3. VERSO UNA TEORIA MICROSCOPICA: INSTABILITA' DELLE COPPIE DI COOPER

3.1 POSSIBILE ORIGINE DI UNA ATTRAZIONE TRA GLI ELETTRONI MEDIATA DAI FONONI

3.2 INTABILITA' E STATI LEGATI DELLE COPPIE DI COOPER IN PRIMA QUANTIZZAZIONE

3.3 COPPIE DI COOPER IN SECONDA QUANTIZZAZIONE SINGOLETTO E TRIPLETTO

Towards a microscopic theory

Qualitative picture of the possible attraction between electrons

Electrostatic repulsion

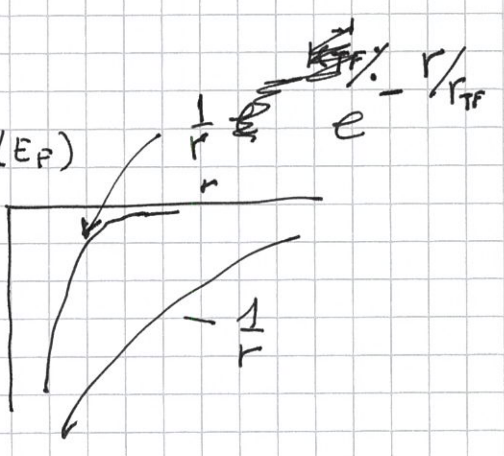
$$V_{bare}(r) = \frac{e^2}{r} \qquad \text{NB: for } r = 1\,\text{Å} \quad V_{bare} \simeq 15\,\text{eV}!$$

$$V_{bare}(q) = \frac{4\pi e^2}{q^2}$$

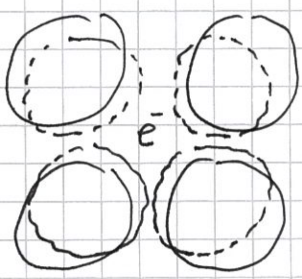
$\Rightarrow$ $\boxed{\text{Thomas Fermi screening}}$

$$\varepsilon_{el}(q) = 1 + \frac{k_s^2}{q^2} \qquad k_s^2 \sim D(E_F)$$

$$V(q) = \frac{4\pi e^2}{q^2 \varepsilon_{el}(q)} = \frac{4\pi e^2}{q^2 + k_s^2}$$



Consider now also the motion of ions



Total dielectric constant of a metal:

(a) conduction electrons $\varepsilon_{el}(q, \omega)$

(b) lattice ions $\varepsilon_{ion}(q, \omega)$

To find the combined effect consider an applied field (external)

$$\phi_a(r,t) = \phi_a(q,\omega)\cos(q\cdot r - \omega t)$$

$$\phi_e(r,t) = \phi_e(q,\omega)\cos(q\cdot r - \omega t)$$ potential due to the electronic space charge

$$\phi_i(r,t) = \phi_i(q,\omega)\cos(q\cdot r - \omega t)$$

The net total potential is

$$\phi = \phi_a + \phi_e + \phi_i$$

Then we can write the following relations

$$\varepsilon_{el}(q,\omega)\,\phi(q,\omega) = \phi_a(q,\omega) + \phi_i(q,\omega) \quad \text{potential seen by electrons}$$

$$\varepsilon_{ion}(q,\omega)\,\phi(q,\omega) = \phi_a(q,\omega) + \phi_e(q,\omega) \quad \text{potential seen by ions}$$

$$-\,\varepsilon(q,\omega)\;\phi(q,\omega) = -\,\phi_a(q,\omega)$$

$$(\varepsilon_{el} + \varepsilon_{ion} - \varepsilon)\,\phi = \phi_a + \phi_i + \phi_e = \phi$$

$$\boxed{\varepsilon(q,\omega) = \varepsilon_{el}(q,\omega) + \varepsilon_{ion}(q,\omega) - 1}$$

Simplest form:

$$\varepsilon_{el}(q\omega) \simeq \varepsilon_{el}(q,0) \simeq 1 + \frac{k_s^2}{q^2} \quad \left(\omega \text{ dependence is weak at small } \omega\right) \quad \omega \ll q v_F$$

$$\varepsilon_{ion}(q,\omega) \simeq \varepsilon_{ion}(0,\omega) \simeq 1 - \frac{\omega_{pi}^2}{\omega^2} \quad \left(q \text{ dependence is weak}\right) \quad \omega \gg q v_{ion}$$

Since $v_F \simeq 10^4 v_{ion}$ there is a large range of ~~of~~ validity of these approximations.

$$\varepsilon(q,\omega) = 1 + \frac{k_s^2}{q^2} - \frac{\omega_{pi}^2}{\omega^2} = \left(1 + \frac{k_s^2}{q^2}\right)\left(1 - \frac{\omega_{phon}^2(q)}{\omega^2}\right)$$

Having used Bohm Staver $\omega_{ph}^2(q) = \omega_{pi}^2/\varepsilon_{el}(q)$

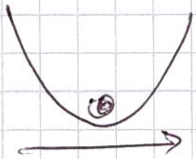
Now consider two electrons at $\vec{r}$. Their Coulomb repulsion is screened by the total $\varepsilon(q,\omega)$

$$\boxed{V_{screen}(q) = \frac{4\pi e^2}{q^2\varepsilon(q,\omega)} = \frac{4\pi e^2}{q^2 + k_s^2}\left(\frac{\omega^2}{\omega^2 - \omega_{phon}^2(q)}\right)}$$

Interpretation:

$$\begin{cases} q = \bar{k} - \bar{k}' \\ \hbar\omega = E_k - E_{k'} \end{cases} \quad \text{for the two electrons}$$

Polarizability of the Harmonic Oscillator



$$E(\vec r,t) = E_0 \cos(q\cdot r - \omega t) =$$

$$\mathrm{Re}\,\{\vec E_0 e^{i(q\cdot r-\omega t)}\}$$

$q\cdot r \approx$ const (small q)

$$F = -fr \qquad \omega_0 = \sqrt{f/m}$$

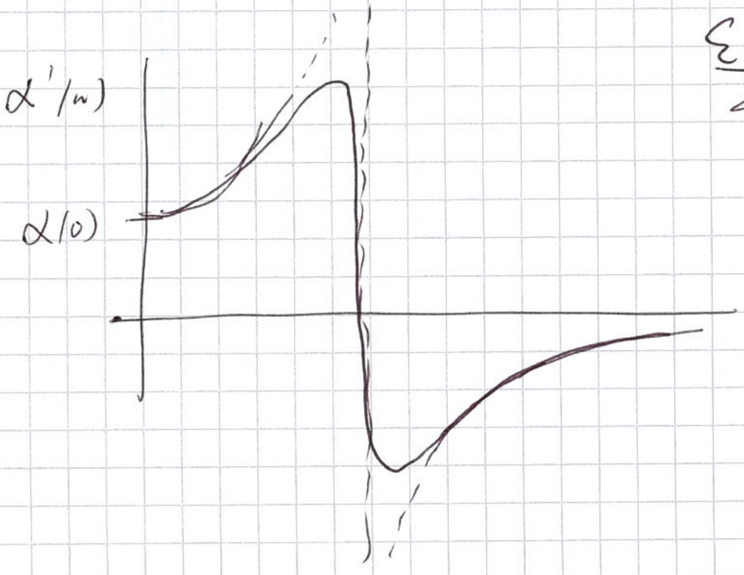
$$\frac{d^2\vec r}{dt^2} = -\omega_0^2\vec r - \frac{e}{m}\vec E_0 e^{-i\omega t} - \gamma\frac{dr}{dt}$$

