (\varepsilon_k - \mu) u_k v_k (b^+_{k\uparrow} b^+_{-k\downarrow} + b_{-k\downarrow} b_{k\uparrow})$$

Then introducing

$$B_k = c_{-k\downarrow} c_{k\uparrow} = (u_k b_{-k\downarrow} - v_k b^+_{k\uparrow})(u_k b_{k\uparrow} + v_k b^+_{-k\downarrow}) =$$

$$= u_k^2 b_{-k\downarrow} b_{k\uparrow} - v_k^2 b^+_{k\uparrow} b^+_{-k\downarrow} + u_k v_k (\underbrace{b_{-k\downarrow} b^+_{-k\downarrow}}_{(1 - b^+_{-k\downarrow} b_{-k\downarrow})} - b^+_{k\uparrow} b_{k\uparrow})$$

The full Hamiltonian is

$$H_{BCS} = 2\sum_k (\varepsilon_k - \mu) v_k^2 + \sum_k (\varepsilon_k - \mu)(u_k^2 - v_k^2) \sum_\sigma b^+_{k\sigma} b_{k\sigma} +$$

$$+ 2\sum_k (\varepsilon_k - \mu) u_k v_k (b^+_{k\uparrow} b^+_{-k\downarrow} + b_{-k\downarrow} b_{k\uparrow}) - \frac{g}{V} \sum_{kk'} B^+_{k'} B_k$$

Introduce the occupation number operators

$$n_{k\sigma} = b^+_{k\sigma} b_{k\sigma}$$

In analogy with the Cooper problem we consider that the b operators represent excitations of the g.-state $|\Psi_0\rangle$

of the BCS Hamiltonian for which $n_{k\sigma}=0$

The energy for a general occupation number eigenstate $n_{k\sigma}$ is then given by

$$E = 2\sum_k (\varepsilon_k-\mu)v_k^2 + \sum_k (\varepsilon_k-\mu)(u_k^2-v_k^2)(n_{k\uparrow}+n_{k\downarrow}) -$$

$$-\frac{g}{V}\left[\sum_k u_k v_k (1-n_{k\uparrow}-n_{k\downarrow})\right]^2 \quad \left[\begin{array}{l}\text{Check sign of the}\\ \text{last term} \quad *\end{array}\right]$$

Since $u_k^2+v_k^2=1 \rightarrow \frac{\partial v_k}{\partial u_k} = -\frac{u_k}{v_k}$

$$\frac{\partial E}{\partial u_k} = 0 = \sum_k \Big[\underbrace{-4(\varepsilon_k-\mu)u_k + 4u_k(\varepsilon_k-\mu)(n_{k\uparrow}+n_{k\downarrow})}_{-4(\varepsilon_k-\mu)u_k(1-n_{k\uparrow}+n_{k\downarrow})}\Big]$$

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$$-\frac{\partial}{\partial u_k}\frac{g}{V}\left[\sum_k u_k v_k(1-n_{k\uparrow}-n_{k\downarrow})\right]^2 =$$

$$= -2\underbrace{\frac{g}{V}\left[\sum_k u_k v_k(1-n_{k\uparrow}-n_{k\downarrow})\right]}_{\Delta}\frac{\partial}{\partial u_k}\sum_k u_k v_k(1-n_{k\uparrow}-n_{k\downarrow}) =$$

$$= -2\Delta\Big[\underbrace{v_k + u_k\Big(-\frac{u_k}{v_k}\Big)}_{\frac{v_k^2-u_k^2}{v_k}}(1-n_{k\uparrow}-n_{k\downarrow})\Big] =$$

$$= 2\Delta\frac{u_k^2-v_k^2}{v_k}(1-n_{k\uparrow}-n_{k\downarrow})$$

$$\frac{\partial E}{\partial u_k} = 0 = \left[-4(\varepsilon_k-\mu)u_k + 2\Delta\frac{u_k^2-v_k^2}{v_k}\right](1-n_{k\uparrow}-n_{k\downarrow}) = 0$$

