4 Nov 2018

"spinless" superconductor or p-wave superconductor

The most general quadratic form is, with the definition

$$\Psi = \begin{pmatrix} C \\ C^\dagger \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \\ c_1^\dagger \\ c_2^\dagger \\ \vdots \\ c_N^\dagger \end{pmatrix} \equiv \left(C^{(s)} \quad C_j^{(s)} \right)$$

$s=1$ for C
$s=2$ for $C^\dagger$

Consider [Bogoliubov-de Gennes form]

$$\hat{H} = \Psi^\dagger H \Psi = (C^\dagger, C) H \begin{pmatrix} C \\ C^\dagger \end{pmatrix}$$

$$= (C^\dagger, C) \begin{pmatrix} H^{11} & H^{12} \\ H^{21} & H^{22} \end{pmatrix} \begin{pmatrix} C \\ C^\dagger \end{pmatrix} = C^\dagger H^{11} C + C^\dagger H^{12} C^\dagger + C H^{21} C + C H^{22} C^\dagger$$

If we identify $H^{21} = \Delta$ then $H^{12} = \Delta^\dagger$

since H must be hermitian and $\Psi^\dagger = (\Psi)^\dagger$

H^{11} and H^{22} is not unique as

$$C H^{22} C^\dagger = \sum_{ij} H^{22}_{ij} C_i C_j^\dagger = \sum_{ij} H^{22}_{ij} (-C_j^\dagger C_i + \delta_{ij})$$

$$= - C_j^\dagger \left(H^{22}\right)^T_{ji} C_i + \text{const.} = - C^\dagger \left(H^{22}\right)^T C + \text{const}$$

We could just set $H^{22} \equiv 0$.

For symmetry reasons we still write $\hat{H} = \Psi^\dagger H \Psi$

$$= (C^\dagger, C) \begin{pmatrix} H^{11} & H^{12} \\ H^{21} & H^{22} \end{pmatrix} \begin{pmatrix} C \\ C^\dagger \end{pmatrix}$$

C = column $\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$ $\quad C^\dagger = \begin{pmatrix} c_1^\dagger \\ c_2^\dagger \\ \vdots \\ c_N^\dagger \end{pmatrix}$

However here C and $C^\dagger$ are row vectors

We need to define the most general Green's function

Consider Green's functions defined with

$$G^{ss'}_{jj'}(\tau,\tau') \equiv -\frac{i}{\hbar}\langle T\, c^{s}_{j}(\tau)\, c^{s'}_{j'}(\tau')\rangle$$

$s = 1, 2$
$j = 1, 2, \cdots N$
τ is contour time

$s=1 \Rightarrow c^1 \equiv c, \quad s^2 = c^+$

So G^{11} is $c\,c \to \Delta$
G^{22} is $c^+ c^+$
G^{12} is $c\,c^+$ the usual one
G^{21} is $c^+ c$ opposite of the usual one

← 2×2

Alternatively we could use $-\frac{i}{\hbar}\langle T\, \psi_j(\tau)\, \psi^+_{j'}(\tau')\rangle$

or $\begin{pmatrix} c \\ c^+ \end{pmatrix}(c\ c^+)^+ = \begin{pmatrix} c \\ c^+ \end{pmatrix}(c^+\ c) \to \begin{pmatrix} cc^+ & cc \\ c^+c^+ & c^+c \end{pmatrix}$

ψ

Which one to use is a matter of taste. Let use the more explicit $G^{ss'}$ defined above

Remember $s=1$ is annihilation operator c
$s=2$ is creation operator c^+

clearly G^{12} and G^{21} are related, not independent.

But if we define the matrix

$$G(\tau,\tau') = -\frac{i}{\hbar}\langle T\, \psi(\tau)\, \psi^+(\tau')\rangle$$

here ψ is column vector in j and s space $\quad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} c \\ c^+ \end{pmatrix}$

then $G \quad \psi_1 = c, \ \psi_2 = c^+$

$\psi^+ = (\psi_1^+\ \psi_2^+) = (c^+,\ c)$

$\psi_1^+ = c^+ \quad \psi_2^+ = c$

still matrix in j-space

With ψ we write $G_{ss'}(\tau,\tau') = -\frac{1}{\hbar}\langle T\, \psi_s(\tau)\, \psi^\dagger_{s'}(\tau')\rangle$

or explicitly

$G_{11} = -\frac{i}{\hbar}\langle T\, c\, c^\dagger\rangle \longrightarrow$

$G_{12} = -\frac{i}{\hbar}\langle T\, c\, c\rangle \;-$ $\quad \psi_1 = c \quad \psi_2 = c^\dagger$

$G_{21} = -\frac{i}{\hbar}\langle T\, c^\dagger c^\dagger\rangle \longleftrightarrow \quad \psi_1^\dagger = c^\dagger \quad \psi_2^\dagger = c$

$G_{22} = -\frac{i}{\hbar}\langle T\, c^\dagger c\rangle \longleftarrow$ make arrow → associated with $c^\dagger$.

In the representation, diagonals are the usual ones. (for electron and hole) and off-diagonals are related to Δ and $\Delta^\dagger$.

If $G(\tau,\tau') = -\frac{i}{\hbar}\langle T\, \psi(\tau)\, \psi^\dagger(\tau')\rangle$ ← Matrix in space j and index s (i.e. Nambu space)

and Hamiltonian $\hat{H} = \psi^\dagger H \psi$

The equation of motion is

$$i\hbar \frac{\partial}{\partial\tau} G(\tau,\tau') - \tilde{H} G(\tau,\tau') = I\,\delta(\tau,\tau')$$

Note $\tilde{H} \neq H$ see page 241 & 217 for definition of $\tilde{H}$.

Heisenberg equation of motion for ψ

$$i\hbar \frac{d\psi}{dt} = [\psi, \hat{H}] \stackrel{?}{=} H\psi$$

look at each component

$$i\hbar \frac{dc}{dt} = [c,\ c^\dagger H'' c + c^\dagger H^{12} c^\dagger + c H^{21} c + c H^{22} c^\dagger]$$

use $[A, BC] = \{A,B\}C - B\{A,C\}$ $\qquad \{c, c\} = 0$

$ABC - BCA = (AB + BA)C - BCAC + CA)$

$$i\hbar \frac{dc}{dt} = \underbrace{\{c, c^\dagger\}}_{1} H'' c + \{c, c^\dagger\} H^{12} c^\dagger + c^\dagger H^{12}\{c, c^\dagger\} + [c,\ c H^{21} c^\dagger]$$

$$= H'' c + H^{12} c^\dagger$$

$$[c, c H^{22} c^\dagger] \Rightarrow [c_i, \sum_{jk} c_j H^{22}_{jk} c^\dagger_k]$$

$$= \sum_{jk} H^{22}_{jk} [c_i, c_j c^\dagger_k] = \sum_{jk} H^{22}_{jk} \big(\underbrace{\{c_i, c_j\}}_{=0} c^\dagger_k - c_j \underbrace{\{c_i, c^\dagger_k\}}_{\delta_{ik}} \big)$$

$$= -\sum_{jk} c_j H^{22}_{jk} \delta_{ik} = -\sum_j c_j H^{22}_{ji}$$

$$= -(c H^{22})^T = -(H^{22})^T c$$

$$i\hbar \frac{dc}{dt} = H^{11} c + H^{12} c^\dagger - (c H^{22})^T - (c^\dagger H^{12})^T$$

$$= \left(H^{11} - (H^{22})^T\right) c + \left(H^{12} - (H^{12})^T\right) c^\dagger$$

$$[c_i, \sum_{jk} c^\dagger_j H^{12}_{jk} c^\dagger_k] = \sum_{jk} H^{12}_{jk} [c_i, c^\dagger_j c^\dagger_k]$$

$$= \sum_{jk} H^{12}_{jk} \left(\underbrace{\{c_i, c^\dagger_j\}}_{\delta_{ij}} c^\dagger_k - c^\dagger_j \underbrace{\{c_i, c^\dagger_k\}}_{i\leftrightarrow k} \right)$$

$$= \sum_k H^{12}_{ik} c^\dagger_k - \sum_j c^\dagger_j H^{12}_{ji} = \sum_k \left(H^{12}_{ik} - H^{12}_{ki}\right) c^\dagger_k$$

$$= \sum_k \left(H^{12}_{ik} - H^{12T}_{ik} \right) c^\dagger_k = H^{12} c^\dagger - (H^{12})^T c^\dagger$$

$$i\hbar \frac{dc^\dagger}{dt} = [c^\dagger, c^\dagger H^{11} c + c^\dagger H^{12} c^\dagger + c H^{21} c + c H^{22} c^\dagger]$$

$$= -(H^{11})^T c^\dagger + H^{21} c - (H^{21})^T c + H^{22} c^\dagger$$

$$= \left(H^{22} - (H^{11})^T\right) c^\dagger + \left(H^{21} - (H^{21})^T\right) c$$

so $$i\hbar \frac{\partial}{\partial t} \psi = \begin{pmatrix} H^{11} - H^{22T} & H^{12} - H^{12T} \\ H^{21} - H^{21T} & H^{22} - H^{11T} \end{pmatrix} \psi \neq H\psi \qquad \psi = \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

Note $\hat{H} = \Psi^\dagger H \Psi$ must be hermitian

$$\hat{H}^\dagger = \hat{H} \Rightarrow (\Psi^\dagger H \Psi)^\dagger = \Psi^\dagger H^\dagger (\Psi^\dagger)^\dagger$$

so $H^\dagger = H$ is hermitian or $\begin{pmatrix} H^{11} & H^{12} \\ H^{21} & H^{22} \end{pmatrix}^\dagger = \begin{pmatrix} H^{11\dagger} & H^{21\dagger} \\ H^{12\dagger} & H^{21\dagger} \end{pmatrix}$

$$H^{12} = (H^{21})^\dagger = (H^{21})^{T*}$$

$$H^{12} - H^{12T} = H^{12} - ((H^{21})^{T*})^T = H^{12} - H^{21*}$$

Let's define

$$i\hbar \frac{d\Psi}{dt} = \tilde{H}\Psi \quad \text{then} \quad \tilde{H} = \begin{pmatrix} H^{11} - H^{22T} & H^{12} - H^{12} \\ H^{21} - H^{21T} & H^{22} - H^{11T} \end{pmatrix} \neq H$$

$$c^\dagger H^{12} c^\dagger = \sum_{jk} H^{12}_{jk} c_j^\dagger c_k^\dagger \quad \text{since } (c_j^\dagger)^2 = 0$$

then diagonal terms H^{12}_{jj} don't enter the expression we can define $H^{12}_{jj} = 0$. diagonal is 0. H^{12} contains only off-diagonal terms.

If H^{12} is symmetric $(H^{12})^T = H^{12}$, then $\tilde{H}$ term will be 0. so we expect H^{12} can only be anti symmetric such as

$$(c_1^\dagger c_2^\dagger)\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} c_1^\dagger \\ c_2^\dagger \end{pmatrix} = c_1^\dagger c_2^\dagger - c_2^\dagger c_1^\dagger$$
$$= c_1^\dagger c_2^\dagger - (-c_1^\dagger c_2^\dagger) = 2 c_1^\dagger c_2^\dagger$$

which is consistent with

$$(c_j^\dagger c_k^\dagger) = -c_k^\dagger c_j^\dagger$$

Without loss of generality we can take

$$H = \begin{pmatrix} H^{11} & \frac{1}{2}H^{12} \\ -\frac{1}{2}H^{21} & 0 \end{pmatrix} \qquad H^{21} = (H^{12})^\dagger \qquad (H^{12})^T = -H^{12}$$

$$H^{11} = (H^{11})^\dagger = (H^{11})^T \quad \text{i.e. take } H^{11} \text{ real}$$

then $\tilde{H} = \begin{pmatrix} H^{11} & H^{12} \\ -H^{12*} & -H^{11T} \end{pmatrix} = \begin{pmatrix} H^{11} & H^{12} \\ H^{21} & -H^{11T} \end{pmatrix} \qquad H^{21} = (H^{12})^\dagger$

Let just define $\tilde{H} = \begin{pmatrix} \tilde{H}_{11} & \tilde{H}_{12} \\ \tilde{H}_{21} & \tilde{H}_{22} \end{pmatrix}$ we will figure out how $\tilde{H}$ is related to the original H in $\hat{H} = \psi^* H \psi$ more carefully. Then the Green's function is

$$i\hbar \frac{\partial}{\partial \tau} G(\tau, \tau') - \tilde{H} G(\tau, \tau') = I\, \delta(\tau, \tau')$$

□ Algebraic property of Nambu-like Ψ operator

We have defined Ψ on page 205, as

$$\Psi = \begin{pmatrix} c \\ c^\dagger \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \\ c_1^\dagger \\ c_2^\dagger \\ \vdots \\ c_N^\dagger \end{pmatrix} \quad \text{and} \quad \Psi^\dagger = (c^\dagger, c)$$

↑ column vector

↑ row vector

$$= (c_1^\dagger c_2^\dagger \cdots c_N^\dagger\ c_1 \cdots c_j \cdots c_N)$$

The anti-commutation relations are

$$\{\Psi, \Psi^\dagger\} = \begin{pmatrix} c \\ c^\dagger \end{pmatrix}(c^\dagger, c) + \text{anti-commutator terms for each matrix element} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} = \mathbb{1}$$

identity matrix of $N \times N$ in j space

↑ 2×2 in Nambu space

$$= \begin{pmatrix} cc^\dagger + c^\dagger c & cc + cc \\ c^\dagger c^\dagger + c^\dagger c^\dagger & c^\dagger c + cc^\dagger \end{pmatrix}$$

The expression $cc + cc$ really means, in component form $c_i c_j + c_j c_i = 0$ for the (i, j) matrix elements.