$$\vec r(t) = \vec r_0 e^{-i\omega t} \qquad p(t) = -e\vec r(t) \equiv$$

$$\vec r_0 = \frac{-(e/m)E_0}{\omega_0^2-\omega^2-i\gamma\omega} \qquad \equiv \alpha(\omega)\vec E_0 e^{-i\omega t}$$

$$\alpha(\omega) = \frac{e^2/m}{\omega_0^2-\omega^2-i\gamma\omega} = \frac{e^2}{m}\frac{(\omega_0^2-\omega^2)+i\gamma\omega}{(\omega_0^2-\omega^2)^2+\gamma^2\omega^2}$$

$$\equiv \alpha'(\omega) + i\alpha''(\omega)$$



$$\frac{\varepsilon-1}{4\pi} = \alpha$$

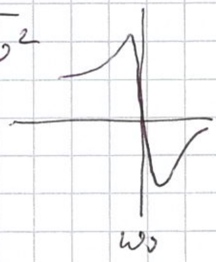
$$\varepsilon \sim 1 + \alpha$$

$\boxed{\varepsilon(\omega) \text{ FOR IONIC CRYSTAL}}$

RETARDATION

$$\frac{\varepsilon - 1}{4\pi} = N\alpha \qquad \boxed{\vec{p} = \alpha_E \vec{E}}$$

$$\left(\alpha_i(\omega) = \frac{e^2/M}{\omega_{0i}^2 - \omega^2} \right) \qquad \alpha_e'(\omega) \simeq \frac{e^2/m}{\omega_0^2 - \omega^2}$$



$$\varepsilon(\omega) = \varepsilon_e + \{\varepsilon(0) - \varepsilon_e\} \frac{\omega_T^2}{\omega_T^2 - \omega^2} =$$

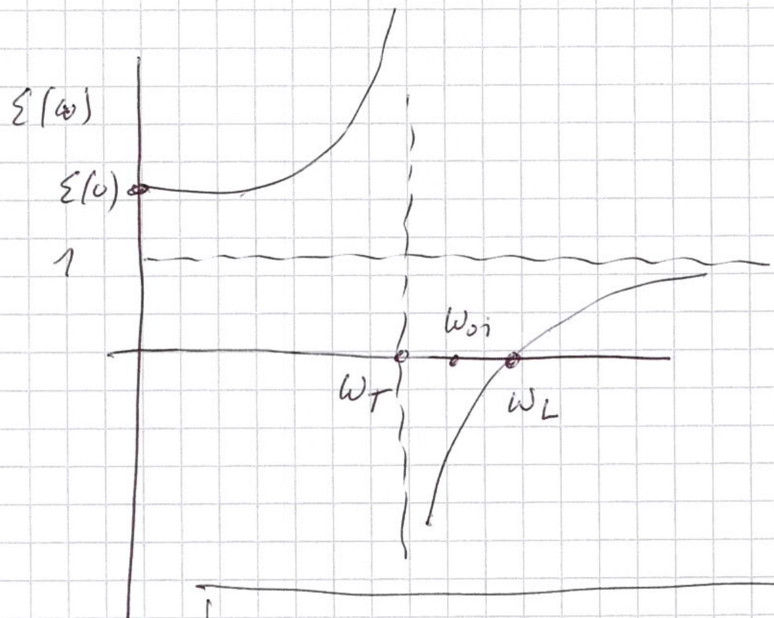
$$= \varepsilon_e \left\{ \frac{\omega_L^2 - \omega^2}{\omega_T^2 - \omega^2} \right\}$$

Dielectric function of ionic crystal (phonons)

$$\omega_T^2 = \omega_{0i}^2 \left\{ \frac{\varepsilon_e + 2}{\varepsilon(0) + 2} \right\} = \omega_{0i}^2 - \left(\frac{\varepsilon_e - 2}{9} \right) \omega_{pi}^2$$

$$\omega_L^2 = \omega_{0i}^2 \left\{ \frac{\varepsilon_e + 2}{\varepsilon(0) + 2} \right\} \frac{\varepsilon(0)}{\varepsilon_e} = \omega_{0i}^2 + 2 \left\{ \frac{\varepsilon_e + 2}{9\varepsilon_e} \right\} \omega_{pi}^2$$

$$\omega_{pi}^2 = \left(\frac{1}{4\pi\varepsilon_0} \right) \frac{4\pi N e^2}{M}$$



$$\boxed{\text{From which at large } \omega \quad \varepsilon_{ion}(\omega) \simeq 1 - \frac{\omega_{pi}^2}{\omega^2}}$$

Therefore:

(a) Since $\omega_{ph} \lesssim \omega_{Deby} \ll E_F$ only electrons with very similar energies are affected by phonons.

(b) When the electronic energy difference is

$$\hbar\omega = E_k - E_{k'} < \hbar\omega_D$$

the phonon contribution has the opposite sign of the electron ~~same~~ screening and the screened $V(q) < 0$!

This is an essential ingredient for the formation of Cooper pairs (but the way we have described it may be more appropriate for the polaron) -

Pair of interacting particles

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(r_2 - r_1)$$

$$\vec{r} = \vec{r}_2 - \vec{r}_1 \qquad R_{CM} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2} \qquad \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$P = M\frac{d\vec{R}}{dt}$$

$$H = -\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + V(r)$$

For a pair of electrons

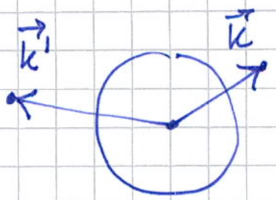
$$H_{pair} = -\frac{\hbar^2}{2(2m)}\nabla_R^2 - \frac{\hbar^2}{m}\nabla_r^2 + V(r)$$

$$\Psi(\vec{r},\vec{R}) = u(\vec{r})\,U(\vec{R}) \qquad \text{separation of the relative motion}$$

$$U(R) = e^{i\vec{K}\cdot\vec{R}} \qquad E_U = \frac{\hbar \mathbf{K}^2}{2(2m)}$$

and for the relative motion

$$\left[-\frac{\hbar^2}{m}\nabla_r^2 + V(r)\right] u(\vec{r}) = E\, u(\vec{r})$$



$\boxed{\text{Cooper pair}}$

Given a free el gas at $T=0$ consider two extra electrons interacting only with a slightly attractive potential $V(r)$

Their wavevectors $\vec{k}_1$ and $\vec{k}_2$ must lie outside the Fermi sphere and their energy is at least $2E_F$

Question : can the attractive interaction lead to a bound pair state ? so that the total energy is less than $2E_F$.