Therefore u_k and v_k are defined by

$$\begin{cases} 2(\varepsilon_k-\mu)u_k v_k = \Delta(u_k^2-v_k^2) \\ u_k^2+v_k^2=1 \end{cases}$$

$$2(\varepsilon_k-\mu)\,u_k v_k = \Delta\,(\overbrace{u_k^2 - v_k^2}^{2u_k^2-1})$$

$$4(\varepsilon_k-\mu)^2 u_k^2 (1-u_k^2) = \Delta^2 (2u_k^2-1)^2 =$$

$$= 4(\varepsilon_k-\mu)(u_k^2-u_k^4) \qquad = \Delta^2(4u_k^4+1-4u_k^2)$$

$$u_k^4\left(-4(\varepsilon_k-\mu)^2-4\Delta^2\right)+u_k^2\left(4(\varepsilon_k-\mu)^2+4\Delta^2\right)-\Delta^2=0$$

$$A=(\varepsilon_k-\mu)^2+\Delta^2$$

$$-4A\,u_k^4+4A\,u_k^2-\Delta^2=0$$

$$u_k^2=\frac{-4A\pm\sqrt{16A^2-4(+4A)\Delta^2}}{-8A}$$

$$=\frac{1}{2}\pm\frac{4\sqrt{A^2-A\Delta^2}}{-8A}=\frac{1}{2}\pm\frac{\sqrt{A}\sqrt{A-\Delta^2}}{A}$$

$$\underset{(v_k^2)}{u_k^2}=\frac{1}{2}\pm\frac{(\varepsilon_k-\mu)}{\sqrt{(\varepsilon_k-\mu)^2+\Delta^2}}$$

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

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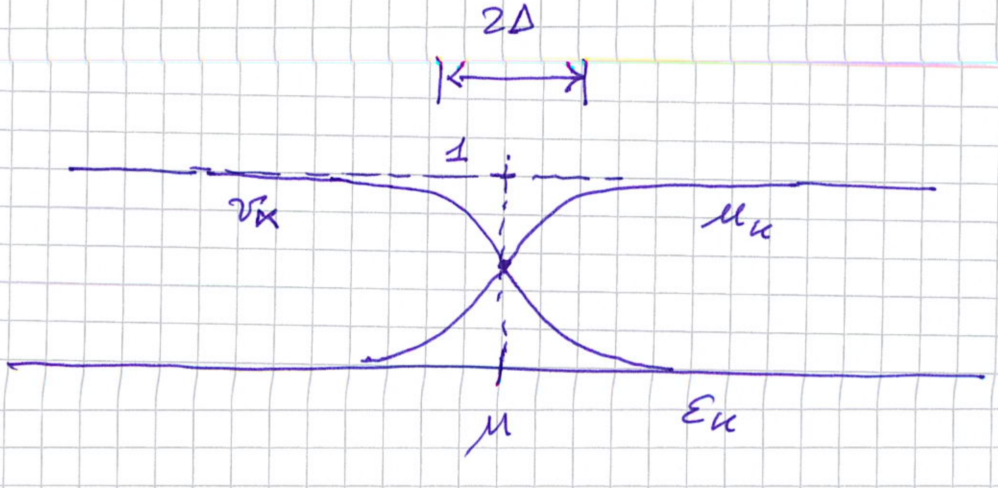
Inserting this in the definition of Δ ~~ted~~ leads to the self consistency condition

$$1=\frac{g}{2V}\sum_k\frac{1-n_{k\uparrow}-n_{k\downarrow}}{\sqrt{(\varepsilon_k-\mu)^2+\Delta^2}}$$

which determines Δ as a function of the BCS coupling constant g, the dispersion of the normal state ε_k and the occupation numbers of $n_{k\sigma}$ of the b quasi-particles of the SC state (related to T).



Formally one could interchange u_k and v_k and still have a solution but this would not be a minimum of the energy.
The second term in E is positive defined, therefore the absolute minimum (g. state) is attained if all the occupation numbers of the b operators are zero.
For the g-state the selfconsistency condition reduces to

$$1 = \frac{g}{2V}\sum_k \frac{1}{\sqrt{(\varepsilon_k-\mu)^2+\Delta_0^2}} = \frac{g N(0)}{2}\int_{-\omega_c}^{+\omega_c} d\omega \frac{1}{\sqrt{\omega^2+\Delta_0^2}} =$$

$$= \frac{g N(0)}{2} \ln \frac{\sqrt{\omega_c^2+\Delta_0^2}+\omega_c}{\sqrt{\omega_c^2+\Delta_0^2}-\omega_c} \simeq \frac{g N(0)}{2} \ln \frac{4\omega_c^2}{\Delta_0^2}$$

With $\Delta_0 \ll \omega_c$

$$\sqrt{\omega_c^2+\Delta_0^2} \simeq \omega_c + \frac{1}{2}(\omega_c^2)^{-1/2}\Delta_0^2 = \omega_c + \frac{1}{2}\frac{\Delta_0^2}{\omega_c}$$

$$\frac{\sqrt{\omega_c^2+\Delta_0^2}+\omega_c}{\sqrt{\omega_c^2+\Delta_0^2}-\omega_c} \simeq \frac{\omega_c+\frac{1}{2}\frac{\Delta_0^2}{\omega_c}+\omega_c}{\cancel{\omega_c}+\frac{1}{2}\frac{\Delta_0^2}{\omega_c}-\cancel{\omega_c}} = \frac{2\omega_c+\frac{1}{2}\frac{\Delta_0^2}{\omega_c}}{\frac{1}{2}\frac{\Delta_0^2}{\omega_c}} \simeq$$

$$\simeq \frac{4\omega_c}{\frac{\Delta_0^2}{\omega_c}} = \frac{4\omega_c^2}{\Delta_0^2}$$

Therefore

$$\Delta_0 = 2\omega_c \exp\left\{-\frac{1}{gN(0)}\right\}$$

for the value of Δ in the g.state at $T=0$.