But $\{\Psi, \Psi^T\} = \begin{pmatrix} c \\ c^\dagger \end{pmatrix}(c, c^\dagger) + \text{anti-commutator terms}$

$$= \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \neq 0$$

since $\{\Psi, \Psi^\dagger\} = \mathbb{1}$, but $\{\Psi, \Psi^T\} = \sigma_x \neq 0$

we see that Ψ is not fermi-like. So its algebraic property differs from that defined for the usual s-wave superconductor, such as that given on page 174 in "Theory of Superconductivity" by J. R. Schrieffer which is $\Psi_{\vec{k}} = \begin{pmatrix} c_{\vec{k}\uparrow} \\ c^\dagger_{-\vec{k}\downarrow} \end{pmatrix}$ Note that

c and $c^\dagger$ refer to different states $\vec{k}\uparrow$ and $-\vec{k}\downarrow$, so

c and $c^\dagger$ anti-commutable, instead of 1.

As a result that Ψ does not anti commute with itself, we find the equation of motion is not Schrödinger-like but with extra terms

If $\hat{H} = \Psi^\dagger H \Psi \rightarrow i\hbar \frac{d}{dt}\Psi \neq H\Psi$

because although $\{\Psi, \Psi^\dagger\} = \mathbb{1}$ we also get contribution from $\{\Psi, \Psi\} = \sigma_x = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$

so $i\hbar \frac{d\Psi}{dt} = [\Psi, \hat{H}] = [\Psi, \Psi^\dagger H \Psi]$

$= \{\Psi, \Psi^\dagger\} H\Psi - \{\Psi, \Psi^T\} H^T (\Psi^\dagger)^T$

$= H\Psi - \sigma_x H^T \underbrace{\Psi^\dagger}_{\text{column vector instead of row here}} \equiv \tilde{H}\Psi$

Here $\tilde{H} \equiv \begin{pmatrix} H_{11} - H_{22}^T & H_{12} - H_{12}^T \\ H_{21} - H_{21}^T & H_{22} - H_{11}^T \end{pmatrix} \neq H$

$H = \begin{matrix} 1 \\ 2 \end{matrix} \overset{\begin{matrix} 1 & 2 \end{matrix}}{\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}}$ With the equation of motion of Ψ

The contour ordered Green's function satisfies

$$G(\tau,\tau') = -\frac{i}{\hbar}\langle T\,\psi(\tau)\,\psi^\dagger(\tau')\rangle$$

$$\begin{pmatrix} c \\ c^\dagger \end{pmatrix}_\tau \begin{pmatrix} c^\dagger & c \end{pmatrix}_{\tau'}$$

$$i\hbar\frac{\partial}{\partial\tau}G(\tau,\tau') - \tilde{H}\,G(\tau,\tau') = I\,\delta(\tau,\tau')$$

In real time, we find [assuming time-translational invariance (i.e. steady state)]

$$i\hbar\frac{\partial}{\partial t}G^{r,a,t}(t) - \tilde{H}\,G^{r,a,t}(t) = I\,\delta(t)$$

The anti time order is $i\hbar\frac{\partial}{\partial t}G^{\bar{t}}(t) - \tilde{H}\,G^{\bar{t}}(t) = -I\,\delta(t)$

and greater/lesser is homogeneous

$$i\hbar\frac{\partial}{\partial t}G^{>,<}(t) - \tilde{H}\,G^{>,<}(t) = 0$$

The retared in energy-space

$$G^r(E) = \int_{-\infty}^{+\infty} G^r(t)\,e^{\frac{i}{\hbar}Et}\,dt \qquad \text{satisfies}$$

Bogoliu-de Gennes

$$G^r(E) = \left(E + i\eta - \tilde{H}\right)^{-1} \leftarrow 2\times 2 \text{ in Nambu space}$$

$$G^{><}(E) \propto \delta(E - \tilde{H}) \leftarrow \text{unfortunately, I don't}$$

know how to fix the constant which is the equilibrium distribution.

Do we still have a "fluctuation-dissipation" theorem here for $G^{><}$? The usual proof breaks down as we cannot have a simultaneous eigen state $|E,N\rangle$ as $\hat{N}$ and $\hat{H}$ do not commute.

What I can think of doing is to diagonalize the Hamiltn in Bogoliubov way. And then do statistical mechanics in the diagonal representation as usual. → then what is the "new" fluctuation-dissipation theorem relating $G^{>,<}$ to G^r G^a?

Heat transfer in super-conductor due to Coulomb interaction

Typical energy scale for super conducting is small, on the order of meV or $kT \sim 10^{-3}$ eV or T few kelvin. while Coulomb interactions are of the order of eV (at least when distance is of the order of nm).

Question. why large Coulomb interaction does not destroy superconductivity?

Anyway we assume that is the case and electron still carries a charge of $-e$ and hole carries $+e$ or $\hat{q}_j = (-e) c_j^\dagger c_j$ or $(+e) c_j c_j^\dagger$. We assume

The Coulomb term is given by

$$H_{int} = \frac{e^2}{2} \sum_{ij} c_i^\dagger c_j^\dagger V_{ij} c_j c_i$$

Bare Coulomb $V_{ij} = \frac{1}{4\pi\varepsilon_0 r_{ij}}$ $\quad r_{ij} \equiv |\vec{r}_i - \vec{r}_j|$

Since we study junction system or system with tip translational invariance is not assumed. In the usually solid state physics, lattice periodicity is assumed so we could work in wave vector space.

If that is the case, we do the Fourier transform

$$c_j = \frac{1}{\sqrt{N}} \sum_{\vec{p}} c_{\vec{p}} e^{i\vec{p}\cdot\vec{R}_j}$$

we assume one electron at each Bravais lattice point $\vec{R}_j$

$\vec{p}$ is discrete in a volume of V, i.e. $\Delta p = \frac{2\pi}{L}$

Putting this fourstrom into H_{int} we get

$$H_{int} = \frac{e^2}{2N^2} \sum_{ij} \sum_{p'k'kp} C^+_{p'} e^{-i\vec{p}'\cdot\vec{R}_i} C^+_{k'} e^{-i\vec{k}'\cdot\vec{R}_j} V(\vec{R}_i - \vec{R}_j) C_k e^{i\vec{k}\cdot\vec{R}_j} C_p e^{i\vec{p}\cdot\vec{R}_i}$$

$$= \frac{e^2}{2N^2} \sum_{p'k'kp} C^+_{p'} C^+_{k'} C_k C_p \sum_{ij} e^{i(\vec{p}-\vec{p}')\cdot\vec{R}_i} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_j} V(\vec{R}_i - \vec{R}_j)$$

Let define $\vec{q} = \vec{p}' - \vec{p}$ $\quad V(\vec{q}) = \sum_j V(\Delta\vec{R}_j) e^{-i\vec{q}\cdot\Delta\vec{R}_j}$ is the Fourier transform of the Coulomb potential. We sum over i first, then

$$\sum_{ij} e^{\cdots} e^{\cdots} V(\vec{R}_i - \vec{R}_j) = \sum_j \left(\sum_i e^{-i(\vec{p}'-\vec{p})\cdot(\vec{R}_i - \vec{R}_j)} V(\vec{R}_i - \vec{R}_j) \right)$$

$$e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_j} = i(\vec{p}'-\vec{p})\cdot\vec{R}_j = \sum_j V(\vec{q}) e^{i(\vec{k}-\vec{k}'-\vec{q})\cdot\vec{R}_j}$$

$$\times e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_j}$$

$= V(\vec{q}) N \delta_{\vec{k}-\vec{k}', \vec{q}}$ ← Kronecker-δ

\# of j values are N

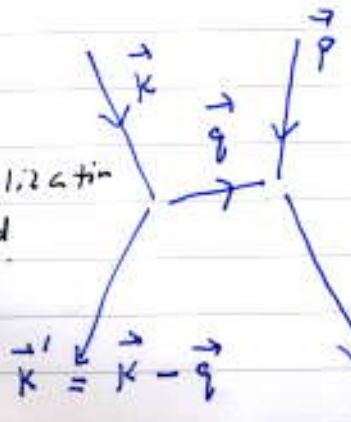
or $\vec{k} - \vec{k}' = \vec{q}$

So the Hamiltonian in the Coulomb interaction in wave vector space is

$$H_{int} = \frac{e^2}{2N} \sum_{\vec{k}\vec{q}\vec{p}} v(\vec{q}) C^+_{\vec{p}+\vec{q}} C^+_{\vec{k}-\vec{q}} C_{\vec{k}} C_{\vec{p}}$$

This has nice physical interpretation of momentum transfer in a Coulomb interaction

Remove the $\vec{q} = 0$ term is equivalent to cancel the neutralization positive ion background



momentum is conserved

$\vec{k} + \vec{p} = \vec{k}' + \vec{p}'$

amount of $\vec{q}$ is transfered from one to another

Dyson equation with the Coulomb interaction — we expect matrix equation of the form

$$G_n = G + G\Sigma G_n$$

Here G is the Green's function without the Coulomb term, i.e. that defined on page 207 - 209 and Σ is self energy. Since G and G_n are 2×2 matrices in Nambu space (indexs) we naturally expect that Σ is also 2×2 in Nambu space and $G\Sigma G_n$ is a MATMUL in Nambu space. This is so far just a guess, we need a proof of it.

$$G_n(\tau,\tau') = (-\tfrac{i}{\hbar})\langle T_\tau\, \psi(\tau)\,\psi^\dagger(\tau')\rangle_{H+H_{int}=H_{tot}}$$

$$=(-\tfrac{i}{\hbar})\langle T_\tau \begin{pmatrix} c(\tau) \\ c^\dagger(\tau)\end{pmatrix}\left(c^\dagger(\tau'),\ c(\tau')\right)\rangle_{H_{tot}}$$

$$= -\tfrac{i}{\hbar}\langle T_\tau \begin{pmatrix} c(\tau)c^\dagger(\tau') & c(\tau)c(\tau') \\ c^\dagger(\tau)c^\dagger(\tau') & c^\dagger(\tau)c(\tau')\end{pmatrix}\rangle_{H_{tot}}$$

$$= \begin{pmatrix} G_n^{11} & G_n^{12} \\ G_n^{21} & G_n^{22}\end{pmatrix}$$

Here time evolution is under the full Hamiltonian

$$\hat{H}_{tot} = \hat{H} + \hat{H}_{int}$$

$$= \psi^\dagger H \psi + \frac{e^2}{2}\sum_{lm} c_j^\dagger c_m^\dagger V_{jm} c_m c_l$$

We work in real space with sites denoted by j, k, l, m etc.

Going into the interaction picture so that the operators now evolve according to the non-interacting Hamiltonian $\hat{H} = \psi^+ H \psi$ and the interaction appears only at the extra factor of exponential we get

$$G_n(\tau, \tau') = -\frac{i}{\hbar} \left\langle T_\tau \psi(\tau) \psi^+(\tau') e^{-\frac{i}{\hbar}\int_c H_{int}(\tau'')\, d\tau''} \right\rangle_H$$

Note now the average is with respect to H not the full one $H + H_{int}$.

$$\langle \cdots \rangle_H = Tr\left(e^{\frac{-\beta(\hat{H} - \mu \hat{N})}{Z}} \cdots \right)$$

$\psi(\tau) \equiv \psi_I(\tau)$ is the interaction picture one, but for notational simplicity I drop the subscript I.

Perturbative expansion means we expand the exponential

$$e^{-\frac{i}{\hbar}\int H_{int}(\tau'')\, d\tau''} = 1 - \frac{i}{\hbar}\int H_{int}(\tau'')\, d\tau'' + \cdots$$

and apply the Wick theorem.

Q: How do we know the Wick theorem is valid under $\hat{H} = \psi^+ H \psi$ which has c^+c^+ and cc terms?

We go ahead do it anyway assuming Wick theorem is valid. The first term is just G

i.e. $$G_n(\tau, \tau') = G(\tau, \tau') +$$

$$\left(-\frac{i}{\hbar}\right) \left\langle T_\tau \psi(\tau) \left(-\frac{i}{\hbar}\right) \int H_{int}(\tau'')\, d\tau'' \, \psi^+(\tau') \right\rangle_H + \cdots$$

Under the contour order sign T_τ we can move the order of operators freely with the rule

ψ ψ^+ or c, c^+ all anti-commute. Since H_{int} contains even # of c's, ψ^+ and H_{int} "commute".

The reason for this rule is that the order of the operators are not fixed yet provided the canon time is not yet specified. When τ, τ', τ'' are fixed, if we remove T_τ operator, the operators must re-arrange themselves according canon time, from past to future from ~~right to left~~ right to left

$$\langle 0 | \hat{O}_1(\tau_1)\, \hat{O}_2(\tau_2) \cdots | 0 \rangle$$

future $\longleftarrow$ past

However, this free moving of the order of operators does not apply at equal time. At equal time. T_τ plays no rule and the order seems arbitrary. In such case we stick to its original order in the Hamilt.

i.e.

$$C_\ell^+(\tau'')\, C_m^+(\tau'')\, C_m(\tau'')\, C_\ell(\tau'')$$

In the Coulomb interaction, the terms are all at equal time τ'', T_τ plays no part we need to keep the order as it is. However, it is ok to note $C_m C_\ell = -C_\ell C_m$ which is true. but $C_m^+ C_m = -C_m C_m^+ + 1$

as operator algebra identity.