Assumptions :

(a) $\vec{k}_1 = -\vec{k}_2$ so that $\vec{K} = \vec{k}_1 + \vec{k}_2 = 0$

Lowest energy state is with $\vec{K}=0$ in the ~~p~~ equation for the pair.

(b) The two electrons have opposite spin (singlet state).

The total wavefunction must be antisymmetrical (fermions)

Then two choices :

- Symmetric spacial with opposite spin (singlet spin antisymmetric)
- Antisymmetric spacial with parallel spins. (triplet spin symmetric)

Spatial part

$$e^{i\vec{k}_1\vec{r}_1} \cdot e^{i\vec{k}_2\vec{r}_2} \pm e^{i\vec{k}_2\vec{r}_1} \cdot e^{i k_1 \cdot r_2} \qquad \bar{r} = \bar{r}_2 - \bar{r}_1$$

$$e^{-i\vec{k}\cdot\bar{r}} \pm e^{i\vec{k}\cdot\bar{r}} = \begin{cases} 2\cos\vec{k}\cdot\bar{r} \text{ with } \uparrow\downarrow \\ -2i\sin\vec{k}\cdot\bar{r} \text{ with } \uparrow\uparrow \end{cases}$$

Looking for an attractive interaction we like to have them close so we take the $\cos(\vec{k}\cdot\bar{r})$ with opposite spin.

Role of Fermi surfaces is only that $|\vec{k}| > k_F$ - crucial for a bound state

For the singlet state we write the wavefunction as a superposition of pair plane wave

$$u(r) = \sum_{k>k_F} a(k)\, e^{ik\cdot r} \qquad (a(k)=0 \text{ for } |\vec{k}| < k_F)$$

$$\left[-\frac{\hbar^2}{m}\nabla_r^2 + V(r)\right] u(\vec r) = E\, u(\vec r)$$

$E_u = E$ because $\vec K = 0$

$$\int d\vec r\, e^{-i\vec k'\cdot\vec r}\left[-\frac{\hbar^2}{m}\nabla_r^2 + V(r)\right]\sum_{k>k_F} a(\vec k)\, e^{i k\cdot r} =$$

$$= \int d\vec r\, e^{-i\vec k'\cdot\vec r}\, E \sum_{k>k_F} a(k)\, e^{i\vec k\vec r}$$ (+ change of labels)

$$\int d\vec r\, e^{-ik'r}\sum_{k>k_F} a(\vec k)\, e^{ikr}\, 2E_k + \int dr\, e^{-ik'r}\, V(r)\sum_{k>k_F} a(\vec k)\, e^{ikr} =$$

$$= \cancel{Ea}\; E\cdot a(k')$$

$$2E_{k'}\cdot a(k') + \sum_{k>k_F}\langle k'|V|k\rangle\, a(k) = E\cdot a(k')$$

$$(2E_k - E)\, a(k) + \sum_{k'>k_F}\langle \vec k|V|\vec k'\rangle\, a(k') = 0$$

$$E_k = \frac{\hbar^2 k^2}{2m}$$

Assumption about $V_{kk'} = V(q)$

$\langle k|V|k'\rangle = -V$ for $E_F \le E_k$; $E_{k'} \le E_F + \Delta$

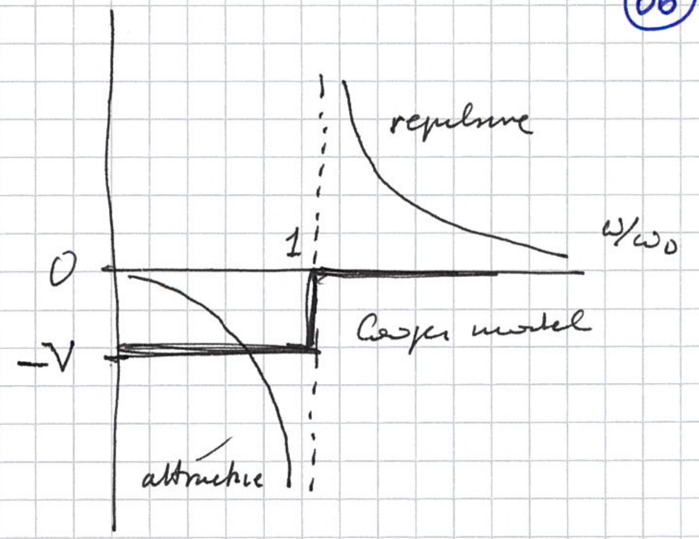
$= 0$ otherwise

where $V > 0$ and $\Delta \approx \hbar\omega_D$

Using it leads to

$$(2E_k - E)\, a(k) = V\sum_{k'} a(k') \quad \text{or}$$

$$\boxed{a(\vec{k}) = \frac{V}{2E_k - E} \sum_{k'} a(\vec{k}')}$$



where the sum extends over a shell of size Δ -

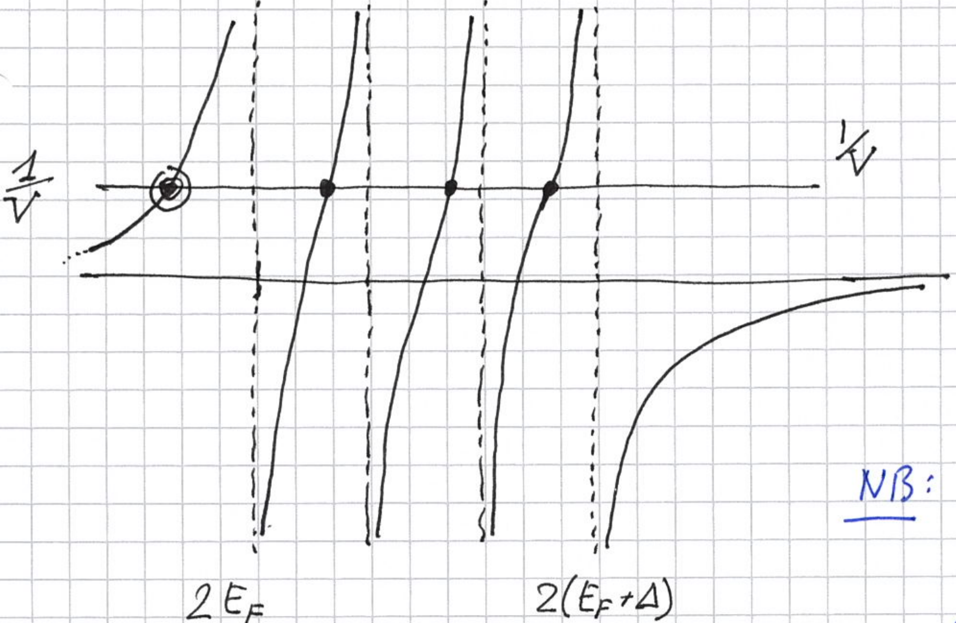
$a(k)$ only depends on $E_k = \frac{\hbar^2 k^2}{2m}$ so it is spherically symmetric (S-state)

Summing over k in a shell Δ and since $\sum_k a(k) = \sum_{k'} a(k')$ we get

$$\boxed{\frac{1}{V} = \sum_k \frac{1}{2E_k - E}} \quad \text{with} \quad \boxed{E_F \leq E_k \leq E_F + \Delta}$$

The Cooper bound state

Plotting the right side as a function of E we have



NB: For the triplet
$a(k) = -a(-k)$
so that $\sum_k a(k) \to \phi$
But for a more complex structure of the interaction there can be a non trivial solution

If $V=0 \rightarrow \frac{1}{V} \rightarrow \infty$ and the roots are simply $E=2E_k$

If $V \neq 0$ we have a quasicontinuum pair states in the region $E > 2E_F$ plus a single root below $2E_F$.