If one replaces the last term $(-g/V)\sum B_{k'}^{+} B_k)$ of the BCS Hamiltonian by the mean field approximation

$$-\frac{g}{V}\sum_{kk'} B_{k'}^{+} B_k \simeq -\Delta \sum_k \left[B_k + B_k^{+}\right]$$

recalling that

$$\Delta = \frac{g}{V}\langle \Psi_0 | \sum_k B_k | \Psi_0 \rangle$$

This means that for one of the B operators we take its average expected value.

This also implies we are neglecting the anomalous terms b^+b^+ or bb. Check on this point better.

In mean field approximation the BCS Hamiltonian is diagonalized by the Bogoliubov-Valatin transformation

$$H_{HF} = 2\sum_k (\varepsilon_k - \mu) v_k^2 + \sum_{k\sigma} (\varepsilon_k - \mu)(u_k^2 - v_k^2)\, b_{k\sigma}^{+} b_{k\sigma} -$$

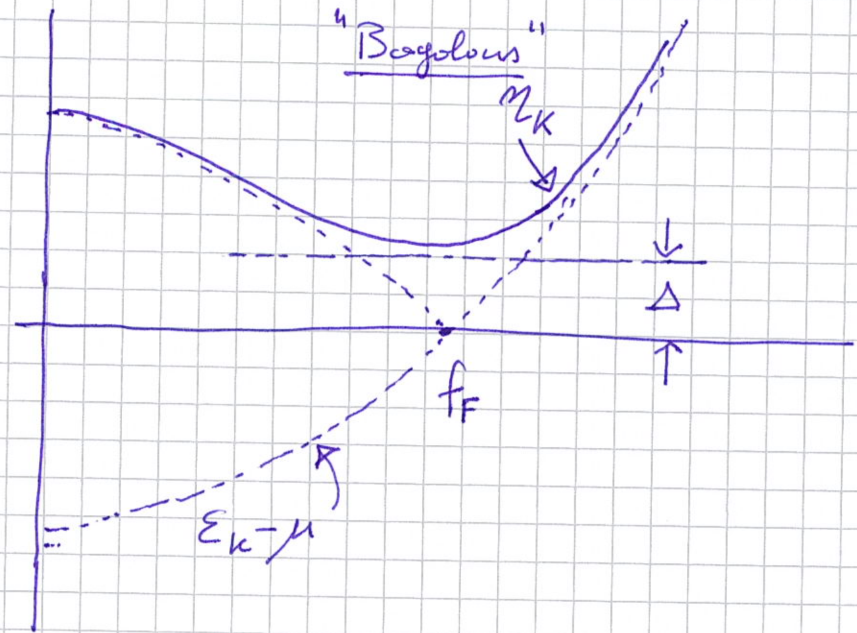
$$- 2\Delta \sum_k u_k v_k \left(1 - \sum_\sigma b_{k\sigma}^{+} b_{k\sigma}\right) =$$

$$= C + \sum_{k\sigma}\left[(\varepsilon_k - \mu)(u_k^2 - v_k^2) + 2\Delta u_k v_k\right] b_{k\sigma}^{+} b_{k\sigma} =$$

$$= C + \sum_{k\sigma} \eta_{k\sigma}\, b_{k\sigma}^{+} b_{k\sigma}$$

$$\boxed{\eta_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}}$$

which is the b quasi particle dispersion relation



The physical meaning of Δ is the gap in the b quasiparticle excitation spectrum of the SC-state.
The fact that the B-V transformation diagonalises the mean field BCS ~~Hamiltonian~~ Hamiltonian justifies a posteriori the assumption that the g-state can be found as an eigenstate of the b occupation number operators.

* Often these relations are found also by diagonalising the mean field BCS Hamiltonian instead of minimizing the energy. Only together these elements provide the solution of the Hamiltonian (in mean field).

The Bogolon may appear partly of a normal state electron and partly a hole, so its charge may not be integer.