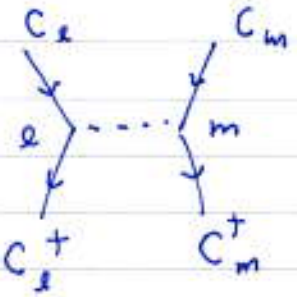
Since $\psi = \begin{pmatrix} c \\ c^+ \end{pmatrix}$ we need to consider 4 possibility for the "end" $\begin{pmatrix} C \cdots C^+ & C \cdots C \\ C^+ \cdots C^+ & C^+ \cdots C \end{pmatrix}$

Let focus the contribution to $G_n^{II}(\tau, \tau')$

which is $\int d\tau'' \left(-\frac{1}{\hbar}\right)^2 \langle T_\tau \, c_j(\tau) \, \frac{e^2}{2} \sum_{l,m} c_l^+(\tau'') \, c_m^+(\tau'') \, V_{lm} \, c_m(\tau'') \, c_l(\tau'') \, c_k^+(\tau') \rangle$

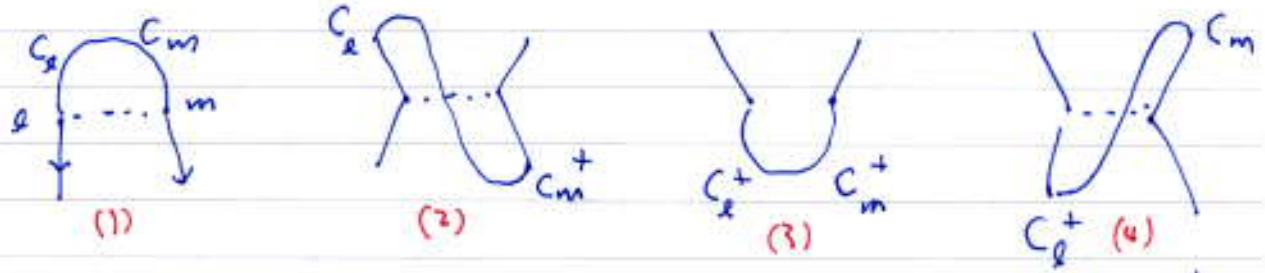
We have 6 c or c^+ which can form 3 Gs, each need a prefactor $\left(\frac{1}{i\hbar}\right)$ but we only have 2 so we should have an over $(i\hbar)$ G G G V form.

Let focus on diagram of Fock type 

The coulomb interaction is of the form 

In order to generate the Fock term, we must connect two ends to the outside, and connect one time internally, but not one of the same space index, since that will give us Hartree term

The 4 possibility are



The other two left over c can be paired with the 1st one $c(\tau)$ or the last one $c^+(\tau')$ so we get 8 graphs but two are equivalent, as a result, it cancel the over $\frac{e^2}{2}$ and obtain finally 4 graphs.

We need to check if we generate extra minus sign when we move the operators in order to do the Wick decomposition.

Consider case (1) $\langle T_\tau\, c_j\, c_\ell^+\, c_m^+\, c_m\, c_\ell\, c_K^+ \rangle$

τ ↑ all at τ'' ↑ τ'

In order to do Wick decomposition we need to move into

$$\langle T_\tau\, c_j\, c_\ell^+\, c_m^+\, c_K^+\, c_m\, c_\ell \rangle$$

since $c_K^+(\tau')$ has τ' $c_m c_\ell$ has τ'' move is OK and no extra sign

Wick theorem

$$= \langle T_\tau c_j c_\ell^+ \rangle \langle T_\tau c_m^+ c_K^+ \rangle \langle T_\tau \underbrace{c_m c_\ell}_{=} \rangle$$

equal time τ'' now $- c_\ell c_m$

$$\to i\hbar\, G^{11}_{j\ell}(\tau,\tau'')\, G^{12}_{\ell m}(\tau'',\tau'')\, G^{21}_{mK}(\tau'',\tau')\,(-1)\, V_{\ell m}$$

Here $G^{11} \to c\,c^+$, $G^{22} \to c^+ c$, $G^{12} \to c\,c$

$G^{21} \to c^+ c^+$. see page 209.

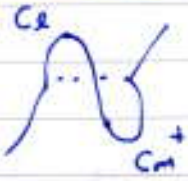
In order to have a MATMUL or convolution we swapped $c_m c_\ell \to - c_\ell c_m$. This generates extra minus sign $(- V_{\ell m})$.

Instead of paring c_j with c_ℓ^+, we could pair it with c_m^+. But ℓ and m are dummy indices

$\ell \leftrightarrow m$ will not change the problem and $V_{\ell m} = V_{m\ell}$ we just get a factor of 2 for this term. The 2 cancel the $\frac{1}{2}$ in $\frac{e^2}{2}$.

We now look at case (2)

$$\langle T_\tau\, c_j\, c_\ell^+\, c_m^+\, c_m\, c_\ell\, c_K^+ \rangle$$



$$= \langle T\, c_j\, c_\ell^+\, c_m^+\, c_\ell\, c_m\, c_K^+ \rangle\,(-1)$$

$$= \langle T_\tau c_j c_\ell^\dagger \rangle \langle T_\tau c_m^\dagger c_\ell \rangle \langle T_\tau c_m c_k^\dagger \rangle \quad (-1)$$

The index order is not in MATMUL form, we like to swap the middle term $\langle T_\tau c_m^\dagger c_\ell \rangle \to \langle T_\tau c_\ell c_m^\dagger \rangle$ (-1)

But we cannot do that as $c_m^\dagger$ and c_ℓ is at equal time τ''. To over come this difficulty we add a little delay to the τ argument $\langle T_\tau c_\ell(\tau'') c_m^\dagger(\tau''+\delta) \rangle$

$\delta > 0$ in conventional sense

Because $\tau''+\delta$ is always later that τ'', it will give $\langle T_\tau c_\ell(\tau'') c_m^\dagger(\tau''+\delta) \rangle = - \langle c_m^\dagger(\tau''+\delta) c_\ell(\tau'') \rangle$ when T_τ operation effect is taken so we get

$$(it)\, G^{11}_{j\ell}(\tau, \tau'')\, G^{11}_{\ell m}(\tau'', \tau''^+)\, G^{11}_{mk}(\tau'', \tau')\, V_{\ell m}$$

Note two minus sign cancelled.

$$\tau''^+ = \tau'' + \delta$$

This term is the usual Fock term or exchange term.

Another possible pairing

$$\langle T_\tau c_j c_\ell^\dagger c_m^\dagger c_m c_\ell c_k^\dagger \rangle$$

$$= - \langle T_\tau c_j c_\ell^\dagger c_k^\dagger c_m^\dagger c_m c_\ell \rangle$$

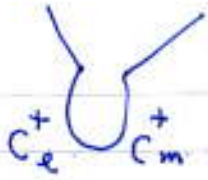
$$= \langle T_\tau c_j c_m c_\ell^\dagger c_k^\dagger c_m^\dagger c_\ell \rangle$$

ok. if we add δ to $c_\ell^\dagger$ and $c_m^\dagger$

$$= \langle T_\tau c_j c_m \rangle \langle T c_\ell^\dagger c_k^\dagger \rangle \langle T c_m^\dagger c_\ell \rangle$$

$$\to\ it\, G^{12}_{jm}(\tau, \tau'')\, G^{22}_{m\ell}(\tau''^+, \tau'')\, G^{21}_{\ell k}(\tau'', \tau')\, V_{\ell m}$$

case (3)



$$\langle T_\tau\, c_j\, c_\ell^+ c_m^+ c_m c_\ell c_k^+ \rangle$$

$$= \langle T_\tau\, c_\ell^+ c_m^+ c_j c_m c_\ell c_k^+ \rangle$$

$$\Rightarrow \langle T_\tau\, c_\ell^+ c_m^+ \rangle \langle T_\tau\, c_j c_m \rangle \langle T_\tau\, c_\ell c_k^+ \rangle$$

$$= \langle T_\tau\, c_j c_m \rangle (-1) \langle T_\tau\, c_m^+ c_\ell^+ \rangle \langle T_\tau\, c_\ell c_k^+ \rangle$$

$$\to (ih)\, G^{12}_{jm}(\tau, \tau'')\, G^{21}_{m\ell}(\tau'', \tau'')\, G^{11}_{\ell m}(\tau'', \tau')\, (-V_{\ell m})$$

Alternative pairing for the ends ii

$$\langle T_\tau\, c_j\, c_\ell^+ c_m^+ c_m c_\ell c_k^+ \rangle$$

By loop symmetry this just give a factor of 2 for the above. Permutation sign?

$$= \langle T_\tau\, c_\ell^+ c_m^+ c_j c_\ell c_m c_k^+ \rangle (-1)$$

$$= \langle T_\tau\, c_j c_\ell \rangle \langle T_\tau\, c_\ell^+ c_m^+ \rangle \langle T_\tau\, c_m c_k^+ \rangle (-1)$$

sign is the same.

Last case (4)

$$\langle T_\tau\, c_j\, c_\ell^+ c_m^+ c_m c_\ell c_k^+ \rangle$$

This term is the same as that on middle of page 235 from case (2).

$$= \langle T_\tau\, c_j c_m^+ c_\ell^+ c_m c_\ell c_k^+ \rangle (-1)$$

$$= \langle T_\tau\, c_j c_m^+ \rangle \langle T_\tau\, c_\ell^+ c_m \rangle \langle T\, c_\ell c_k^+ \rangle (-1)$$

$$= \langle T_\tau\, c_j c_m^+ \rangle \langle T_\tau\, c_m(\tau'') c_\ell^+(\tau''+\delta) \rangle \langle T\, c_\ell c_k^+ \rangle$$

$$\to ih\, G^{11}_{jm}(\tau, \tau'')\, G^{11}_{\ell k}(\tau'', \tau'^+)\, G^{11}(\tau'', \tau')\, V_{\ell m}$$

Last case alternative pairing

$$\langle T_\tau \; c_j \; c_\ell^+ c_m^+ c_m c_\ell \; c_k^+ \rangle$$

$$= - \langle T_\tau \; c_\ell^+ c_m^+ c_m c_j c_\ell \; c_k^+ \rangle$$

$$= \langle T_\tau \; c_\ell^+ c_m \; c_m^+ c_k^+ \; c_j c_\ell \rangle \qquad (\tau^{0+})$$

we can do this if we add δ to time of c_m^+

$$= \langle T_\tau \; c_\ell^+ c_m \rangle \langle T_\tau c_m^+ c_k^+ \rangle \langle T_\tau \; c_j \; c_\ell \rangle$$

$$= \langle T_\tau \; c_j \; c_\ell \rangle \langle T_\tau \; c_\ell^+ c_m \rangle \langle T_\tau \; c_m^+ c_k^+ \rangle$$

$$\to \; i\hbar \, G^{12}_{j\ell}(\tau\,\tau'') \, G^{22}_{\ell m}(\tau'', \tau'') \, G^{21}_{mk}(\tau'', \tau') \, V_{\ell m}$$

This term is the same as that on page 235, cancel the $\frac{e^2}{2}$.

Now putting the δ term together

case 1) $2 \cdot i\hbar \, G'' G^{12} G^{21} (-1) V$

2) $\begin{cases} i\hbar \, G'' G^{11} G'' V \\ i\hbar \, G^{12} G^{22} G'' V \end{cases}$ Same

3) $2 \, i\hbar \, G^{12} G^{21} G'' (-1) V$ Same

4) $\begin{cases} i\hbar \, G'' G'' G'' V \\ i\hbar \, G^{12} G^{22} G^{21} V \end{cases}$

It is obvious case 2) & 4) are the same as it is a permutation of $\ell \leftrightarrow m$. We have total of 4 difference term, each has a prefactor 2. this 2 will cancell the $\frac{1}{2}$ in $\frac{e^2}{2} \sum_{\ell m} \cdots$

Finally we can write the Green's function expansion for the 11-component as

$$G^{11}_{jk}(\tau,\tau') = G^{11}_{jk}(\tau,\tau') + \sum_{lm}\int d\tau'' G^{11}_{jl}(\tau\tau'')\, i\hbar\, G^{11}_{lm}(\tau'',\tau'')\, V_{lm} e^2 G^{11}_{mk}(\tau'',\tau')$$

$$+ \sum_{lm}\int d\tau'' G^{11}_{jl}(\tau\tau'')\cdot i\hbar\, G^{12}_{lm}(\tau'',\tau'')(-V_{lm})e^2 G^{21}_{mk}(\tau'',\tau')$$

$$+ \sum_{lm}\int d\tau'' G^{12}_{jl}(\tau\tau'')\, i\hbar\, G^{21}_{lm}(\tau'',\tau'')(-V_{lm}) e^2 G^{11}_{mk}(\tau'',\tau')$$

$$+ \sum_{lm}\int d\tau'' G^{12}_{jl}(\tau,\tau'')\, i\hbar\, G^{22}_{lm}(\tau''\tau'')\, V_{lm} e^2 G^{21}_{mk}(\tau'',\tau')$$

We see we can write this as a convolution in both j,τ,s if we also work out all 4 $G^{ss'}$

so the Dysm equation in matrix multiplication form is

$$G^n(\tau,\tau') = G(\tau,\tau') + \int d\tau_1 \int d\tau_2\, G(\tau\tau_1)\Sigma(\tau_1\tau_1) G(\tau_2\tau') + \cdots$$

provided we define the self energy in Nambu space as

$$\sum^{s_1 s_2}_{lm}(\tau_1,\tau_2) = e^2\, i\hbar\, G^{s_1 s_2}_{lm}(\tau_1,\tau_2)\left[V_{lm}(-1)^{s_1-s_2}\delta(\tau_1,\tau_2)\right]$$

The $\delta(\tau_1,\tau_2)$ means the Coulomb interaction is instantaneous and in Nambu space the Coulomb interaction need to the the form

$$\underbrace{\quad\quad}_{l\tau_1 s_1\; m\tau_2 s_2} = V_{lm}(-1)^{s_1-s_2}\delta(\tau_1,\tau_2)$$

or

$$V \underset{s_1=1}{\overset{s_2=1}{=}} \begin{matrix} 2 \\ \end{matrix}\begin{bmatrix} V & -V \\ -V & V \end{bmatrix}\delta(\tau_1,\tau_2)$$

Due to the δ-function in V, the Green's function is evaluated at equal time $G^{s_1 s_2}(\tau_1, \tau_1)$

However, the makes the contour order ill-defined we must follow the prescription to take

$$G^{11}(\tau_1, \tau_1) \to G^{11}(\tau_1, \tau_1^+) \to -\langle c^+ c \rangle$$

$$G^{12}(\tau_1, \tau_1) \to G^{12}(\tau_1^+, \tau_1) \to \langle c c \rangle$$

no change

$$G^{21}(\tau_1, \tau_1) \to G^{21}(\tau_1^+, \tau_1) \to \langle c^+ c^+ \rangle$$

no change

$$G^{22}(\tau_1, \tau_1) \to G^{22}(\tau_1^+, \tau_1) \to \langle c\, c^+ \rangle$$

no change

I think this problem of adding an infinitesimal δ to τ will be not needed when the Coulomb interaction is screened, required a D which does has time argument.