This is a bound state which occurs no matter how small is V!

This is remarkable because in general two interacting particles in free space only form a bound state if the attractive interaction has some strength above some value.

i.e Screened Coulomb interaction between electron and +e heavy charge gives a bound state only if the screening length is longer than the Bohr radius a_0.

The bound state of the Cooper pair is due to the presence of the filled Fermi sphere which excludes the use of one electron states below E_F.

Cooper pair binding energy E_B

In the region $E < 2E_F$ the denominators are positive and regular → continuum limit OK.

$$\frac{1}{V} \int_{E_F}^{E_F+\Delta} \frac{\overbrace{(1/2)\, D(E')}^{\text{one spin}}\, dE'}{2E'-E} \simeq \frac{1}{4} D(E_F) \int_{E_F}^{E_F+\Delta} \frac{d(2E')}{2E'-E} =$$

[S. Weinberg triplet etc?]

$$= \frac{1}{4} D(E_F) \ln \frac{2E_F - E + 2\Delta}{2E_F - E} = \frac{1}{4} D(E_F) \ln \frac{E_B + 2\Delta}{E_B}$$

$$\boxed{E_B = \frac{2\Delta}{e^{4/VD(E_F)} - 1} \simeq 2\Delta\, e^{-4/VD(E_F)}}$$

NB: Impossible to get a perturbative solution for small V. Non analiticity.

in the limit of weak coupling $VD(E_F) \ll 1$

* Superposition with $a(k)$ distribution

$\Delta \simeq \hbar\omega_{Debye}$

NB: We have considered $q=0$; If $k+k'=q\neq 0$ $k_1 = k + q/2$; $k_2 = -k + \frac{q}{2}$

$E(k_1) = E(k) + (k \cdot q/2)/m$ → denominator $\boxed{E - 2E(k) - \hbar q \cdot v_F}$

$E(k_2) = E(-k) - (k \cdot q/2)/m$

Note the importance of the Fermi sphere for the stability of Cooper pair.
If the lower cutoff were not E_F but 0, then, since $D(0)=0$
there would be no solution for weak coupling.
Also note that this explains why the critical temperature
is so low, much lower than T_{Debye}.

Non perturbative solution.

Spatial extent of a Cooper pair

The pair wavefunction $u(r)$ is made of functions with
energy range between E_F and $E_F + \hbar\omega_D$
The spread of momenta is then

$$\hbar\omega_D \simeq \delta\left(\frac{p^2}{2m}\right) \simeq 2\,\delta p\left(\frac{p_F}{2m}\right) \qquad \delta p \simeq \frac{m(\hbar\omega_D)}{p_F}$$

The spatial range is then of order

$$\xi \simeq \frac{\hbar^2}{\delta p} \simeq \frac{\hbar p_F}{m(\hbar\omega_D)} \simeq \frac{\hbar^2 k_F}{m(\hbar\omega_D)} \simeq \frac{1}{k_F}\frac{E_F}{\hbar\omega_D} \simeq (10^{-8})(10^3)\,\text{cm}$$

$$\simeq 1000\,\text{Å} \qquad \underline{\text{very large}}$$

This means that in the global BCS state a pair interacts
with <u>many</u> other pairs. (<u>mean field ≃ OK</u>)

* NB: Interpretation of Cooper pair in real space ?

* Check second quantization approach - Note Esling (V. Scarola)

SECOND QUANTIZATION FOR FERMIONS

→ COOPER'S PAIR

Consider a one particle wave eq. solution $\varphi_j(x)$

$$H\varphi_j(x) = E_j\varphi_j(x)$$

when j includes orbital and spin degrees of freedom

Field operators

$$\Psi(x) = \sum_j c_j \varphi_j(x) \quad ; \quad \Psi^+(x) = \sum_j c_j^+ \varphi_j^*(x)$$

The field operator $\Psi(x)$ and the fermion operator c_j operate on a state vector Φ, while $\varphi_j(x)$ is a C-number.

$$\Phi_{vac} = |0,0,0,\cdots,0\rangle = |\phi\rangle$$

The ground state of N fermions is

$$\Phi_0 = |1_1\, 1_2\, 1_3 \cdots 1_N\, 0_{N+1} 0_{N+2} \cdots 0\rangle$$

where states are ordered for increasing energy.

$\Psi^+(x)$ is an operator which adds a particle at x

$$\Psi^+(x')|\phi\rangle \to \delta(x-x')$$

Consider the density operator

$$\rho(x) \equiv \int dx'' \Psi^+(x'')\delta(x-x'')\Psi(x'')$$

and then

$$\rho(x)\Psi^+(x')|\phi\rangle = \int dx'' \Psi^+(x'')\delta(x-x')\underbrace{\Psi(x'')\Psi^+(x')}_{\delta(x''-x')}|\phi\rangle =$$

$$= \delta(x-x')\Psi^+(x')|\phi\rangle \quad ✓$$

From Pauli principle$^{(*)}$ → anticommutation relations

$$[C_\ell, C_m^+]_+ = C_\ell C_m^+ + C_m^+ C_\ell = \delta_{\ell m}$$

$$[C_\ell, C_m]_+ = C_\ell C_m + C_m C_\ell = 0$$

$$[C_\ell^+, C_m^+]_+ = C_\ell^+ C_m^+ + C_m^+ C_\ell^+ = 0$$

[For a single state one can represent C^+, C in terms of the Jordan Wigner matrices.]