However the true b quasiparticle operators are

$$\begin{cases} \beta_{k\sigma} = u_k c_{k\sigma} - \sigma v_k P c^+_{-k-\sigma} \\ \beta^+_{k\sigma} = u_k c^+_{k\sigma} - \sigma v_k c_{-k-\sigma} P^+ \end{cases}$$ (Josephson)

Where P annihilates and P^+ creates a bound pair with zero momentum and zero spin as in Cooper.

A Bogolon is annihilated, (i.e. a hole bogolon is created) by partially creating a normal state hole and partially annihilating an electron pair and replacing it with a normal state electron.

The second part of the process also creates a positive charge, so the hole bogolon ($|k| < k_F$) carries an integer quantum charge.

Electron Bogolon ($|k| > k_F$) is created by partially creating a normal state electron and partially creating an electron pair and simultaneously annihilating a normal state electron.

The P operators make the Bogolon be surrounded by a SC backflow of charge which ensures that charges are integer.

<u>NB</u>: It remains to show that the new g.-state $|\Psi_S\rangle$ is indeed SC (!).

BCS ground state and Bogoliubov-Valatin transformation for the excited states

In the B-V description the BCS ground state $|\Psi_0\rangle$ was assumed to be an occupation number eigenstate of $n_{k\sigma} = b^+_{k\sigma} b_{k\sigma}$ when $b_{k\sigma}$ were determined by B-V. Then it was found that all occupation numbers $n_{k\sigma}$ are zero in the g-state. This implies that

$$\langle \Psi_0 | b^+_{k\sigma} b_{k\sigma} | \Psi_0 \rangle = 0$$

and also $\quad b_{k\sigma} |\Psi_0\rangle = 0 \quad$ for all $k\sigma$

The mean field BCS g-state is the uniquely defined b-vacuum. We can show that

$$|\Psi_0\rangle = \prod_k (u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow}) |0\rangle$$

is the properly defined g-state. The normal metal g-state is

$$|0\rangle = \prod_{k\sigma}^{\varepsilon_k < \mu} c^+_{k\sigma} |0\rangle = \prod_{k}^{\varepsilon_k < \mu} c^+_{k\uparrow} c_{-k\downarrow} |0\rangle$$

and has the shape of $|\Psi_0\rangle$ with $u_k = 0$ for $\varepsilon_k < \mu$ and $u_k = 1$ for $\varepsilon_k > \mu$ and the opposite for v_k

Normalization

$$\langle |(u_k + v_k c_{-k\downarrow} c_{k\uparrow})(u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow})\rangle =$$

$$u_k^2 + u_k v_k c^+_{k\uparrow} c^+_{-k\downarrow} + u_k v_k c_{-k\downarrow} c_{k\uparrow} +$$

$$+ v_k^2 c_{-k\downarrow} c_{k\uparrow} c^+_{k\uparrow} c^+_{-k\downarrow} = u_k^2 + v_k^2$$

Then

$$b_{k'\uparrow} |\Psi_0\rangle = \left[\prod_{k \neq k'} (u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow})\right] (u_{k'} c_{k'\uparrow} - v_{k'} c^+_{-k'\downarrow}) \cdot$$

$$\cdot (u_{k'} + v_{k'} c^+_{k'\uparrow} c^+_{-k'\downarrow}) |\tilde{k}\rangle$$

state in which neither $k\uparrow$ nor $k\downarrow$ is occupied

One gets four terms

$u_k^2 c_{k\uparrow} \to \emptyset$

$u_k v_k c_{k\uparrow} c^+_{k\uparrow} c^+_{-k\downarrow} = u_k v_k \left((1 - c^+_{k\uparrow} c_{k\uparrow}) c^+_{-k\downarrow} \right) = u_k v_k c^+_{-k\downarrow}$

$-u_k v_k c^+_{-k\downarrow}$

$-v_k^2 c^+_{-k\downarrow} c^+_{k\uparrow} c^+_{-k\downarrow} \to \emptyset$

$\Sigma \to \emptyset$

Therefore the operator $b_{k'\uparrow}$ annihilates the ground state because, since it describes an excitation, it is orthogonal to the g-state.