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01 Hartree term

To obtain the Hartree graph we need to make a loop at the same site, there are just two equivalent ways to do this

It is not possible to have cc or c^+c^+ terms with a loop on the same sites consider contribution to G_n^{11}

$$\langle T_\tau\, c_j(\tau)\, c_l^+(\tau'')\, c_m^+(\tau'')\, c_m(\tau')\, c_l(\tau'')\, c_k^+(\tau') \rangle$$

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$$\langle T_\tau\, c_j(\tau)\, c_l^\dagger(\tau'')\rangle \langle T_\tau\, c_m^\dagger(\tau'')\, c_m(\tau'')\rangle \langle T_\tau\, c_l(\tau'')\, c_k^\dagger(\tau')\rangle$$

$$= \langle T_\tau\, c_j(\tau)\, c_l^\dagger(\tau'')\rangle \left(-\langle T_\tau\, c_m(\tau'')\, c_m^\dagger(\tau''^+)\rangle\right) \langle T_\tau\, c_l(\tau'')\, c_k^\dagger(\tau')\rangle$$

add δ to τ so that $c^\dagger$ is late than c for

$$\to (-i\hbar) e^2\, G^{11}_{jl}(\tau, \tau'')\, G^{11}_{mm}(\tau'', \tau''^+)\, G^{11}_{lk}(\tau'', \tau')\, V_{lm}$$

This is the real term for  with $(-i\hbar)$ factor

Alternative decomposition

$$\langle T_\tau\, c_j\, c_l^\dagger\, c_m^\dagger\, c_m\, c_l\, c_k^\dagger\rangle$$

$$= \langle T_\tau\, c_l^\dagger\, c_m^\dagger\, c_m\, c_j\, c_l\, c_k^\dagger\rangle (-1)$$

$$= \langle T_\tau c_l^\dagger c_k^\dagger\, c_m^\dagger c_m\, c_j\, c_l\rangle (-1)$$

$$= \langle T_\tau\, c_l^\dagger c_k^\dagger\rangle \langle T_\tau\, c_m^\dagger c_m\rangle \langle T_\tau\, c_j\, c_l\rangle (-1)$$

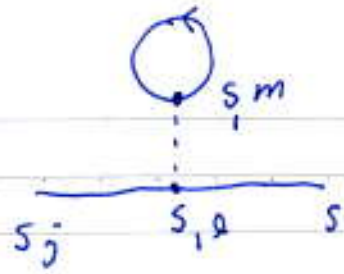
$$\Rightarrow (-i\hbar) e^2\, G^{21}_{lk}(\tau'', \tau')\, G^{22}_{mm}(\tau''^+, \tau'')\, G^{12}_{jl}(\tau, \tau'')\, V_{lm}$$

$$\to (-i\hbar) e^2\, G^{12}_{jl}(\tau,\tau'')\, G^{22}_{mm}(\tau''^+,\tau'')\, G^{21}_{lk}(\tau'',\tau)\, V_{lm}$$

The $c_l^\dagger c_l$ term is equivalent to this one after $l \leftrightarrow m$ swap cancel the factor of $\frac{1}{2}$ in $\frac{e^2}{2}$.

The 2 term can be written as a sum

$$\sum_{s=1,2} (-i\hbar) e^2\, G^{1s}_{jl}\, G^{ss}_{mm}\, G^{s1}_{lk}\, V_{lm}$$



This means i.e. we got an s-index

why we don't have a term  with $s_1 \neq s_2$?

That is, for the Hartree term we don't have off diagonal term for the $V = \begin{bmatrix} V & -V \\ -V & V \end{bmatrix}$ matrix?

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polarization diagram 

To get the polarization diagrams, we need 2nd order terms in H_{int} with 2 V's.

$$\langle T \cdots C_l^+ C_m^+ V_{lm} C_m C_l \; C_p^+ C_q^+ V_{pq} C_q C_p \cdots \rangle \left(\frac{1}{2}\right)^3$$

we need contract one site of first term with one site of the 2nd term say l and p. The m and q sites need to be connected exactly

$$\pm \langle T \cdots \quad C_l^+ C_l C_p^+ C_p \cdots \rangle$$

sign we cannot contract with the same side, we must connect to different site so we have the possibility of

$C_l^+ C_l \; C_p^+ C_p$ or $C_l^+ C_l \; C_p^+ C_p$

$$\rightarrow -\langle T_\tau C_l C_p^+ \rangle \langle T_\tau C_p C_l^+ \rangle \quad - \langle T_\tau C_l^+(\tau_1) C_p^+(\tau_2) \; C_l(\tau_1) C_p(\tau_2) \rangle$$

$$+ \langle T_\tau C_l^+(\tau_1) C_p^+(\tau_2) \rangle$$

The 2nd ten is $+ G^{21}_{\beta\rho}(\tau_1 \tau_2)\, G^{12}_{\rho\beta}(\tau_2 \tau_1)$

A better graphic rule for the Feynman diagram.

Let use a line —— for C

use arrow $\longrightarrow$ for C^+

Then the 4 Bogoliubov - de Gennes space Green's functions are denoted

$G^{11} = \langle C\, C^+ \rangle$ $\longrightarrow$

$G^{22} = \langle C^+ C \rangle$ $\longleftarrow$

$G^{12} = \langle C\, C \rangle$ ——

$G^{21} = \langle C^+ C^+ \rangle$ $\longleftrightarrow$

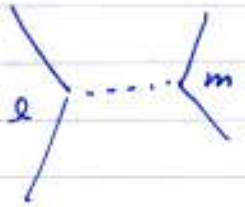
the arrows are always point outward of the line

The begin & end also have site and contour time label. i.e.

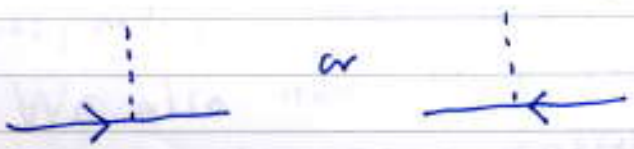
$$G^{11}_{jk}(\tau\tau') = -\frac{i}{\hbar}\langle T_c C_j(\tau)\, C^+_k(\tau')\rangle \rightarrow \overset{C}{j\tau} \longrightarrow \overset{C^+}{k\tau'}$$

The Coulomb interaction is

$$C^+_\ell C^+_m V_{\ell m} C_m C_\ell$$

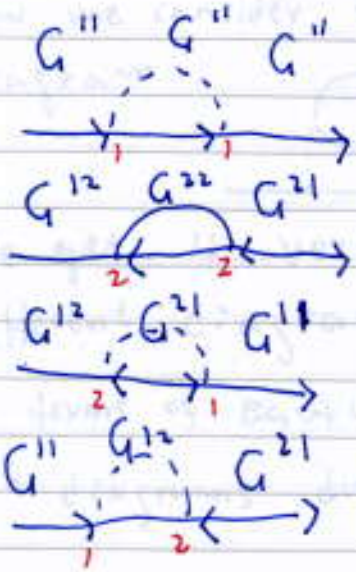


Two sites ℓ and m are involved. Since each site must have pair $C^+_m C_m$ or $C^+_\ell C_\ell$ we should have only one arrow goes into the vertex



Two arrows  or no arrows 
are not possible since it is $G_{\ell}^{+} G_{\ell}^{+}$ or $C_{\ell} C_{\ell}$ which is 0. For the Fock diagram

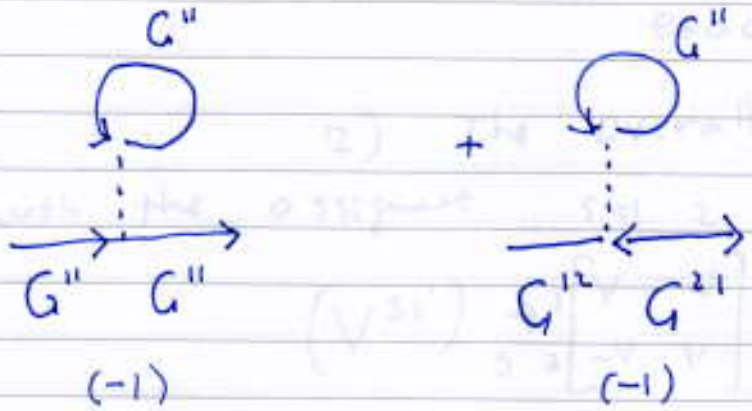
each vertex can have two possible arrow, this gives 4 graphs



We note that each graph appears exactly once (no prefactor of, say 2). But some have negative sign. Here

 always means $V_{\ell m}$ with extra sign

Following "one arrow on each vertex" rule the Hartree diagram is



Note reverse the arrow in the loop produces same diagram!

We can add a $s = 1, 2$ variable on each vertex These give the corresponding Green's function $G^{ss'} \rightarrow$  . We also note that the direction of the arrow correlated

forward 1 backward 2

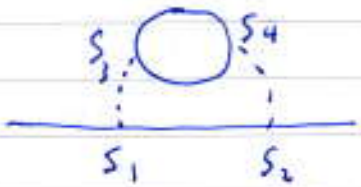
[For this reason, we can think of each vertex has three labels associated with it, a site label j, a contour time τ, and BdG label s.] This does not actually work correctly

---

Now we consider the second order term involving polarization diagram

Each vertex has two possible arrow, or labels.

We get 4 vertexes so we should have $2^4 = 16$ wrong $= 8$ different diagrams. fixing the two end as — and → In terms of equivalent s-label picture, we also have 2^{16} diagrams due to the choice of s-label



$s_{1,2,3,4} = 1, 2$ } wrong

We need to make sure 1) each diagram appears exactly once

2) The overall sign is consistent with the assignment $s' = 1\ 2$

$$(V^{ss'}) \begin{matrix} \to 1 \\ s\ 2 \end{matrix} \begin{bmatrix} V & -V \\ -V & V \end{bmatrix}$$

Of cause, loop ◯ in our extra minus sign as usual.

If this is true, we have convolution in s label for the screening equation $D = V + V \Pi D$ } wrong

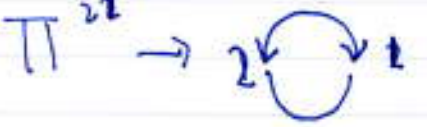
or $D^{ss'} = V^{ss'} + \sum_{s_3, s_4} V^{s s_3} \Pi^{s_3 s_4} D^{s_4 s'}$

We should have 4 different Π by the choose of S_1 and S_4

$\Pi^{11} \rightarrow$  $= G^{11} G^{11}$ 2nd G read backward

$\Pi^{22} \rightarrow$  $= G^{22} G^{22}$

$\Pi^{12} \rightarrow$  $= G^{12} G^{21}$

$\Pi^{21} \rightarrow$  $= G^{21} G^{12}$

clearly by symmetry we have $\Pi^{11} = \Pi^{22}$ $\Pi^{12} = \Pi^{21}$
They are not indept diagram due to this symmetry
we should have only 8 diagram should we then divide them by 2? → NO

Number of distinct graphs for the polarization bubble diagrams.

We note the polarization bubble can have only two possibility this

 or

Not 4 as the other arrow reverse one is the same diagram. Do we in fact extra minus sign compare the usual one?

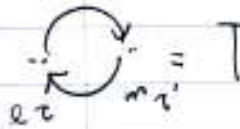
$= i\hbar e^2 G^{11}_{lm}(\tau, \tau') G^{22}_{lm}(\tau, \tau')$

and $G^{22}_{lm}(\tau, \tau') = -\frac{i}{\hbar} \langle T_\tau c^+_l(\tau) c_m(\tau') \rangle$

$= \frac{i}{\hbar} \langle T c_m(\tau') c^+_l(\tau) \rangle = -G^{11}_{ml}(\tau', \tau)$

We have the symmetry $G^{22}_{gm}(\tau,\tau') = -G^{11}_{mg}(\tau',\tau)$

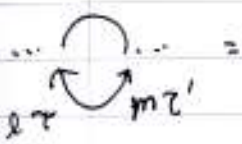
Thus, we define



$$= \Pi^{11}_{gm}(\tau,\tau') \equiv ihe^2 G^{11}_{gm}(\tau,\tau') G^{22}_{gm}(\tau,\tau') \equiv \Pi^{22}_{gm}(\tau,\tau')$$

$$= -ihe^2 G^{11}_{gm}(\tau,\tau') G^{11}_{mg}(\tau',\tau)$$

The other graph has the explicit expression



$$= \Pi^{12}_{gm}(\tau\tau') = -ihe^2 G^{12}_{gm}(\tau,\tau') G^{21}_{gm}(\tau,\tau') = \Pi^{21}_{gm}(\tau,\tau')$$

↑ see page 249 to see why we need a minus sign here

We also have the symmetry

$$G^{21}_{gm}(\tau,\tau') = -\frac{i}{\hbar}\langle T_\tau c^+_g(\tau) c^+_m(\tau')\rangle = \frac{i}{\hbar}\langle T_\tau c^+_m(\tau') c^+_g(\tau)\rangle$$

$$= -G^{21}_{mg}(\tau',\tau)$$

or $$\Pi^{12}_{gm}(\tau,\tau') = +ihe^2 G^{12}_{gm}(\tau,\tau') G^{21}_{mg}(\tau',\tau)$$

↑ plus '+' sign here

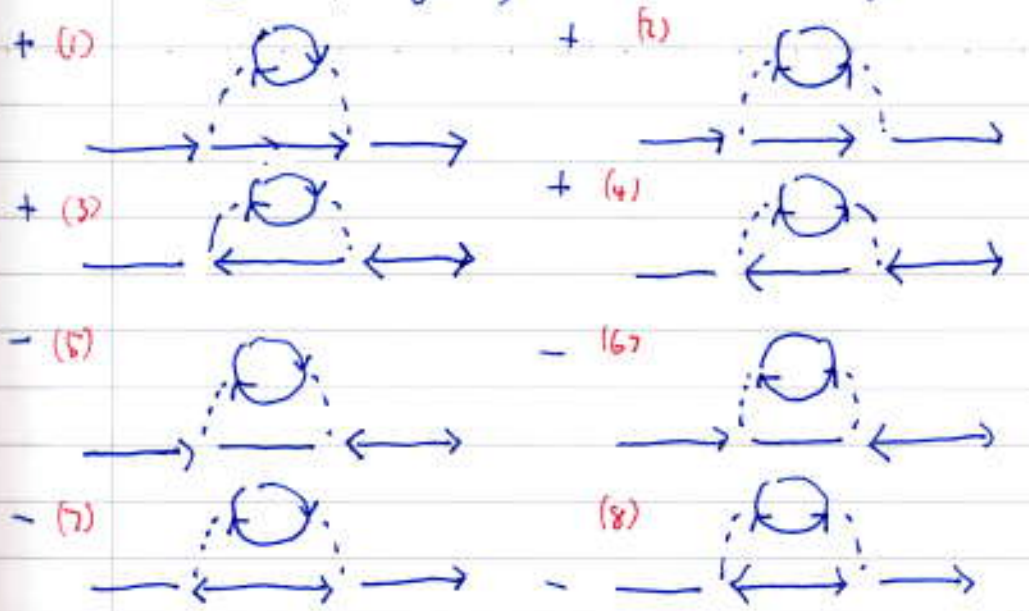
Let define Π with Nambu indices as a sum

$$\Pi_{gm}(\tau,\tau') = \Pi^{11}_{gm}(\tau,\tau') + \Pi^{12}_{gm}(\tau,\tau') \rightarrow \Pi = \Pi^{11} + \Pi^{12}.$$

We see no extra sign associated with the polarization diagram. The 8 diagrams are generated by putting 2 loop diagram onto 4 line vertex diagram with 4 choices of the middle pure.