Construct a state with one state k occupied

$$\Phi = C_k^+ |\phi\rangle = C_k^+ |0,0,0,\ldots 0_k,\ldots\rangle = |0,0,0,\cdots 1_k,\cdots\rangle$$

The ground state of an unperturbed Fermi sea is

$$\Phi_0 = \left(\prod_{|k|<k_F} C_k^+\right)|\phi\rangle = C_1^+ C_2^+ \cdots C_k^+ \cdots C_{k_F}^+ |\phi\rangle$$

~~Then~~ If there are many particle $C_i^+ C_j$ is unchanged but there is a problem with the sign of C_i^+ and C_j

i.e. consider

$$\Phi = C_1^+ C_2^+ |\phi\rangle$$

(*) Pauli principle and anticommutation

$\psi(a)|\phi\rangle = |a\rangle$ creates a particle in state a

$\psi(b)\psi(a)|\phi\rangle = \psi(b)|a\rangle = |a,b\rangle$

$\psi(a)\psi(b)|\phi\rangle = |b,a\rangle$

Since ψ anticommute

$$\psi(a)\psi(b) + \psi(b)\psi(a) = 0 \quad \rightarrow |a,b\rangle = -|b,a\rangle$$

Fermi statistics

If $b = a$

$$\psi(a)\psi(a) + \psi(a)\psi(a) = 2\psi(a)\psi(a) = 0$$

$$|a,a\rangle = 0 \rightarrow \text{Pauli principle.}$$

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Operating with c_2

$$c_2\Phi = c_2 c_1^+ c_2^+|\emptyset\rangle = -c_1^+ c_2 c_2^+|\emptyset\rangle =$$
$$= -c_1^+(1-c_2^+c_2)|\emptyset\rangle = -c_1^+|\emptyset\rangle$$

while with c_1

$$c_1\Phi = c_1 c_1^+ c_2^+|\emptyset\rangle = (1-c_1^+c_1)\,c_2^+|\emptyset\rangle = c_2^+|\emptyset\rangle$$

We have a $\ominus$ sign for every occupied state i which is on the left of the state j on which we operate. This implies a definite order.
Normal product: all creation are on the left.

In general

$$c_j|\dots n_j \dots\rangle = n_j\theta^j|\dots 0_j \dots\rangle$$

$$c_j^+|\dots n_j \dots\rangle = (1-n_j)\,\theta^j|\dots 1_j \dots\rangle$$

$$\theta^j = (-1)^{p_j}$$

where p_j is the number of occupied states on the left of j in the state vector Φ

$$[\Psi(x),\Psi^+]_+ = \delta(x-x')$$

$$[\Psi(x),\Psi^+(x')]_+ = \sum_{jl}[c_j^+c_l]_+\varphi_j(x)\varphi_l^*(x') = \sum_j \varphi_j(x)\varphi_j^*(x')$$

and $\sum_j \varphi_j(x)\varphi_j^*(x') = \delta(x-x')$ by closure or normalization.

One-Particle density operator

$$\rho(x) = \int dx'\,\Psi^+(x')\,\delta(x-x')\,\Psi(x') = \Psi^+(x)\Psi(x) =$$
$$= \sum_{ij} c_i^+c_j\,\varphi_i^*(x)\varphi_j(x)$$

The Hamiltonian in the second quantization representation is obtained by the general theorem that quantum operators are obtained directly from their classical analogs. For example

$$H = \int d^3x\, \psi^+(x) \frac{p^2}{2m} \psi(x) = \int dx \sum_{jl} c_j^+ c_l\, \varphi_j^*(x) \frac{p^2}{2m} \varphi_l(x)$$

$$p = -i\nabla$$

$$\rightarrow H = \sum_j \left(\frac{k_j^2}{2m}\right) c_j^+ c_j$$

<u>Coulomb interaction</u>

$$H = \frac{1}{2m}\sum_j p_j^2 + \frac{1}{2}\sum_{\substack{ij \\ i\neq j}}{}' \frac{e^2}{|x_i - x_j|} + v(x)$$ (removes the $q=0$ term)

$$= \frac{1}{2m}\sum_i p_i^2 + \frac{1}{2}\sum_{ij}{}' \sum_{q\neq 0} \frac{4\pi e^2}{q^2} e^{iq\cdot(x_i - x_j)}$$

$$\rho(x) = \sum_q \rho_q e^{iqx} = \sum_i \delta(x - x_i)$$

$$H = \frac{1}{2m}\sum_i p_i^2 + \sum_{q\neq 0} \frac{2\pi e^2}{q^2}\left(\rho_q^+ \rho_q - n\right)$$ electron concentration (positive background)

$$\rho_q(x) = \sum_k c_k^+ c_{k+q}$$

$$\rho_q^+ = \sum_k c_{k+q}^+ c_k = \rho_{-q}$$

Coulomb energy

$$\sum_q \frac{2\pi e^2}{q^2}\left(\rho_k^+ \rho_k - n\right) \rightarrow \sum_q{}' \left(\sum_{kk'} \frac{2\pi e^2}{q^2} c_{k+q}^+ c_k c_{k'-q}^+ c_{k'} - n\right)$$

Fermi Liquid and Cooper Pair in II Quantization

IInd Q : manipulate states without knowing the wavefunction

very suitable for non fixed number of particles.

FL g. state : occupied if $\varepsilon_k < \mu$ and empty if $\varepsilon_k > \mu$ –

Adding a fermion with $\varepsilon > \mu \to$ excited state

Removing " $\varepsilon < \mu \to$ hole

Dressed excitations with polarization cloud (FL) – $\boxed{\text{g. state } |\emptyset\rangle}$

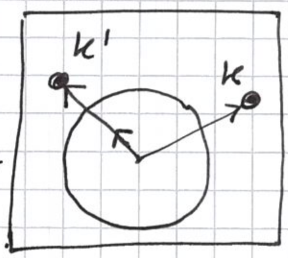
$$\varepsilon_k < \mu \qquad c^\dagger_{k,\sigma}|\emptyset\rangle = 0 \qquad c^\dagger_{k,\sigma} c_{k\sigma}|\emptyset\rangle = |\emptyset\rangle$$

$$\varepsilon_k > \mu \qquad c_{k\sigma}|\emptyset\rangle = 0 \qquad c_{k,\sigma} c^\dagger_{k,\sigma}|\emptyset\rangle = |\emptyset\rangle$$

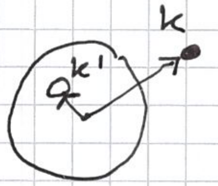
Effective Hamiltonian

$$H = \sum_{k,\sigma} c^\dagger_{k,\sigma}(\varepsilon_k - \mu) c_{k,\sigma} +$$

Cooper pair

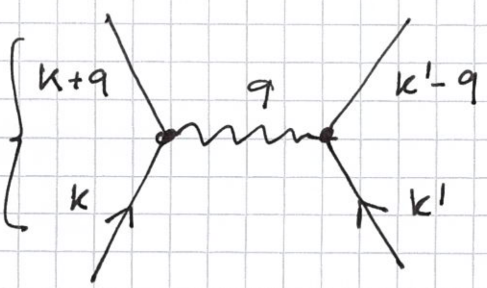


$$+ \frac{1}{2} \sum_{\substack{\varepsilon_k > \mu \;\; \varepsilon_{k'} > \mu \\ k,\sigma,k'\sigma',q}} c^\dagger_{k+q,\sigma} c^\dagger_{k'-q,\sigma'} W_{kk'} c_{k'\sigma'} c_{k\sigma} +$$



$$+ \sum_{\substack{\varepsilon_k > \mu, \; \varepsilon_{k'} < \mu \\ k\sigma,k'\sigma',q}} c^\dagger_{k+q,\sigma} c_{k'-q\sigma'} W_{kk'q} c^\dagger_{k'\sigma} c_{k\sigma} +$$

$$+ \frac{1}{2} \sum_{\substack{\varepsilon_k < \mu ; \; \varepsilon_{k'} < \mu \\ k\sigma,k'\sigma',q}} c_{k+q,\sigma} c_{k'-q,\sigma'} W_{kk'q} c^\dagger_{k',\sigma'} c_{k\sigma}$$