Pair States

Find the wavefunctions contained in $|\Psi_0\rangle$

$c^\dagger_{k\sigma}$ creates an electron in a state $\sim e^{ik\cdot r}\chi_\sigma(s)$

$$\psi^\dagger(r,s)=\sum_{k\sigma} c^\dagger_{k\sigma}\, e^{(ik\cdot r)}\chi_s(s)$$

$$\Psi_0(x_1,x_2,\dots x_N)=\langle x_1\dots x_N|\Psi_0\rangle =$$

$$=\langle|\psi(x_N)\cdots\psi(x_1)\underbrace{\prod_k(u_k+v_k c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow})|\rangle}_{=0 \text{ if not } k_i\sigma_i\neq k_j\sigma_j\ (i\neq j)}$$

$$\Psi_0(x_1\dots x_N)=\sum_{k_1,\dots k_N} e^{ik_Nr_N}c_{k_N\sigma_N}\,e^{ik_{N-1}r_{N-1}}c_{k_{N-1}\sigma_{N-1}}\cdots e^{ik_1\sigma_1}c_{k_1\sigma_1}\times$$

$$\times\prod_k(1+g_k c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow})\prod_k u_k|0\rangle=$$

$$=\sum_{k_1\dots k_N} e^{i(k_1r_1+\dots+k_Nr_N)}\underbrace{\langle|c_{k_N\sigma_N}\cdots c_{k_1\sigma_1}\prod_k^{N/2} g_k c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}|\rangle}_{\text{sum over all possible contractions}}\left(\prod_k u_k\right)\simeq$$

$$\simeq\sum_{\{k_{2i}\}}{}'\left(e^{ik_2(r_1-r_2)}g_{k_2}\delta_{\sigma_1-\sigma_2}\cdots\cdots e^{ik_N(r_{N-1}-r_N)}g_{k_N}\delta_{\sigma_{N-1}-\sigma_N}\pm\dots\right)=$$

$$=\mathcal{A}\,\phi(r_1-r_2)\chi_{singlet}\,\phi(r_3-r_4)\chi_{singlet}\cdots\phi(r_{N-1}-r_N)\chi_{singlet}$$

$$\phi(\rho)\simeq\sum_k g_k e^{ik\cdot\rho}\ ;\quad g_k=\frac{v_k}{u_k}$$

$|\Psi_0\rangle$ consists of pairs of electrons in the general pair orbital state $\phi(\rho)\chi_{singlet}$

But u_k and v_k may be written as functions of Δ_0 and $(\varepsilon_k - \mu)/\Delta_0 \simeq \hbar v_F k/\Delta_0$

From this $\quad g_k \simeq \tilde{g}\left(\frac{\hbar v_F k}{\Delta_0}\right)$

$$\phi(\rho) \sim \int d^3k \, g_k \, e^{ik\rho} \sim \int_0^\infty dk\, k^2 g_k \int_{-1}^{+1} d\xi \, e^{i\rho\xi} =$$

$$= \int_0^\infty dk\, k^2 g_k \frac{e^{ik\rho} - e^{-ik\rho}}{ik\rho} \simeq$$

$$\simeq \frac{1}{\rho}\int_0^\infty dk\, k\, \tilde{g}\left(\frac{\hbar v_F k}{\Delta_0}\right) \sin k\rho \sim \frac{1}{\rho}\int dx \; x\,\tilde{g}(x)\sin\left(\frac{\Delta_0 x \rho}{\hbar v_F}\right) \sim$$

$$\sim f(\rho/\xi_0) \qquad \text{with} \qquad \xi_0 \approx \frac{1}{\pi\delta k} = \frac{\hbar v_F}{\pi\Delta_0}$$

ρ is the distance vector of the two electrons in the pair. Its average is ξ_0, the orbital ϕ does not depend on the center of mass position. Plane wave with $K=0$

All $N/2 \sim 10^{23}$ electron pairs occupy the same delocalised pair orbital ϕ in the BCS g-state $|\Psi_0\rangle$

This is the condensate wave function of the SC state and the structure of the wavef. $|\Psi_0\rangle$ ensures that the solution of the BCS model is a superconductor.

NB: all N electrons or only those near the F.S. (?)

BCS WAVEFUNCTION

NB: particle number is not fixed

Basically this should correspond to the antisymmetrisation of a function of type

$$\phi(x_1-x_2)\,\phi(x_3-x_4)\cdots\phi(x_{N-1}-x_N)|0\rangle$$

Each function ϕ has the structure

$$\phi \longleftrightarrow \sum_k g_k\, a^+_{k\uparrow} a^+_{-k\downarrow}$$

and the ~~a~~ full function has the shape

$$A \sum_{k_1,k_2\cdots k_N} g_{k_1} g_{k_2} \cdots g_{k_N} (a^+_{k_1\uparrow} a^+_{-k_1\downarrow})(a^+_{k_2\uparrow} a^+_{-k_2\downarrow})\cdots(a^+_{k_N\uparrow} a^+_{-k_N\downarrow})|0\rangle$$

this is already an approximation but not easy to handle.