→ or ← or — or ⟷

The 8 topologically distinct diagrams are

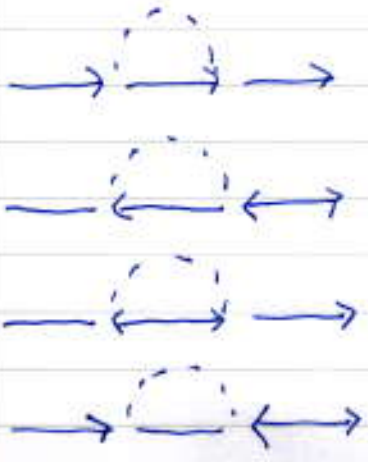


recall $G^{11} \rightarrow$
$G^{22} \leftarrow$
G^{12} —
$G^{21} \leftrightarrow$

arrow is associated with G^+.

For normal metal $G^{12} = G^{21} = 0$ we see only graph (1) is not zero, which is correct!

We now discuss the extra sign associated with these diagrams. Since the bubble diagram do not have extra sign if we define them as given for Π^{11}, Π^{12} as page 3. The extra + or - sign has the same origin of permutation the c or c^+ operate to form the line —:—:—. Thus the extra sign for the 2nd order diagrams are the same as for the 1st order diagram i.e. see page 251



This means the signs are a common factor, we can then define D not in Nambu space but the usual space indices only so that

$$D = V + V\Pi D \quad \leftarrow \begin{matrix} 1\times 1 \\ \text{not } 2\times 2 \end{matrix}$$

Here $\Pi = \Pi^{11} + \Pi^{22} = \Pi^{22} + \Pi^{21}$

$\Sigma =$  $s, s' = 1, 2$

However the minus sign is needed to get GW self energy as

$$\Sigma = GD(ie^2) \quad \text{or} \quad \Sigma^{ss'} = G^{ss'} D^{ss'} ie^2$$

Here $\mathbb{D} = \begin{bmatrix} D & -D \\ -D & D \end{bmatrix}$ or $\Sigma^{11} = G^{11} D ie^2$ $\Sigma^{22} = G^{22} D ie^2$

$$\Sigma^{12} = -G^{12} D ie^2 \quad \Sigma^{21} = -G^{21} D ie^2$$

The conclusion is that normal metal and superconducting contribution should be added to get a total Π

$$\Pi = \Pi^{11} + \Pi^{12}$$

and compute $D = v + v \Pi D$ as usual, not in Nambu or Bogoliubov - de Gennes space and $\mathbb{V} = \begin{bmatrix} V & -V \\ -V & V \end{bmatrix}$ is not used here. But $\mathbb{D} = \begin{bmatrix} D & -D \\ -D & D \end{bmatrix}$ is need to get GW self-energy Σ. Note Σ has Nambu indices. Π does not.

The physical meaning of Π or χ

To zeroth order of Coulomb interaction $\Pi = \chi$ and is given by charge-charge correlation so

$$\chi_{lm}(\tau, \tau') = -\frac{i}{\hbar} \langle T_\tau q_l(\tau) q_m(\tau') \rangle_H$$

τ - contour time

$q_l(\tau) = \sum_\sigma c_{l\sigma}^\dagger(\tau) c_{l\sigma}(\tau)$

$$= -\frac{i}{\hbar} \langle T_\tau c_{l\sigma}^\dagger(\tau) c_{l\sigma}(\tau) c_{m\sigma'}^\dagger(\tau') c_{m\sigma'}(\tau') \rangle e^2$$

Apply Wick theorem we have

$$\langle T c_{l\sigma}^\dagger c_{l\sigma} c_{m\sigma'}^\dagger c_{m\sigma'} \rangle + \langle T c_{l\sigma}^\dagger c_{l\sigma} c_{m\sigma'}^\dagger c_{m\sigma'} \rangle$$

$$= \langle T c_{l\sigma}^\dagger(\tau) c_{m\sigma'}(\tau') \rangle \langle T c_{l\sigma}(\tau) c_{m\sigma'}^\dagger(\tau') \rangle + \langle T c_{l\sigma}^\dagger c_{m\sigma'}^\dagger \rangle \langle c_{l\sigma} c_{m\sigma'} \rangle (-1)$$

so $\chi_{gm}(\tau,\tau') = -\frac{i}{\hbar}\langle T_\tau q_g(\tau) q_m(\tau')\rangle$

$= i\hbar e^2 G^{11}_{gm}(\tau,\tau') G^{22}_{gm}(\tau,\tau')$

$+ i\hbar e^2 G^{12}_{gm}(\tau,\tau') G^{21}_{gm}(\tau,\tau')(-1) \equiv \Pi_{gm}(\tau,\tau')$ ← minus sign

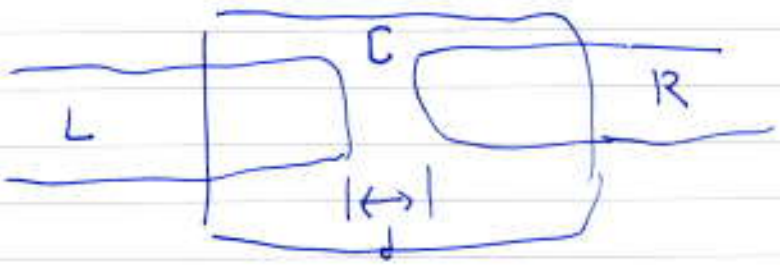
We see they are identical to the polarization bubble diagram result 

provided we take the sum of normal metal and superconducting contribution to Π, the rest does look the same as before.

The decomposition $\langle T\, C^{\dagger}_{in}(\tau) C^{+}_{m}(\tau') C_{m}(t')\rangle = \langle n\rangle^2$ is constant in time domain, a $\delta(\omega)$ in frequency domain so it should not contribute to transport. If we use $\delta\hat{q} = \hat{q} - \hat{q}_{background}$ this term is 0. So that $\langle \delta q\rangle = 0$

□ Current formula

To get transport, we divide the system into three parts, left, center, right



We assume only the center part experience Coulomb interaction. Baths L & R have no Coulomb interaction

$$\Psi = \begin{pmatrix} \Psi_L \\ \Psi_C \end{pmatrix} \qquad \Psi_L = \begin{pmatrix} c_{1L} \\ c_{2L} \\ \vdots \\ c_{nL} \\ c^{\dagger}_{1L} \end{pmatrix} \Big\} \equiv \begin{pmatrix} c_L \\ c_L^{\dagger} \end{pmatrix}$$

We classify Ψ_j according to there physical positions

1. Each Ψ_α $\alpha = L, C, R$ still are BdG vectors.

We need to work out the Meir-Wingreen formula for the energy current in terms of Green's function of the Center and Lead self energies. Particularly what happen to the BdG structure. The starting point is to compute

$$K_L = H_L - M_L N_L \qquad \hat{H}_{tot} = \hat{H}_L + \hat{H}_C + \hat{H}_R + \hat{V}_{LC} + \hat{V}_{RC} + \cdots$$

$$I_L = -\left\langle \frac{d\hat{H}_L}{dt} \right\rangle \rightarrow \text{Need use } \left\langle - \frac{d\hat{K}_L}{dt} \right\rangle$$

$$= -\left\langle \frac{1}{i\hbar} [\hat{H}_L \; \hat{H}_{tot}] \right\rangle = (\Psi_L^\dagger \Psi_C^\dagger \Psi_R^\dagger) \begin{pmatrix} H_L & V_{LC} & 0 \\ V_{CL} & H_C & V_{CR} \\ 0 & V_{RC} & H_R \end{pmatrix} \begin{pmatrix} \Psi_L \\ \Psi_C \\ \Psi_R \end{pmatrix}$$

$$= -\frac{1}{i\hbar} \left\langle [\hat{H}_L, \hat{V}_{LC} + \hat{V}_{CL}] \right\rangle$$

$\hat{V}$ — these are the only terms that do not commute with $\hat{H}_L$.

$$= \frac{1}{i\hbar} \left\langle [\hat{V}, \hat{H}_L] \right\rangle \equiv \langle \dot{\hat{V}} \rangle$$

Here we define the "left" derivative by

$$\dot{\hat{V}} = \frac{1}{i\hbar} [\hat{V}, \hat{H}_L]$$

The meaning of the expression is clear, it is the Heisenberg evolution according $\hat{H}_L$, while holding $\hat{H}_C + \hat{H}_R$ constant

as a result, $\hat{H}_L$ acctions only on Ψ_L or $\Psi_L^\dagger$

since $\hat{V} = \Psi_L^\dagger V^{LC} \Psi_C + \Psi_C^\dagger V^{CL} \Psi_L$

Here $\dot{\Psi}_L$ evolves according to H_L

$$\dot{\hat{V}} = \dot{\Psi}_L^\dagger V^{LC} \Psi_C + \Psi_C^\dagger V^{CL} \dot{\Psi}_L$$

The equation of motion for ψ_L is ← need tilde side dot

$$\dot{\psi}_L = \frac{1}{i\hbar}[\psi_L, H_L] = \frac{1}{i\hbar}\tilde{H}_L \psi_L \qquad \tilde{H}_L = \tilde{H}_L^{+}$$

$$\dot{\psi}_L^{+} = -\frac{1}{i\hbar}\psi_L^{+}\tilde{H}_L$$

The full time evolution is

$$\dot{\psi}_L = \frac{d\psi_L}{dt} \equiv \frac{1}{i\hbar}[\psi_L, \hat{H}_{tot}] = \frac{1}{i\hbar}[\psi_L, \hat{H}_L + \hat{V}_{LC} + \hat{V}_{CL}]$$

$$= \dot{\psi}_L + \frac{1}{i\hbar}[\psi_L, \hat{V}]$$

This equation relate the left derivative (evolve according to $\hat{H}_L$) and that of full derivative (evolve according to $\hat{H}_{tot}$)

$\hat{V}_{LC} + \hat{V}_{CL} = \hat{V}$

Take hermitian conjugate of above we get

$$\frac{d\psi_L^{+}}{dt} = \dot{\psi}_L^{+} - \frac{1}{i\hbar}[\psi_L, \hat{V}]^{+}$$

so $\dot{\hat{V}} = \dot{\psi}_L^{+} V^{LC} \psi_C + \psi_C^{+} V^{CL} \dot{\psi}_L$

$$= \frac{d}{dt}\psi_L^{+} V^{LC}\psi_C + \psi_C^{+} V^{CL}\frac{d\psi_L}{dt} +$$

$$-\frac{1}{i\hbar}[\psi_L, \hat{V}]^{+} V^{LC}\psi_C + \psi_C^{+} V^{CL}\frac{1}{i\hbar}[\psi_L, \hat{V}]$$

We show the last two terms cancel exactly

$$[\psi_L, \hat{V}] = [\psi_L, \psi_L^{+} V_{LC}\psi_C + \psi_C^{+} V_{CL}\psi_L]$$

$$= \underbrace{\{\psi_L, \psi_L^{T}\}}_{I} V_{LC}\psi_C + \sigma_x V_{CL}^{T}\psi_C^{+T} \equiv \tilde{V}_{LC}\psi_C$$

Here we define $\tilde{V}_{LC}$ if we write out BdG explicitly.

Thus, the last two terms are

$$-\frac{1}{i\hbar}\psi_c^+ \tilde{V}_{Lc}^+ V^{Lc}\psi_c + \frac{1}{i\hbar}\psi_c^+ V^{cL}\tilde{V}_{Lc}\psi_c$$

Is $\left[-\tilde{V}_{Lc}^+ V^{Lc} + V^{cL}\tilde{V}_{Lc}\right] = 0$? $\quad \hat{V}_{Lc}^+ = \tilde{V}_{cL}$

If the last two terms can be omitted, then

then current is

$$I_L = -\left\langle \frac{dH_L}{dt}\right\rangle = \langle \dot{\hat{V}}\rangle = \frac{d}{dt}\Big\{\langle \psi_L^+(t) V^{Lc}\psi_c(t')\rangle + \langle \psi_c^+(t') V^{cL}\psi_L(t)\rangle\Big\}\Big|_{\substack{t'=0\\ t=0}}$$

$$= \frac{d}{dt}\left\{\sum_{jk}\langle \psi_{Lj}^+(t)\psi_{ck}(t')\rangle V_{jk}^{Lc} + \sum_{jk}\langle \psi_{cj}^+(t)\psi_{Lk}(t)\rangle V_{jk}^{cL}\right\}$$

$$-i\hbar G^<_{ck\,Lj}(t',t)V_{jk}^{Lc} + -i\hbar G^<_{Lk\,cj}(t,t')V_{jk}^{cL}$$

$$= (-i\hbar)\frac{d}{dt}\left\{ Tr\left(G^<_{cL}(t',t)V^{Lc} + V^{cL}G^<_{Lc}(t,t')\right)\right\}$$

Here the trace is in space index as well as BdG index s.