Consider now a Cooper pair made by two additional electrons

For the non interacting state

$$H_0|\phi\rangle = |\phi\rangle E_0 \quad E_0 = \langle\phi|H|\phi\rangle = \sum_{k\sigma}^{\varepsilon_k<\mu} (\varepsilon_k - \mu)$$

and we subtract this term from the original Hamiltonian

$$\hat{H} = H_0 - E_0 \quad \hat{H}|\phi\rangle = 0|\phi\rangle$$

We may create a quasiparticle above μ in this g. state

$$\varepsilon_{k_1} > \mu \quad |k_1\sigma_1\rangle = c^{+}_{k_1\sigma_1}|\phi\rangle$$

$$\hat{H}|k_1\sigma_1\rangle = |k_1\sigma_1\rangle(\varepsilon_{k_1} - \mu)$$

$$\hat{H}|k_1\sigma_1\rangle = \sum_{k\sigma} c^{+}_{k\sigma}(\varepsilon_k - \mu) c_{k\sigma} c^{+}_{k_1\sigma_1}|\phi\rangle$$

but $c^{+}_{k\sigma} c_{k\sigma} c^{+}_{k_1\sigma_1} = c^{+}_{k_1\sigma_1} c^{+}_{k\sigma} c_{k\sigma}$

and $c^{+}_{k\sigma} c_{k\sigma}|\phi\rangle = |\phi\rangle$

For the case of a hole $\varepsilon_{k_1} < \mu$

$$|k_1\sigma_1\rangle = c_{k_1\sigma_1}|\phi\rangle$$

$$H|k_1\sigma_1\rangle = |k_1\sigma_1\rangle |\varepsilon_{k_1} - \mu|$$

In this case the term $c^{+}_{k_1\sigma_1} c_{k_1\sigma_1} c_{k_1\sigma_1} = 0$ so one term has to be removed from the sum of energies in the Hamiltonian. So the ~~#~~ single particle spectrum of the effective Hamiltonian above $|\phi\rangle$ is just

$$\eta_k = |\varepsilon_k - \mu|$$

and the excited states are $|k_1\sigma_1\rangle$ independent on the wavefunction of $|\phi\rangle$ ($\simeq$ approximation).

*

Consider now a state with two excited particles

$$|k_1\sigma_1, k_2\sigma_2\rangle = c^\dagger_{k_1\sigma_1} c^\dagger_{k_2\sigma_2}|\phi\rangle$$

Here we consider two electrons but other cases would be analogous

Consider

$$\sum_{k,\sigma} c^\dagger_{k\sigma}(\varepsilon_k-\mu)c_{k\sigma}\, c^\dagger_{k_1\sigma_1} c^\dagger_{k_2\sigma_2}|\phi\rangle$$

$$c^\dagger_{k_1\sigma_1}(\varepsilon_{k_1}-\mu)c_{k_1\sigma_1}\, c^\dagger_{k_1\sigma_1} c^\dagger_{k_2\sigma_2}|\phi\rangle$$

$$+\, c^\dagger_{k_2\sigma_2}(\varepsilon_{k_2}-\mu)c_{k_2\sigma_2}\, c^\dagger_{k_1\sigma_1} c^\dagger_{k_2\sigma_2}|\phi\rangle$$

NB: k_1 and k_2 are not within the shell

$$c^\dagger_{k_1\sigma_1}(\varepsilon_{k_1}-\mu)c^\dagger_{k_2\sigma_2}\underbrace{c_{k_1\sigma_1}c^\dagger_{k_1\sigma_1}|\phi\rangle}_{=|\phi\rangle \text{ for } \varepsilon_k>0} =$$

$$= c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}|\phi\rangle(\varepsilon_{k_1}-\mu)$$

and the term with k_2 gives

$$c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}|\phi\rangle = (\varepsilon_{k_2}-\mu)$$

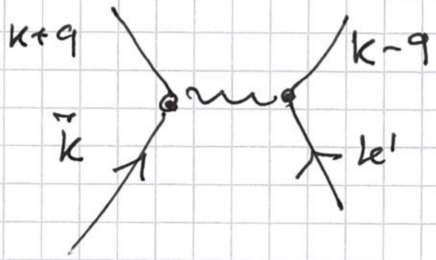
Therefore

$$H_0\, c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}|\phi\rangle = c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}|0\rangle(\eta_{k_1}+\eta_{k_2})$$

$$\eta_k = |\varepsilon_k-\mu|$$

Considering the first interaction term

$$H'_{\cdot\cdot} = \frac{1}{2} \sum_{\substack{\varepsilon_k>\mu,\ \varepsilon_{k'}>\mu \\ k\sigma, k'\sigma', q}} c^{+}_{k+q,\sigma} c^{+}_{k'-q,\sigma'} w_{kk'q} c_{k'\sigma'} c_{k\sigma} c^{+}_{k_1\sigma_1} c^{+}_{k_2\sigma_2} |0\rangle$$



(a) $k\sigma = k_1\sigma_1$; $k'\sigma' = k_2\sigma_2$

(b) $k'\sigma' = k_1\sigma_1$; $k\sigma = k_2\sigma_2$

$$\frac{1}{2} c^{+}_{k_1+q,\sigma_1} c^{+}_{k_2-q,\sigma_2} w_{k_1k_2q} c_{k_2\sigma_2} c_{k_1\sigma_1} c^{+}_{k_1\sigma_1} c^{+}_{k_2\sigma_2} |0\rangle$$

$$c_{k_i\sigma_i} c_{k_i\sigma_i} |0\rangle = |0\rangle \qquad \underbrace{c_{k_2\sigma_2} c^{+}_{k_2\sigma_2}}_{|0\rangle} \,\&\, \underbrace{c_{k_1\sigma_1} c^{+}_{k_1\sigma_1}}_{|0\rangle} |0\rangle$$

$$= \boxed{\frac{1}{2} c^{+}_{k_1+q\sigma_1} c^{+}_{k_2-q,\sigma_2} w_{k_1k_2q} |0\rangle}$$

$$\frac{1}{2} c^{+}_{k_2+q\,\sigma_2} c^{+}_{k_1-q,\sigma_1} w_{k_2k_1q} c_{k_1\sigma_1} c_{k_2\sigma_2} c^{+}_{k_1\sigma_1} c^{+}_{k_2\sigma_2} |0\rangle$$

$$\underbrace{c_{k_1\sigma_1} c^{+}_{k_1\sigma_1}}_{-|0\rangle} \quad \underbrace{c_{k_2\sigma_2} c^{+}_{k_2\sigma_2}}_{|0\rangle} |0\rangle$$

$$\boxed{= -\frac{1}{2} c^{+}_{k_2+q,\sigma_2} c^{+}_{k_1-q,\sigma_1} w_{k_2k_1q} |0\rangle}$$

$$= +\frac{1}{2} c^{+}_{k_1-q} c^{+}_{k_2+q} w_{k_1k_2q} |0\rangle$$

$$(\Sigma) \quad = \frac{1}{2} c^{+}_{k_1+q} c^{+}_{k_2-q} w_{k_1k_2q} |0\rangle$$