Schrieffer proposal:

$$|\Phi\rangle = \prod_k (u_k + v_k a^+_{k\uparrow} a^+_{-k\downarrow})|0\rangle$$

the product is on all k's, not just those outside the Fermi sphere.

u_k is the prob. that the state k is empty

and v_k the prob. that it is occupied by a pair.

Consider

$$|\Phi\rangle = N \prod_k (1 + g_k a^+_{k\uparrow} a^+_{-k\downarrow})|0\rangle$$

which is equivalent to the one written above.

check

$$\langle\tilde\phi|\tilde\phi\rangle = \prod_{k',k} \langle 0|(1+g_{k'}a_{-k'\downarrow}a_{k'\uparrow})(1+g_k a^+_{k\uparrow}a^+_{-k\downarrow})|0\rangle N^2$$

$$= \prod_{k,k'} \langle 0|1 + g_{k'}\underbrace{a_{-k'\downarrow}a_{k'\uparrow}}_{\emptyset} + g_k \underbrace{a^+_{k\uparrow}a^+_{-k\downarrow}}_{\emptyset} + g_k g_{k'} a_{-k'\downarrow}a_{k'\uparrow}a^+_{k\uparrow}a^+_{-k\downarrow}|0\rangle$$

$$1 = \langle\tilde\phi|\tilde\phi\rangle = N^2 \prod_k (1+g_k^2)$$

$$N = \prod_k \frac{1}{\sqrt{1+g_k^2}}$$

$$\langle\tilde\phi|\tilde\phi\rangle = \prod_{k'} \langle 0|(u_{k'} + v_{k'}a^+_{-k'\downarrow}a^+_{k'\uparrow}) \prod_k (u_k + v_k a^+_{k\uparrow}a^+_{-k\downarrow})|0\rangle$$

$$u_k = \frac{1}{\sqrt{1+g_k^2}} \quad ; \quad v_k = \frac{g_k}{\sqrt{1+g_k^2}}$$

and therefore

$$u_k^2 + v_k^2 = 1$$

Only terms with $k = k'$

Number of particles with spin $\uparrow$

$$\langle N_\uparrow\rangle = \sum_k \langle 0|(u_k + v_k a_{-k\downarrow}a_{k\uparrow})a^+_{k\uparrow}a_{k\uparrow}(u_k + v_k a^+_{k\uparrow}a^+_{-k\downarrow})|0\rangle$$

$$= \sum_k v_k^2 \langle 0|a_{-k\downarrow}a_{k\uparrow}(a^+_{k\uparrow}a_{k\uparrow})a^+_{k\uparrow}a^+_{-k\downarrow}|0\rangle = \sum_k v_k^2$$

Let us now consider the variance of

$$N = N_\uparrow + N_\downarrow$$

$$\Delta N^2 = \langle N^2\rangle - \langle N\rangle^2 = \langle N_\uparrow^2 + N_\downarrow^2 + 2N_\uparrow N_\downarrow\rangle - 4\langle N_\uparrow\rangle^2 =$$

$$= 2\left(\langle N_\uparrow^2\rangle + \langle N_\uparrow N_\downarrow\rangle - 2\langle N_\uparrow\rangle^2\right)$$

$$\langle N_\uparrow^2\rangle = \langle 0|\prod_l (u_l + v_l a_{-l\downarrow} a_{l\uparrow}) \sum_{kk'} n_{k\uparrow} n_{k'\uparrow} \prod_m (u_m + v_m a^\dagger_{m\uparrow} a^\dagger_{-m\downarrow})|0\rangle =$$

$$= \sum_{k\neq k'} \langle 0|(u_k + v_k a_{-k\downarrow} a_{k\uparrow})(u_{k'} + v_{k'} a_{-k'\downarrow} a_{k'\uparrow})\, n_{k\uparrow} n_{k'\uparrow} \cdot$$

$$\cdot (u_k + v_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow})(u_{k'} + v_{k'} a^\dagger_{k'\uparrow} a^\dagger_{-k'\downarrow})|0\rangle +$$

$$+ \sum_k \langle 0|(u_k + v_k a_{-k\downarrow} a_{k\uparrow})\, n_{k\uparrow}^2\, (u_k + v_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow})|0\rangle =$$

$$= \sum_{k\neq k'} v_k^2 v_{k'}^2 + \sum_k v_k^2 = \sum_{k,k'} v_k^2 v_{k'}^2 + \sum_k (v_k^2 - v_k^4)$$