We see there is a distinction between the Hamiltonian $\hat{H} = \psi^+ H\psi$ and equation of motion of the operator $i\hbar\frac{d\psi}{dt} = \tilde{H}\psi$. If this distinction is real and not superficial, we may run into trouble in deriving the Meir-Wingreen formula, as $\tilde{V}_{Lc}$ and V_{Lc} may not be the same matrix.

We need a more careful analysis as what is $\tilde{H}$.
We note that $\psi^\dagger = (c^\dagger, c)$ and $\psi = \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$ are essentially the same thing with a permutation of the position in Bogoliubov-de Gennes space. In particular we can relate them as

$$(\psi^\dagger)^T = \sigma_x \begin{pmatrix} c \\ c^\dagger \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} = \begin{pmatrix} c^\dagger \\ c \end{pmatrix} = \sigma_x \psi$$

or take the transpose $\psi^\dagger = \psi^T \sigma_x$ or $\psi = \sigma_x (\psi^\dagger)^T$

i.e. σ_x multiplied from left permute row
σ_x multiplied from right permute the column

Thus $\hat{H} = \psi^\dagger H \psi = \psi^T \sigma_x H \psi = \psi^\dagger H \sigma_x (\psi^T)^T$

we can think of $\hat{H}$ as bilinear in $\psi^\dagger$ and ψ or ψ and ψ or ψ^T and $\psi^\dagger$. They are all equivalent with proper adjustment of single particle Hamilton and H or $\sigma_x H$ or $H\sigma_x$.

{ For this reason we might change notation to define H to mean $\frac{1}{2}\psi^\dagger H \psi = \hat{H}$. with a $\frac{1}{2}$ divided. But it is too late to change notation. I prefer we stick to my original notation $\hat{H} = \psi^\dagger H \psi$.

The commutation relation for ψ is

$$\{\psi, \psi^\dagger\} = I$$
$$\{\psi, \psi^T\} = \sigma_x$$
$$\{\psi^\dagger, \psi^{\dagger T}\} = \sigma_x$$

use the commutation relation we compute

$$i\hbar \frac{d\psi}{dt} = [\psi, \hat{H}]$$

or look at each component ψ_{js} j space, s BdG space, $\psi_{j1} = c_j$, $\psi_{j2} = c_j^\dagger$

$$[\psi_{js}, \psi^\dagger H \psi] = \sum_{\substack{s's'' \\ k\ell}} [\psi_{js}, \psi^\dagger_{ks'} H^{s's''}_{k\ell} \psi_{\ell s''}]$$

$$= \sum_{\substack{s's'' \\ k\ell}} \Big\{ \{\psi_{js}, \psi^\dagger_{ks'}\} H^{s's''}_{k\ell} \psi_{\ell s''} - \psi^\dagger_{ks'} H^{s's''}_{k\ell} \{\psi_{js}, \psi_{\ell s''}\} \Big\}$$

Here we use the identity $[A, BC] = \{A, B\}C - B\{A, C\}$ which can be verified to be true for any A, B, C operators

left side is $A(BC) - (BC)A$

right side is $(AB + BA)C - B(AC + CA) = ABC + BAC - BAC - BCA$

$\{A, B\}$ $\{A, C\}$

Pauli $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

left = right.

so $[\psi_{js}, \psi^\dagger H \psi] = \sum_{\substack{s's'' \\ k\ell}} \delta_{jk} \delta_{ss'} H^{s's''}_{k\ell} \psi_{\ell s''} - \psi^\dagger_{ks'} H^{s's''}_{k\ell} \delta_{j\ell} (\sigma_x)^{ss''}$

$$= \sum_{s''\ell} H^{ss''}_{j\ell} \psi_{\ell s''} - \sum_{\substack{s's'' \\ k\ell}} \delta_{j\ell} (\sigma_x)^{ss''} H^{s's''}_{k\ell} \psi^\dagger_{ks'}$$

$$= (H\psi)_{j\ell} - \sum_{\substack{s's'' \\ k\ell}} \delta_{j\ell} (\sigma_x)^{ss''} (H^T)^{s''s'}_{\ell k} \psi^\dagger_{ks'}$$

$$(H^T)^{s''s'}_{jk} = H^{s's''}_{kj}$$

$$= H\psi - (\sigma_x H^T (\psi^\dagger)^T)$$

Here $\sigma_x = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$ is Pauli matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ in BdG space and identity I position space

i.e. σ_x is $2N \times 2N$ matrix in both BdGs & real space.

using $\psi^{\dagger T} = \sigma_x \psi$ we find

$$i\hbar \frac{d\psi}{dt} = \tilde{H}\psi, \quad \text{here } \tilde{H} = H - \underbrace{\sigma_x H^T \sigma_x}_{2N \times 2N}$$

all matrices here are $2N \times 2N$ in the combined space.

$\tilde{H} = H - \sigma_x H^T \sigma_x$ here H^T is matrix transpose in both j and s space i.e.

$$H^T = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}^T = \begin{pmatrix} H_{11}^T & H_{21}^T \\ H_{12}^T & H_{22}^T \end{pmatrix} \quad 2\times 2 \text{ in BdG space}$$

Multiply by σ_x from left & right causes a permutation of the rows & columns we have

$$\sigma_x H^T \sigma_x = \begin{pmatrix} H_{22}^T & H_{12}^T \\ H_{21}^T & H_{11}^T \end{pmatrix} \quad \text{or} \quad \tilde{H} = \begin{pmatrix} H_{11} - H_{22}^T & H_{12} - H_{12}^T \\ H_{21} - H_{21}^T & H_{22} - H_{11}^T \end{pmatrix}$$

This agrees with that obtained on page 217 or page 211.

My claim is that we can redefine or choosing the parameter without a loss of generality at $\tilde{H} = 2H$. i.e. $\tilde{H}$ and H essentially the same. To see this, we note the term $C^\dagger H_{11} C + C H_{22} C^\dagger$ split is not unique, we can split half each to the other to

ie $\frac{1}{2} C^\dagger H_{11} C + \frac{1}{2} C^\dagger H_{11} C = \frac{1}{2} C^\dagger H_{11} C + \frac{1}{2} \sum_{jk} C_j^\dagger H''_{jk} C_k$

$= \frac{1}{2} C^\dagger H_{11} C + \frac{1}{2} \sum_{jk} (-C_k C_j^\dagger) H''_{jk}$ $\quad = \frac{1}{2} C^\dagger H_{11} C - \frac{1}{2} C H_{11}^T C^\dagger$ + const

similarly $\frac{1}{2} C H_{22} C^\dagger + \frac{1}{2} C H_{22} C^\dagger = \frac{1}{2} C H_{22} C^\dagger - \frac{1}{2} C^\dagger H_{22}^T C +$ const

Since adding a constant to the Hamilton do not change physics, we drop the constant thus

$$C^\dagger H_{11} C + C H_{22} C^\dagger = \frac{1}{2} \left[C^\dagger (H_{11} - H_{22}^T) C + C (H_{22} - H_{11}^T) C^\dagger \right] + \text{const}$$

The $C H_{12} C$ term must be antisymmetric $\Rightarrow H_{12} = -H_{12}^T$

since $\sum_{jk} C_j H_{jk}^{12} C_k = -\sum_{jk} C_k H_{jk}^{12} C_j = - C H_{12}^T C = C H_{12} C$

Thus we find $C H_{12} C = \frac{1}{2} C H_{12} C + \frac{1}{2} C H_{12} C$

similarly for $C^+ H_{21} C^+$ term $= \frac{1}{2} C H_{12} C - \frac{1}{2} C H_{12}^T C$

So we can write our Hamiltn H, without any loss of generality

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \quad \text{as} \quad H' = \frac{1}{2}\begin{bmatrix} H_{11} - H_{22}^T & H_{12} - H_{12}^T \\ H_{21} - H_{21}^T & H_{22} - H_{11}^T \end{bmatrix}$$

with the identy $\psi^+ H \psi = \psi^+ H' \psi$

In the alternate symmetrized form, we find $H' = \frac{1}{2}\tilde{H}$ or $\tilde{H} = 2H'$ so $\tilde{H}$ and H' are the same apart from a factor of 2. Let introduce a new notation

of $h = H_{11} - H_{22}^T$ then $h^T = H_{11}^T - H_{22}$

and $\Delta = H_{21} - H_{21}^T$

$\Delta^T = H_{21}^T - H_{21} = -\Delta$ is antisymmetric

we can then write

$$H' = \frac{1}{2}\begin{bmatrix} h & \Delta^+ \\ \Delta & -h^T \end{bmatrix} \quad \text{and} \quad \tilde{H} = \begin{bmatrix} h & \Delta^+ \\ \Delta & -h^T \end{bmatrix}$$

Since $\psi^+ H' \psi$ must be hermitin the off digal are related by hermitn conjugate

$$C \Delta C \rightarrow (C \Delta C)^+ = C^+ \Delta^+ C^+$$

H is hermtn $H^T = H \Rightarrow H_{11}^+ = H_{11} \quad H_{22}^+ = H_{22}$

$H_{21}^+ = H_{12} \quad H_{12}^+ = H_{21}$ so $H_{12} - H_{12}^T = H_{21}^+ - \left(H_{21}^+\right)^T$

$= \left(H_{21} - H_{21}^T\right)^+ = \Delta^+$ Note H_{11} and H_{22} are related by time inversion $t \rightarrow -t$

To summarize we can write the Hamiltn as

$\hat{H} = \frac{1}{2}\Psi^{+}\tilde{H}\Psi$ and equation of motion is

$i\hbar\frac{d\Psi}{dt} = \tilde{H}\Psi$ here we have special symmetry

taking into account $\tilde{H} = \begin{bmatrix} h & \Delta^{+} \\ \Delta & -h^{T} \end{bmatrix}$ $h = h^{+}$, $\Delta^{T} = -\Delta$

$H' = \frac{1}{2}\tilde{H}$ is the symmetrized version of original H.

note $-h^{T} = -h^{*}$

We can now go back to the derivation of Meir-Wingreen formula on page 15. Since we have shown we can make $2H = \tilde{H}$ the calculation on page 15 is true as V_{LC} and $\tilde{V}_{LC}$ are the same except a factor of 2. Since the equations of motion and Dyson equations on page 219 requiring the use of $\tilde{H}$. It is then more convenient we stick to $\tilde{H}$ and also express H_L in terms of $\tilde{H}$, i.e. we are going to consider the notation

$$\hat{H} = \frac{1}{2}\Psi^{+}\tilde{H}\Psi$$

with a pre factor $\frac{1}{2}$. Similarly $\hat{H}_L = \frac{1}{2}\Psi_L^{+}\tilde{H}_L\Psi_L$, this extra factor of $\frac{1}{2}$ appears in the current formula as in the phonon case. If we use tilde version of the Hamiltonian so the formula on page 15 becomes

$$I_L = (-i\hbar)\frac{1}{2}\frac{d}{dt}\left\{ Tr\left(G^{<}_{CL}(t',t)\tilde{V}^{LC} + \tilde{V}^{CL}G^{<}_{LC}(t,t') \right) \right\}_{\substack{t'\to 0 \\ t\to 0}}$$

Note $V^{LC} = \frac{1}{2}\tilde{V}^{LC}$ we use time translated invariance $\frac{d}{dt}G^{<}_{CL}(t'-t) = -\frac{d}{dt'}G^{<}(t'-t)$ then

Since we have time translational invariance at steady states $G(t,t') = G(t-t')$, we can use Fourier transform representation,

$$G(t) = \int_{-\infty}^{+\infty} \frac{dE}{2\pi\hbar}\, G(E)\, e^{-\frac{i}{\hbar}Et}$$

so $$\frac{d}{dt} G^{<}_{LL}(t,t')\Big|_{\substack{t'=0\\ t=0}} = \int_{-\infty}^{+\infty} \frac{dE}{2\pi\hbar} \left(-\frac{i}{\hbar}\right) E\, G^{<}_{LC}(E)$$

So $$I_L = \frac{1}{2} \int_{-\infty}^{+\infty} \frac{dE}{2\pi\hbar} E\, \mathrm{Tr}_{js}\left(G^{<}_{LL}(E)\, \tilde{V}^{LC} - \tilde{V} G^{<}_{LC}(E) \right)$$

Here the trace $\mathrm{Tr}_{js}[\cdots]$ is in the $2N \times 2N$ BdG & nambu space (s,j)

We now follow standard procedure to eliminate G_{CL} in favor of G_{CC}, the Green's function involving the center only. We split the Hamiltonian $\tilde{H}$ and Green's function in TD 3×3 blocks of L, C, R so

$$\tilde{H} = \begin{pmatrix} \tilde{H}_L & \tilde{V}_{LC} & 0 \\ \tilde{V}_{CL} & \tilde{H}_C & \tilde{V}_{CR} \\ 0 & \tilde{V}_{RC} & \tilde{H}_R \end{pmatrix} \qquad G = \begin{pmatrix} G_{LL} & G_{LC} & G_{LR} \\ G_{CL} & G_{CC} & G_{CR} \\ G_{RL} & G_{RC} & G_{RR} \end{pmatrix}$$

Then the equation of motion on page 215, 219 becomes

$$i\frac{\partial}{\partial\tau} \begin{bmatrix} G_{LL} & G_{LR} \\ & G_{CC} \\ & \ddots \end{bmatrix} - \begin{bmatrix} \tilde{H} \end{bmatrix} \begin{bmatrix} G_{LL} & G_{LC} \\ & G_{CC} \\ & \ddots \end{bmatrix} = \begin{bmatrix} 1 & 0 & \\ 0 & 1 & 0 \\ & 0 & 1 \end{bmatrix} \delta(\tau,\tau')$$