Therefore the application of the effective Hamiltonian gives

$$\boxed{\begin{aligned} H c^+_{k_1\sigma_1} c^+_{k_2\sigma_2}|0\rangle &= c^+_{k_1\sigma_1} c^+_{k_2\sigma_2}|0\rangle + \\ &+ \sum_q c^+_{k_1+q,\sigma_1} c^+_{k_2-q,\sigma_2}|0\rangle\, w_{k_1 k_2, q} \end{aligned}}$$

Cooper problem

- Total zero momentum $k_2 = -k_1$

$$|\psi\rangle = \sum_k a_k |k\sigma; -k\sigma'\rangle = \sum_k a_k c^+_{k\sigma} c^+_{-k\sigma'}|0\rangle$$

The idea is that this state should be an eigenstate of $\tilde{H}$

$\hat{H}|\psi\rangle = E\psi$

$$H|\psi\rangle = \sum_k c^+_{k\sigma} c^+_{-k\sigma'}|0\rangle\, 2\eta_k a_k + \sum_{k,q} c^+_{k+q,\sigma} c^+_{-k-q,\sigma'}|0\rangle\, w_{k,-k,q}\, a_k$$

multiplying by

$$\langle 0| c_{-k'\sigma'} c_{k'\sigma} \cdots$$

$$\langle 0| c_{-k'\sigma'} c_{k'\sigma} c^+_{k\sigma} c^+_{-k\sigma'}|0\rangle = \langle 0| c_{-k'\sigma'} (\delta_{kk'} - c^+_{k\sigma} c_{k'\sigma}) \times$$

$$\times c^+_{-k\sigma'}|0\rangle = \delta_{kk'} \langle 0| c_{-k'\sigma'} c^+_{-k\sigma'}|0\rangle - \quad (\delta_{kk'} - c^+_{-k\sigma'} c_{-k'\sigma'})$$

$$- \langle 0| c_{-k'\sigma'} c^+_{k\sigma} \underbrace{c_{k'\sigma} c^+_{-k\sigma'}}_{(\delta_{-kk'}\delta_{\sigma\sigma'} - c^+_{-k\sigma'} c_{k'\sigma})}|0\rangle$$

$$\left(= \delta_{kk'} - \langle 0|(\delta_{-kk'}\delta_{\sigma\sigma'} - c^+_{k\sigma} c_{-k'\sigma'})\, \delta_{-kk'}\delta_{\sigma\sigma'}|0\rangle = \right.$$

$$\left. = \delta_{kk'} - \delta_{-kk'}\delta_{\sigma\sigma'} \right)$$

$$\delta_{\kappa\kappa'} - \langle\phi| c^+_{-\kappa\sigma'} c_{-\kappa'\sigma'}|\phi\rangle -$$

$$- \langle\phi| c_{-\kappa'\sigma'} c^+_{\kappa\sigma} \delta_{-\kappa,\kappa'}\delta_{\sigma\sigma'}|\phi\rangle +$$

$$+ \langle\phi| c_{-\kappa'\sigma'} c^+_{\kappa\sigma} c^+_{-\kappa\sigma'} c_{\kappa'\sigma}|\phi\rangle$$

$$= \delta_{\kappa\kappa'} - \delta_{-\kappa\kappa'}\delta_{\sigma\sigma'}$$

$$E(a_{\kappa'} - a_{-\kappa'}\delta_{\sigma\sigma'}) = 2\eta_{\kappa'}(a_{\kappa'} - a_{-\kappa}\delta_{\sigma\sigma'}) +$$

$$+ \sum_q w_{\kappa'-q,-\kappa'+q,q}(a_{\kappa'-q} - a_{-\kappa'+q}\delta_{\sigma\sigma'})$$

when we also used again $w_{-\kappa'-q,\kappa'+q,q} = w_{\kappa'+q,-\kappa'-q,-q}$ and then replaced $\sum_q \to \sum_{-q}$

A nontrivial solution with even parity $a_{-\kappa} = a_\kappa$ (even angular momentum is only possible at $\delta_{\sigma\sigma'} = 0$, that is for a singlet state $\sigma' = -\sigma$. For a spin triplet $\sigma' = \sigma$ only a non trivial solution with odd parity is possible

Consider the singlet case

$$a_{\vec\kappa} = a_\kappa Y_{lm}\left(\frac{\vec\kappa}{\kappa}\right) \quad \text{with even } l$$

rename $\kappa' \to \kappa$; $\kappa' - q \to \kappa'$ the matrix element

$$w_{\kappa',-\kappa',\kappa-\kappa'} \approx \lambda_l w^l_\kappa$$

$$a_\kappa = \frac{\lambda_l w^l_\kappa C}{E_{lm} - 2\eta_\kappa} \; ; \; C = \sum_{\kappa'} w^{l*}_\kappa a_{\kappa'} \quad \text{inserting}$$

$$1 = \lambda_l \sum_\kappa |w^l_\kappa|^2 \frac{1}{E_{lm} - 2\eta_\kappa} = \lambda_l F(E_{lm})$$

More on the Cooper Pair problem

Towards the BCS wavefunction

Cooper pair : essentially two body problem not self-consistent with respect to the full many body problem.

But it indicates the path for the many body wavefunction

Consistent model : guess the solution has the shape of Cooper wavefunctions but neglect in the interaction term all those terms involving operators referring to states within the Fermi sea.

Cooper: If Fermi sea is filled both extra electrons lie just at the Fermi level

Most general wavefunction of this type

$$\sum_{\substack{k,k'\\ \sigma,\sigma'}} \alpha_{\sigma\sigma'}(k,k')\, c^{*}_{k\sigma} c^{+}_{k'\sigma'} |\underbrace{\phi}_{}\rangle$$

└ Filled Fermi sea

Hamiltonian conserves spin and momentum so ~~lowest state~~ the wavefunction is an eigenstate of momentum and spin.

For the lowest state we expect $K_{tot}=0$ and assume singlet for the spin

$$|\Psi\rangle = \sum_{k} \alpha(k)\, c^{+}_{-k\downarrow} c^{+}_{k\uparrow} |\phi\rangle$$

when $\sum |\alpha(k)|^2 = 1$ for normalization

The energy in this state is

check

$$E = 2\sum_{\varepsilon > \varepsilon_F} \varepsilon_k |\alpha(k)|^2 - \frac{1}{2}\sum_{k,q} \underbrace{\left(W_{k,k,-q} + W_{-k,k,-q}\right)}_{} \alpha^*(k+q)\,\alpha(k)$$

The $q=0$ terms in the interaction lead to self-energy that is absorbed in ε_k, so we assume that $W=0$ for $q=0$

For E to be a minimum with respect to $\alpha(k)$ (normalized) the function

? check $$E - \lambda \sum |\alpha(k)|^2$$

must be minimized

$$\frac{\partial E}{\partial \alpha(k)} = \lambda \, \alpha(k)$$

$$2\varepsilon_k \alpha(k) - \frac{1}{2}\sum_q \left(w_{k-q,\,k+q,\,q} + w_{-k+q,\,k-q,\,-q} \right)\alpha(k-q) - \lambda\alpha(k) = 0$$

Multiplying by $\alpha^*(k)$ and $\sum_k \longrightarrow E = \lambda$

So if the variational equations have a solution with $\lambda < 0$ the pair of electrons will tend to form a bound state.
→ Fermi sea would then be unstable.