Since for fermions $n_{k\uparrow} n_{k\uparrow} = n_{k\uparrow}$

$$\langle N_\uparrow N_\downarrow\rangle = \langle 0|\prod_l (u_l + v_l a_{-l\downarrow} a_{l\uparrow}) \sum_{k,k'} a^\dagger_{k\uparrow} a_{k\uparrow} a^\dagger_{k'\downarrow} a_{k'\downarrow} \cdot$$

$$\cdot \prod_m (u_m + v_m a^\dagger_{m\uparrow} a^\dagger_{-m\downarrow})|0\rangle =$$

$$= \sum_{k\neq k'} v_k^2 v_{k'}^2 + \sum_k v_k^2 = \sum_{k,k'} v_k^2 v_{k'}^2 + \sum_k (v_k^2 - v_k^4)$$

Using that $N_\uparrow = N_\downarrow$

Therefore $\Delta N^2 = \langle N^2\rangle - \langle N\rangle^2 =$

$$= \langle N_\downarrow^2\rangle + \langle N_\uparrow^2\rangle + 2\langle N_\uparrow N_\downarrow\rangle - \langle N\rangle^2 =$$

$$= \sum_{kk'} 4 v_k^2 v_{k'}^2 + \sum_k 4 v_k^2 (1 - v_k^2) - 4\sum_{k,k'} v_k^2 v_{k'}^2 =$$

$$= 4\sum_k v_k^2 (1 - v_k^2) = 4\sum_k v_k^2 u_k^2$$

$$u_k^2 v_k^2 = \frac{1}{4} \frac{\Delta^2}{(\varepsilon_k - \mu)^2 + \Delta^2}$$

$$\langle N^2 \rangle - \langle N \rangle^2 = 4 \sum_k \frac{1}{4} \frac{\Delta^2}{\omega_k^2 + \Delta^2} = \underbrace{\frac{\Omega}{(2\pi)^3}}_{\propto N} \int d\omega \, \frac{\Delta^2 N(\omega)}{\omega^2 + \Delta^2}$$

This integral converges because $DOS(\omega) \sim \sqrt{\omega}$

Therefore $\quad \dfrac{\Delta N^2}{\langle N \rangle^2} \sim \dfrac{1}{\langle N \rangle}$

So for large N one can fix the value of N with a chemical potential

<u>Implications of a non fixed N:</u>

We can write the wavefunction as

$$|\tilde{\phi}\rangle = \sum_{N=0}^{\infty} \lambda_N |\phi_N\rangle$$

where λ_N are peaked around N^* and the fluctuations are of order $\sqrt{N^*}$

$$\lambda_{N+p} \sim \lambda_N \quad \text{if } p \ll \sqrt{N^*}$$

This means that the wavefunction with non fixed N for some properties behaves as if $N \sim N^*$ is fixed but for other properties it shows non zero values for operators that change N

$$\langle \tilde{\phi} | F | \tilde{\phi} \rangle = \sum_{N, N'} \lambda_N^* \lambda_{N'} \langle \phi_{N'} | F | \phi_N \rangle$$

If F conserves the value of N

$$\langle \tilde{\phi} | F | \tilde{\phi} \rangle = \sum_N |\lambda_N|^2 \langle \phi_N | F | \phi_N \rangle \simeq$$

$$\simeq \langle \phi_{N^*} | F | \phi_{N^*} \rangle \sum_N |\lambda_N|^2 = \langle \phi_{N^*} | F | \phi_{N^*} \rangle$$

having assumed that $\langle \phi_N | F | \phi_N \rangle$ varies slowly with N –

If the operator changes the value of N

$$\langle \Phi | F | \Phi \rangle = \sum_N \lambda^*_{N+p} \lambda_N \langle \phi_{N+p} | F | \phi_N \rangle \simeq$$

$$\simeq \sum_N |\lambda_N|^2 \langle \phi_{N+p} | F | \phi_N \rangle = \langle \phi_{N^*+p} | F | \phi_{N^*} \rangle$$

Therefore in this situation one can have nonzero value also for anomalous operators like $a^+ a^+$ which for a normal Fermi liquid give zero –

FINITE TEMPERATURE BCS

The transformed Hamiltonian shows that the bogolons created by operators $\beta^+_{k\sigma}$ and have an energy dispersion

$$\eta_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}$$

are fermionic excitations with charge e and spin σ above the BCS ground state $|\Psi_0\rangle$. Since they may recombine into Cooper pairs ϕ, the chemical potential of the Cooper pair must be 2μ where μ ~~is~~ is the chemical potential of bogolons.