We define isolated subsystem Green's function by symbol g as

$$i\frac{\partial}{\partial\tau} \begin{bmatrix} g_L & 0 & 0 \\ 0 & g_C & 0 \\ 0 & 0 & g_R \end{bmatrix} - \begin{bmatrix} \tilde{H}_L & 0 & 0 \\ 0 & \tilde{H}_C & 0 \\ 0 & 0 & \tilde{H}_R \end{bmatrix} \begin{bmatrix} g_L & 0 & 0 \\ 0 & g_C & 0 \\ 0 & 0 & g_R \end{bmatrix} = \begin{bmatrix} 1 & 0 & \\ 0 & 1 & 0 \\ & 0 & 1 \end{bmatrix} \delta(\tau,\tau')$$

We split $\tilde{H}$ into diags and off-diags

$$\tilde{H} = \begin{bmatrix} \tilde{H}_L & 0 & 0 \\ 0 & H_C & 0 \\ 0 & 0 & \tilde{H}_R \end{bmatrix} + \begin{bmatrix} 0 & \tilde{V}_{LC} & 0 \\ \tilde{V}_{CL} & 0 & \tilde{V}_{CR} \\ 0 & \tilde{V}_{RC} & 0 \end{bmatrix} = \tilde{H}_d + \tilde{V}$$

↑ off diag me

then $\left(i\hbar \frac{\partial}{\partial t} I - \tilde{H}_d\right) G + \tilde{V} G = I\, \delta(t, t')$

symbolically the operator $I i\hbar \frac{\partial}{\partial t} - \tilde{H}_d$ is g^{-1}

since $g^{-1} g = I\, \delta(t, t')$ so we get the solution

$$g^{-1} G + \tilde{V} G = I \rightarrow G + g\tilde{V} G = g$$

or $G = g + \underbrace{g\tilde{V} G}$ ← Dyson equation for G flip side ↓

convolution in τ, j and s

$= g + G\tilde{V} g$ Note $G = g + g\tilde{V} G$

$= g + G\tilde{V} g$

In particular we get

$$G_{CL} = G_{CC} \tilde{V}^{CL} g_L \quad \text{or} \quad G_{LC} = g_L \tilde{V}^{LC} G_{CC}$$

These two equations are in contour time, i.e.

$$G_{CL}(\tau, \tau') = \int d\tau''\, G_{CC}(\tau, \tau'') \tilde{V}^{CL} g_L(\tau'', \tau')$$

Use Langreth rule we get

$$G^<_{CL} = G^r_{CC} \tilde{V}^{CL} g^<_L + G^K_{CC} \tilde{V}^{CL} g^a_L \qquad \text{similarly for } G^<_{LC}$$

For notational simplicity we'll drop the CC subscript so G means Green's function of the center. Now we define the lead self energy by

$$\Sigma_L = \tilde{V}^{CL} g_L \tilde{V}^{LC}$$ work in E space the trace term means

$\leftarrow \mathrm{Tr} \equiv \mathrm{Tr}_{j,s}(\dots)$

$$\mathrm{Tr}\left(G^<_{cL}\tilde{V}^{Lc} - \tilde{V}^{cL}G^<_{Lc}\right)$$

$$= \mathrm{Tr}\left(G^r\Sigma^<_L + G^<\Sigma^a_L - \Sigma^r_L G^< - \Sigma^<_L G^a\right)$$

Use $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ we get

$$= \mathrm{Tr}\left(G^<(\Sigma^a_L - \Sigma^r_L) + (G^r - G^a)\Sigma^<_L\right)$$

use the relation $G^r - G^a = G^> - G^<$

$$\Sigma^r_\alpha - \Sigma^a_\alpha = \Sigma^>_\alpha - G^<_\alpha \qquad \alpha = L, R$$

we get

$$= \mathrm{Tr}\left(G^<(\Sigma^<_L - \Sigma^>_L) + (G^> - G^<)\Sigma^<_L\right)$$

$$= \mathrm{Tr}\left(G^<\Sigma^<_L - G^<\Sigma^>_L + G^>\Sigma^<_L - G^<\Sigma^<_L\right)$$

The energy current out of the left lead is then

$$I_L = \frac{1}{2}\int_{-\infty}^{+\infty}\frac{dE}{2\pi\hbar}\cdot E\,\mathrm{Tr}_{j,s}\left(G^>\Sigma^<_L - G^<\Sigma^>_R\right)$$

Here trace is in both the space indices j as well as Nambu/BdG index s. Note the extra $\frac{1}{2}$ due to our choice of written the Hamilton as

$$\hat{H} = \frac{1}{2}\Psi^+\tilde{H}\Psi \qquad \text{and used associate } \tilde{V}_{Lc}.$$

In conclusion we do have the Meir-Wingreen formula expressed as a trace over ordinary space index j but also in Nambu space index s. Except we need to watch out for the extra $\frac{1}{2}$ factor due to our particular choice of using Hamilton $\tilde{H}$.

Fluctuation-dissipation theorem (FDT)

Following up to the question of FDT mentioned on page 219 we discuss the validity the theorem. According to the definition of contour ordered Green's function on page 207 the greater component is

$$G^{>}(t) \equiv -\frac{i}{\hbar}\langle \psi(t)\psi^{\dagger}(0)\rangle = -\frac{i}{\hbar}\mathrm{Tr}\left[\frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z} e^{\frac{i}{\hbar}\hat{H}t}\psi e^{-\frac{i}{\hbar}\hat{H}t}\psi^{\dagger}\right]$$

Here $\psi(t) = e^{\frac{i}{\hbar}\hat{H}t}\psi e^{-\frac{i}{\hbar}\hat{H}t}$ satisfies the Heisenberg equation of motion $i\hbar\frac{d\psi}{dt} = [\psi, \hat{H}]$

If $[\hat{H}, \hat{N}] = 0$ we can find eigen states $|n\rangle$ which is simultaneously the eigen states of $\hat{H}$ and $\hat{N}$.

$$\hat{H}|n\rangle = E_n|n\rangle$$
$$\hat{N}|n\rangle = N_n|n\rangle$$

Using Lehrmann representation. i.e. compute trace with $|n\rangle$ as basis, we can show

$$G^{<}(E) = -e^{-\beta(E-\mu)}G^{>}(E)$$ since

$$-iA = G^{>} - G^{<} = G^{r} - G^{a} \quad \text{or} \quad -iA = -(e^{\beta(E-\mu)}+1)G^{<}$$

$$\text{or} \quad G^{<} = \frac{1}{e^{\beta(E-\mu)}+1} iA = if(E)A = -f(E)(G^{r}-G^{a})$$

This is the fluctuation-dissipation theorem for the usual electrons.

The above derivation breaks down when $[\hat{H}, \hat{N}] \neq 0$

A proof for the normal metal case so $[\hat{H}, \hat{N}] = 0$

$$G^{>}(t) = -\frac{i}{\hbar}\left\langle \begin{pmatrix} C(t)C^{\dagger}(0) & C(t)C(0) \\ C^{\dagger}(t)C^{\dagger}(0) & C^{\dagger}(t)C(0) \end{pmatrix} \right\rangle$$

so $G^{>} = \begin{pmatrix} G^{>}_{11} & G^{>}_{12} \\ G^{>}_{21} & G^{>}_{22} \end{pmatrix}$ ← 2×2 in BdG or Nambu space

By general theorem of quantum-mechanics, different eigenvalues of $\hat{N}$ are orthogonal $\langle n | e^{-\beta(H-\mu N)} \underbrace{c\, c}_{c^\dagger c^\dagger} | n \rangle = 0$

i.e. for normal metal we have

$$G_{12} = G_{21} = 0$$

$$G^{>}_{11}(t) = -\frac{i}{\hbar} \langle c(t)\, c^\dagger(0) \rangle \qquad G^{>}_{22}(t) = -\frac{i}{\hbar} \langle \left(c^\dagger(t)\right)^T c(0)^T \rangle$$

or $G^{11,>}_{jk}(t) = -\frac{i}{\hbar} \langle c_j(t)\, c^\dagger_k(0) \rangle \qquad G^{22,>}_{jk}(t) = -\frac{i}{\hbar} \langle c^\dagger_j(t)\, c_k(0) \rangle$

since $G^{11,<}_{jk}(t) = \frac{i}{\hbar} \langle c^\dagger_k(0)\, c_j(t) \rangle$ we find the relation

$$G^{22,>}_{jk}(t) = -\frac{i}{\hbar} \langle c^\dagger_j(0)\, c_k(-t) \rangle = -G^{11,<}_{kj}(-t)$$

i.e. $G^{22,>}(t) = -\left[G^{11,<}(-t)\right]^T$ reverse time & space and a (-1)

We can focus on $G^{11,>}$ only the usual one

$$G^{11,>}_{jk}(t) = -\frac{i}{\hbar} \mathrm{Tr}\left(\frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z} e^{\frac{i}{\hbar}\hat{H}t}\, c_j\, e^{-\frac{i}{\hbar}\hat{H}t}\, c^\dagger_k \right)$$

$$= -\frac{i}{\hbar} \sum_{n,m} \frac{1}{Z} e^{-\beta(E_n - \mu N_n) + \frac{i}{\hbar}E_n t} \langle n | c_j | m \rangle e^{-\frac{i}{\hbar}E_m t} \langle m | c^\dagger_k | n \rangle$$

$G(E) = \int_{-\infty}^{\infty} G(t)\, e^{+\frac{i}{\hbar}Et}\, dt$

In order to have a non-zero value $|m\rangle$ must have one particle more than $|n\rangle$ i.e. $N_m = N_n + 1$

Going to E space by Fourier transform in t we get

$$G^{11,>}_{jk}(E) = -\frac{i}{\hbar} \sum_{n,m} \frac{e^{-\beta(E_n - \mu N_n)}}{Z} \langle n | c_j | m \rangle \langle m | c^\dagger_k | n \rangle\, 2\pi\hbar\, \delta(E_n - E_m + E)$$

We now work out $G^{11,<}$

$$G^{11,<}_{jk}(t) = +\left(\frac{i}{\hbar}\right)\langle c^+_k(0)\, c_j(t)\rangle = \frac{i}{\hbar}\mathrm{Tr}\left(\frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z} c^+_k e^{\frac{i}{\hbar}\hat{H}t} c_j e^{-\frac{i}{\hbar}\hat{H}t}\right)$$

$$= \frac{i}{\hbar}\sum_{n,m}\langle m|\, e^{-\beta(\hat{H}-\mu\hat{N})}\, c^+_k \sum_n |n\rangle\langle n|\, e^{+\frac{i}{\hbar}\hat{H}t} c_j e^{-\frac{i}{\hbar}\hat{H}t}|m\rangle$$

$$= \frac{i}{\hbar}\sum_{n,m}\frac{e^{-\beta(E_m-\mu N_m)}}{Z}\langle m|c^+_k|n\rangle\langle n|c_j|m\rangle e^{\frac{i}{\hbar}(E_n-E_m)t}$$

$$\rightarrow G^{11,<}_{jk}(E) = \frac{i}{\hbar}\sum_{n,m}\frac{e^{-\beta(E_n-\mu N_m)}}{Z}\langle m|c^+_k|n\rangle\langle n|c_j|m\rangle 2\pi\hbar\,\delta(\underbrace{E_n - E_m}_{\wedge} + E)$$

We try to bring $G^<$ into a form similar to $G^>$. Due to the δ-function in energy eigenvalues. $E_n = E_m - E$

reorder the $\langle\cdots|c|\cdots\rangle$ term we get

$$G^{11,<}_{jk}(E) = \frac{i}{\hbar}\sum_{n,m}\frac{e^{-\beta(E_m-\mu N_m)}}{Z}\langle n|c_j|m\rangle\langle m|c^+_k|n\rangle 2\pi\hbar\,\delta(\underbrace{E_n - E_m}_{\wedge} + E)$$

we see now the are nearly the same except $N_n \rightarrow N_m$

The factor in the distribution

$$E_m - \mu N_m = E_n + E - \mu(N_n + 1) = E_n - \mu N_n + E - \mu$$

so we can factor a common factor to get

$$G^{11,<}(E) = -e^{-\beta(E-\mu)} G^{11,>}(E)$$ this is the usual FD relation

using complet similar steps, we find

$$G^{22,<}(E) = -e^{-\beta(E+\mu)} G^{22,>}(E)$$

we notice chemical potential need to flip a sign

so as a matrix of 2x2 $\begin{bmatrix} G^{11} & 0 \\ 0 & G^{22} \end{bmatrix}$

$G^< = -e^{\cdots} G^>$ as a common factor is false

Thus the correct form is

$$G^<(E) = -\begin{bmatrix} e^{\pm\beta(E-\mu)} & 0 \\ 0 & e^{\beta(E+\mu)} \end{bmatrix} G^>(E)$$

or

$$G^< = -\begin{bmatrix} \frac{1}{e^{\beta(E-\mu)}+1} & 0 \\ 0 & \frac{1}{e^{\beta(E+\mu)}+1} \end{bmatrix} (G^> - G^a)$$

$G^{11} \to E-\mu$

$G^{22} \to E+\mu$

so $G^< = -f(G^> - G^a)$ with a common $f \equiv \frac{1}{e^{\beta(E-\mu)}+1}$ is false! (unless, of course when $\mu \equiv 0$).

Now we discuss for the superconductor with the mean field Hamiltonian such that $[\hat{H}, \hat{N}] \neq 0$. In such case, I believe the fluctuation-dissipation theorem is false. We can check up with a double quantum dots with concrete calculations. However, we can recover FDT if we redefine our Green's functions. In particular, we need to modify the Heisenberg evolution as not in $\hat{H}$, but in $\hat{K} = \hat{H} - \mu\hat{N}$. For ordinary case when $[\hat{H}, \hat{N}] = 0$, this is not a big deal as $\hat{N}$ is a constant, and we simply redefine 0 of energy of the particular. However If $[\hat{H}, \hat{N}] \neq 0$, $\hat{H}$ and $\hat{K}$ are really different dynamics, which one represent real physics?

we see $-\frac{d\hat{K}}{dt}$ is heat

while $-\frac{d\hat{H}}{dt}$ is energy.