Then $$|\varepsilon_k - \varepsilon_{k+q}| < \hbar\omega_q$$

$$w_{k,-k,q} = V \quad |\varepsilon_k|, |\varepsilon_{k+q}| < \hbar\omega$$
$$= 0 \text{ otherwise}$$

$$(2\varepsilon_k - \lambda)\alpha(k) = V \sum_{0<\varepsilon_k<\hbar\omega} \alpha(k') \quad \text{for } 0<\varepsilon_k<\hbar\omega$$
$$= 0 \text{ otherwise}$$

$$\sum \alpha(k') = A = \text{constant}$$

$$\alpha(k) = \frac{AV}{2\varepsilon_k - \lambda} \quad \varepsilon_k < \hbar\omega$$

$$A = \sum \alpha(k) = \sum_{0<\varepsilon_k<\hbar\omega} \frac{AV}{2\varepsilon_k - \lambda}$$

$$1 = V_0 \sum_{0<\varepsilon<\hbar\omega} \frac{1}{2\varepsilon_k - \lambda}$$

$$\rightarrow \quad -\lambda = 2\hbar\omega\, e^{-2/VN(0)}$$

Essential singularity at $V=0$

Only one solution for $\lambda < 0$ others are in the continuum

Energy $|\lambda|$ is required to break a pair – suggests that a proper many body wavefunction should have a gap in the spectrum.

Triplet: consider now the alternative possibility

$$|\psi\rangle = \sum_k \alpha(k)\, c^+_{k\uparrow} c^+_{-k\uparrow} |\emptyset\rangle \qquad \left[\sum |\alpha(k)|^2 = 1\right]$$

$$\alpha(k) = -\alpha(-k) \quad \text{given the sum}$$

$$E = 2\sum{}' \varepsilon_k |\alpha(k)|^2 - \frac{1}{2}\sum_{k,q}{}' \left(w_{k-q,-k+q,q} + w_{-k+q,k-q,q}\right)\alpha^*(k)\,\alpha(k-q)$$

Prime in the sum is that it is taken over half k-states

For the minimum of E

$$(2\varepsilon_k - \lambda)\,\alpha(k) = \frac{1}{2}\sum_q \left(w_{k-q,-k+q,q} + w_{-k+q,k-q,-q}\right)\alpha(k-q)$$

and

$$(2\varepsilon_k - \lambda)\,\alpha(k) = V \sum_{0<\varepsilon'<\hbar\omega}^{\text{(whole k space)}} \alpha(k') = 0$$

But if the potential has angular dependence

i.e.
$$w_{k,-k,q} = V_1 + V_2\, \frac{\bar{k}\cdot(\bar{k}+\bar{q})}{k\cdot|\bar{k}+\bar{q}|}$$

Then the solution can be written as

$$(2\varepsilon_k - \lambda)\,\alpha(k) = N(0)\,V_2 \int d\varepsilon \int \frac{d\Omega}{4\pi}\,\alpha(k')\,\frac{\bar{k}'\cdot\bar{k}}{kk'}$$

The solution has the form

$$\alpha(\vec{k}) = (\bar{k}\cdot\bar{a})\,\beta(\varepsilon)$$

($\bar{a}$ = arbitrary vector)

Then

$$\frac{1}{3}N(0)V_2(\bar{k}\cdot\bar{a})\int_0^{\hbar\omega} d\varepsilon\,\beta(\varepsilon)$$

$$(2\varepsilon_k - \lambda)\,\beta(\varepsilon) = \frac{1}{3}N(0)V_2\int_0^{\hbar\omega} d\varepsilon\,\beta(\varepsilon)$$

$$\boxed{-\lambda = 2\hbar\omega\, e^{-6/N(0)V_2}} \longrightarrow \text{Triplet state}$$

Since $\vec{a}$ is arbitrary the solution is triply degenerate.

Nature of BCS wavefunction

Key point : isolate the small interaction responsible for the phenomenon. Neglect all other terms even if large. Creating many pairs (macroscopically) there is interference and one cannot discuss them independently.

Key to the problem is that the g-state of the unperturbed system is almost degenerate - many states with similar energies so that the potential gained ~~by~~ is not balanced by increase of kinetic energy. If the elements of the potential were all negative and equal we could have

$$|\Psi\rangle = \sum a_m |\Psi_m\rangle \qquad \sum |a_m|^2 = 1$$

↳ energies E_m with respect to the g. state.

When $|\Psi_m\rangle$ have all small negative energies

Now interested in macroscopic change in the energy.

Total energy

$$E = \sum_m E_m |a_m|^2 - V \sum_{m,n} a_m^* a_n$$

As in Cooper energy is minimized if

$$E_m a_m - V \sum_n a_n = \lambda a_m$$

$$a_m = -\frac{V \sum_n a_n}{E_m - \lambda}$$

equation for the solution with $\lambda < 0$ is

$$1 = V \sum_m \frac{1}{E_m - \lambda}$$

If

$$V \sum_m \frac{1}{E_m} > 0$$

the new solution has lower energy than the original state
If the g. state is N-fold degenerate, the E_k would be zero an
a solution would be

$$E = \lambda = -NV$$

But for our model interaction, because of the commutation properties,
not all matrix elements will be negative.
Sign of wavefunction is not defined so for one pair one
can chose it to make a particular interaction negative
But this cannot be done for N wavefunctions
For example

$$\bar{V} = -\frac{1}{2} V \sum C^+_{k+q,\sigma} C^+_{k',\sigma'} C_{k'+q,\sigma'} C_{k\sigma} \qquad (V>0)$$

and consider

$$|1\rangle = C^+_{k_1\uparrow} C^+_{k_2\uparrow} C^+_{-k_1-k_2\downarrow} |F\rangle$$

$$|2\rangle = C^+_{k_1\uparrow} C^+_{k_3\uparrow} C^+_{-k_1-k_3\downarrow} |F\rangle$$

$$|3\rangle = C^+_{k_2\uparrow} C^+_{k_3\uparrow} C^+_{-k_2-k_3} |F\rangle$$

The signs of all these 3 states cannot be choosen so that
all matrix elements $\langle i|\bar{V}|j\rangle$ are negative
In this case $\langle 1|\bar{V}|2\rangle$ and $\langle 2|\bar{V}|3\rangle$ are negative while $\langle 1|\bar{V}|3\rangle > 0$.

* So one has to consider if one can find a subset of states which are
negative a make a coherent superposition of them.
One way of doing this is to pair Bloch states and choose only
those many body states in which the two members of the many
body states are either both occupied or both unoccupied

$$\sum_k \underbrace{g_k a^+_{k\uparrow} a_{-k\downarrow}}_{\text{Cooper pair}}$$

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