At temperature T the distrib. of bogolons is

$$n_{k\uparrow} = n_{k\downarrow} = \frac{1}{e^{\eta_k/k_BT} + 1}$$

The gap equation then becomes

$$1 = \frac{g}{2V} \sum_k \frac{1 - 2\left(e^{\eta_k/kT} + 1\right)^{-1}}{\eta_k} =$$

$$= \frac{g N(0)}{2} \int_{-\omega_c}^{+\omega_c} \frac{d\omega}{\sqrt{\omega^2 + \Delta^2}} \; \frac{e^{\sqrt{\omega^2+\Delta^2}/kT} - 1}{e^{\sqrt{\omega^2+\Delta^2}/kT} + 1} =$$

$(\omega = \varepsilon_k - \mu)$

$$= g N(0) \int_0^{\omega_c} \frac{d\omega}{\sqrt{\omega^2 + \Delta^2}} \tanh\left(\frac{\sqrt{\omega^2 + \Delta^2}}{2kT}\right)$$

$$\left[\begin{aligned} \sinh x &= \frac{e^x - e^{-x}}{2} \\ \cosh x &= \frac{e^x + e^{-x}}{2} \\ \mathrm{tgh}\, x &= \frac{e^x - e^{-x}}{e^x + e^{-x}} \end{aligned}\right]$$

(ω is symmetric)

For $T \to 0$ $\tanh \to 1$ for $x \to \infty$ it reproduces the gap equation of the g-state.

For increasing temperature the numerator of the basic gap eq. decreases, so also Δ must decrease. It becomes zero at the transition temperature T_c

$$1 = gN(0)\int_0^{\omega_c} \frac{d\omega}{\omega} \tanh\frac{\omega}{2k_BT_c} =$$

$$= gN(0)\int_0^{\omega_c/2k_BT_c} \frac{dx}{x} \tanh x =$$

Integration by parts ($\int u\,dv = uv - \int v\,du$)

$$= \ln\frac{\omega_c}{2kT_c}\tanh\frac{\omega_c}{2kT_c} - \int_0^{\omega_c/2kT_c} dx\,\frac{\ln x}{\cosh^2 x} \simeq \qquad \left[\frac{d\tanh x}{dx} = \frac{1}{\cosh^2 x}\right]$$

$$(kT_c \ll \omega_c)$$

$$\simeq \ln\left(\frac{\omega_c}{2kT_c}\right) - \int_0^{\infty} dx\,\frac{\ln x}{\cosh^2 x} =$$

$$= \ln\frac{4\gamma}{\pi} + \ln\frac{\omega_c}{2k_BT_c} = \frac{2\gamma\,\omega_c}{\pi\,k_BT_c}$$

where $\ln\gamma = C = 0.577$ is the Euler constant

$$\gamma = \lim_{n\to\infty}\left(\sum_{k=1}^{n}\frac{1}{k} - \ln n\right)$$

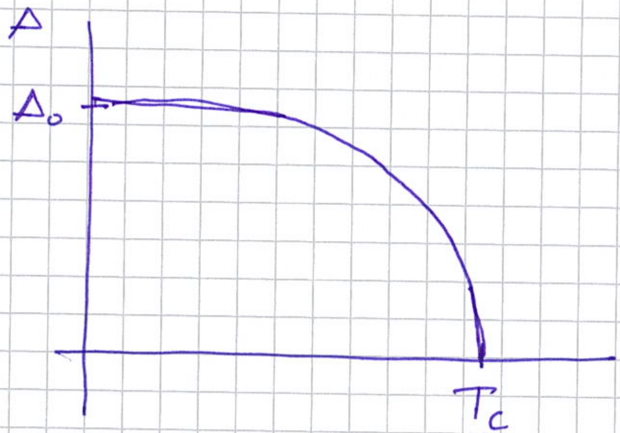
$$\boxed{kT_c = \frac{2\gamma}{\pi}\,\omega_c \exp\left\{-\frac{1}{gN(0)}\right\} = \frac{\gamma}{\pi}\Delta_0}$$

with $2\gamma/\pi \simeq 1.13$ and

$$\boxed{\frac{2\Delta_0}{kT_c} \simeq 3.52}$$

The gap $\Delta(T)$ as a function of T should be computed numerically. A good approximation is

$$\Delta(T) \simeq \Delta_0 \sqrt{1-\left(\frac{T}{T_c}\right)^3}$$



From the energy expression the thermodynamical quantities can be calculated, once $\Delta(T)$ and $\eta_n(T)$ are given

Condensation energy at $T=0$

$$\frac{B_c(0)^2}{2\mu_0} = \frac{1}{2} N(0)\,\Delta_0^2$$

which leads to the thermodynamic critical field at $T=0$.

The specific heat jump at T_c

$$\frac{C_s - C_n}{C_n} = 1.43$$

and the exponential behaviour of the specific heat at low temperature

$$C_s(T) \simeq T^{-3/2} e^{-\Delta_0/kT} \qquad \text{for } T \ll T_c$$