If the system evolves according to $\hat{K}$, then heat is conserved since $i\hbar \frac{d\hat{K}}{dt} = [\hat{K}, \hat{K}] = 0$

but energy is not conserved $i\hbar \frac{d\hat{H}}{dt} = [\hat{H}, \hat{K}]$

$= [\hat{H}, -\mu\hat{N}] \neq 0$

The fact that total energy is not conserved in the dynamics of $\hat{K}$ is alarming. However, in $\hat{H}$, the particle # is not conserved any way

$$i\hbar \frac{d\hat{N}}{dt} = [\hat{N}, \hat{K}] = [\hat{N}, \hat{H} - \mu\hat{N}] = [\hat{N}, \hat{H}] \neq 0$$

as far as $\hat{N}$ is conserved evolving under $\hat{H}$ or $\hat{K}$ are completely equivalent. So since the particle number is not conserved, it seems to me alright to have a situation that the energy is not conserved. Then we need to ask, where the energy goes?

There may still be conceptual issue to use $\hat{K} = \hat{H} - \mu\hat{N}$ to evolve the dynamics operationally, we go ahead with a new definition of Green's function by

$$G_K(\tau, \tau') = -\frac{i}{\hbar} \langle \psi_K(\tau) \psi_K^{\dagger}(\tau') \rangle$$

Here our Heisenberg evolution now is

$$i\hbar \frac{d\psi}{dt} = [\psi, \hat{K}] \qquad \hat{K} = \hat{H} - \mu\hat{N}$$

with this new definition of Green's fluctuation-dissipation theorem is valid.

$$G^<(E) = -e^{-\beta E} G^>(E) \rightarrow G^<(E) = -\frac{1}{e^{\beta E}+1}\left(G^>(E) - G^a(E)\right)$$

here $G^<, G^>, G^r, G^a$ are 2×2 matrix in BdG space and the fermi function is a common function. Notice we don't have a chemical potential μ here. The reason is that μ is absorbed into $\hat{K}$ and into energy spectrum $\xi = \varepsilon - \mu$.

Let us try to prove this, focusing on the expression of $G^>$ we have

$$G^>_{js\,ks'}(t) = -\frac{i}{\hbar} \mathrm{Tr}\left[\frac{e^{-\beta \hat{K}}}{Z} e^{\frac{i}{\hbar}\hat{K}t} \psi_{js} e^{-\frac{i}{\hbar}\hat{K}t} \psi^+_{ks'}\right]$$

(explicit BdG indices; we have $\hat{K} = \hat{H} - \mu\hat{N}$ everywhere)

Since we cannot find simultaneous eigen value for $\hat{H}$ and $\hat{N}$, we just look for eigen state of $\hat{K}$ so that

$$\hat{K}|n\rangle = K_n|n\rangle \qquad n = 1, 2, 3, \cdots$$

since $\hat{K}$ is hermitian K_n is real and $|n\rangle$ is complete $\sum_n |n\rangle\langle n| = \hat{1}$ as usual.

Since $|n\rangle$ may not have a fixed particle number, such as the BCS ground state type

$$\langle n|c\,c|n\rangle \neq 0$$

Any way we do the usual Lehmann expansion to get

$$G^>_{js\,ks'}(t) = -\frac{i}{\hbar}\sum_{n,m} \frac{e^{-\beta K_n + \frac{i}{\hbar}K_n t}}{Z} \langle n|\psi_{js}|m\rangle e^{-\frac{i}{\hbar}K_m t} \langle m|\psi^+_{ks'}|n\rangle$$

we do Fourier transform $G(E) = \int_{-\infty}^{+\infty} G(t)\, e^{\frac{i}{\hbar}Et}\, dt$

use $\int_{-\infty}^{+\infty} e^{i\omega t}\,dt = 2\pi\delta(\omega)$

in E-space, we find

$$G^{>}_{js,ks'}(E) = -\frac{i}{\hbar}\sum_{n,m}\frac{e^{-\beta K_n}}{Z}\langle n|\psi_{js}|m\rangle\langle m|\psi^{\dagger}_{ks'}|n\rangle\, 2\pi\hbar\,\delta(E+K_n-K_m)$$

swap the order

$G^{<}$ by definition is

$$G^{<}_{js\,ks'}(t) = +\frac{i}{\hbar}\,\mathrm{Tr}\left(\frac{e^{-\beta\hat{K}}}{Z}\,\psi^{\dagger}_{ks'}\,e^{\frac{i}{\hbar}\hat{K}t}\,\psi_{js}\,e^{-\frac{i}{\hbar}\hat{K}t}\right)$$

Take trace with $\langle m|\ldots|m\rangle$ insert $\sum_n |n\rangle\langle n| = \hat{1}$

we get

$$= +\frac{i}{\hbar}\sum_{n,m}\frac{e^{-\beta K_m}}{Z}\langle m|\psi^{\dagger}_{ks'}|n\rangle\, e^{\frac{i}{\hbar}K_n t}\langle n|\psi_{js}|m\rangle\, e^{-\frac{i}{\hbar}K_m t}$$

go to E-space we get

$$G^{<}_{js\,ks'}(E) = \frac{i}{\hbar}\sum_{n,m}\frac{e^{-\beta K_m}}{Z}\langle n|\psi|_{js}|m\rangle\langle m|\psi^{\dagger}_{ks'}|n\rangle\, 2\pi\hbar\,\delta(E+K_n-K_m)$$

If we compare $G^{>}$ with $G^{<}$, the only difference is an overall minus sign '$-$' and the Boltzmann factor. Because of the δ-function constraint, we have

$$E + K_n - K_m = 0 \quad \text{or}$$

$$K_m = E + K_n \quad \text{so}$$

$$G^{<}(E) = -G^{>}(E)\,e^{-\beta E}$$ ← This is the same for all indices js, ks' so it is a matrix equation in space & Nambu space with a common numerical factor

Since $G^{>} - G^{<} = G^{r} - G^{a} = -iA$ (2x2 matrix)

using the $G^{<} = -G^{>}e^{-\beta E}$ relation we have $-e^{\beta E}G^{<} - G^{<} = G^{r} - G^{a}$

or $$G^{<} = -\frac{1}{e^{\beta E}+1}\left(G^{r} - G^{a}\right)$$ This is the desired FDT.

An alternative derivation following L P Kanaroff & G Baym "Quantum Statistical Mechanics", Benjamin (1962).

Let's define $G^{>}_{\hat{A}\hat{B}}(t_1,t_2) = \frac{(-i/\hbar)}{} \mathrm{Tr}\left(\frac{e^{-\beta\hat{K}}}{Z} e^{\frac{i}{\hbar}\hat{K}t_1}\hat{A}\, e^{-\frac{i}{\hbar}\hat{K}t_1} e^{\frac{i}{\hbar}\hat{K}t_2}\hat{B}\, e^{-\frac{i}{\hbar}\hat{K}t_2}\right)$

$$= \mathrm{Tr}\left(\frac{1}{Z} e^{\frac{i}{\hbar}\hat{K}(t_1-t_2+i\hbar\beta)}\hat{A}\, e^{-\frac{i}{\hbar}\hat{K}(t_1-t_2)}\hat{B}\right)\left(\frac{-i}{\hbar}\right)$$

It is obvious that we have time translation invariance, the function depends only on the difference $t_1 - t_2 = t$ so we write

$$G^{>}_{\hat{A}\hat{B}}(t) = -\frac{i}{\hbar}\mathrm{Tr}\left(\frac{1}{Z} e^{\frac{i}{\hbar}\hat{K}(t+i\hbar\beta)}\hat{A}\, e^{-\frac{i}{\hbar}\hat{K}t}\hat{B}\right)$$

We'll let t run over the complex plane provided the expression converges. We assume $\hat{A}$ or $\hat{B}$ are fermi c or c^+

so $G^{<}_{\hat{A}\hat{B}}(t) \equiv \frac{i}{\hbar}\mathrm{Tr}\left(\frac{e^{-\beta\hat{K}}}{Z}\hat{B}\, e^{\frac{i}{\hbar}\hat{K}t}\hat{A}\, e^{-\frac{i}{\hbar}\hat{K}t}\right)$

$$= \frac{i}{\hbar}\mathrm{Tr}\left[\frac{1}{Z} e^{\frac{i}{\hbar}\hat{K}t}\hat{A}\, e^{-\frac{i}{\hbar}\hat{K}(t-i\beta t)}\hat{B}\right]$$

do cyclic permutation

If we make a replacement $t \to t + i\hbar\beta$ we find it is $-G^{>}$, ie

$$G^{<}_{\hat{A}\hat{B}}(t+i\hbar\beta) = -G^{>}_{\hat{A}\hat{B}}(t) \quad \leftarrow \text{KMS condition}$$

This is the Kubo-Martin-Schwinger boundary condition

Do Fourier transform to t

$$\int_{-\infty}^{+\infty} G^{<}_{\hat{A}\hat{B}}(t+i\hbar\beta)\, e^{i\frac{E}{\hbar}t}\, dt = -\int_{-\infty}^{+\infty} G^{>}_{\hat{A}\hat{B}}(t)\, e^{i\frac{E}{\hbar}t}\, dt$$

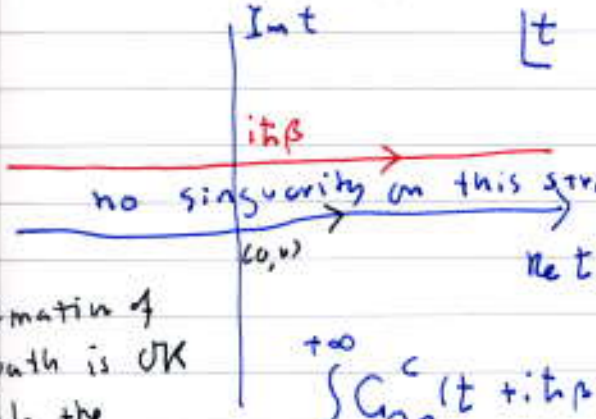
$$= \int_{-\infty}^{\infty} G^{<}_{\hat{A}\hat{B}}(t+i\hbar\beta)\, e^{i\frac{E}{\hbar}(t+i\hbar\beta)+\beta E}\, dt = -G^{>}_{\hat{A}\hat{B}}(E)$$

Here we make analytic continuation assuption

Since $G^<_{\hat{A}\hat{B}}(t)$ is defined on the complex plane

we can make the integral at real axis $\mathrm{Im}\, t = 0$

or at $t + i t_\beta$



We assume the integral on the complex path equal to that on real path. i.e. we assume

$$\int_{-\infty}^{+\infty} G^<_{\hat{A}\hat{B}}(t + i t_\beta) e^{i\frac{E}{\hbar}(t + i t_\beta)} dt = \int G^<_{\hat{A}\hat{B}}(t) e^{i\frac{E}{\hbar}t} dt$$

$$= G^<_{\hat{A}\hat{B}}(E)$$

Deformation of the path is OK provide the function is analytic inside it.

Thus we obtain

$$e^{\beta E} G^<_{\hat{A}\hat{B}}(E) = - G^>_{\hat{A}\hat{B}}(E)$$

$\hat{A} = c$ or c^+

$\hat{B} = c$ or c^+

Here $\hat{A}, \hat{B}$ are arbitrary operators like c, c^+. This expression agreed with the Lehmann representation argument which is more explicit. So in the Matsubara matrix form the equality is element wise, i.e.

$$G^<(E) = - e^{-\beta E} G^>(E)$$

$$G^{<,>} = \begin{matrix} \\ 1 \\ 2 \end{matrix} \begin{matrix} \begin{matrix} 1 & 2 \end{matrix} \\ \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} \end{matrix} \quad \begin{matrix} \\ s \\ s' \end{matrix}$$

Same as that on page 43 or 45.

The fluctuation-dissipation theorem is nothing but the Kubo-Martin-Schwinger condition in E space!

Surface Green's function of a Kitaev chain

We consider the simple 1D Kitaev chain with semi infinite end..

$$\hat{K} = \hat{H} - \mu \hat{N}$$

$$= -t\left(c_0^\dagger c_1 + c_1^\dagger c_2 + c_2^\dagger c_3 + \cdots \right) \Big\} + \text{h.c.}$$
$$- \Delta\left(c_0 c_1 + c_1 c_2 + c_2 c_3 + \cdots \right)$$
$$- \mu\left(c_0^\dagger c_0 + c_1^\dagger c_1 + c_2^\dagger c_2 + \cdots \right)$$

Let write in a more symmetric form by write half of $c_0^\dagger c_1$ as $-c_1 c_0^\dagger$, then

$$\hat{K} = -\frac{t}{2}\left(c_0^\dagger c_1 + c_1^\dagger c_2 + c_2^\dagger c_3 + \cdots \right.$$
$$\left. c_1^\dagger c_0 + c_2^\dagger c_1 + c_3^\dagger c_2 + \cdots \right)$$
$$+ \frac{t}{2}\left(c_1 c_0^\dagger + c_2 c_1^\dagger + c_3 c_2^\dagger + \cdots \right.$$
$$\left. c_0 c_1^\dagger + c_1 c_2^\dagger + c_2 c_3^\dagger + \cdots \right)$$
$$- \frac{\Delta}{2}\left(c_0 c_1 + c_1 c_2 + c_2 c_3 + \cdots \right)$$
$$+ \frac{\Delta}{2}\left(c_1 c_0 + c_2 c_1 + c_3 c_2 + \cdots \right)$$
$$- \frac{\Delta}{2}\left(c_1^\dagger c_0^\dagger + c_2^\dagger c_1^\dagger + c_3^\dagger c_2^\dagger + \cdots \right)$$
$$+ \frac{\Delta}{2}\left(c_0^\dagger c_1^\dagger + c_1^\dagger c_2^\dagger + c_2^\dagger c_3^\dagger + \cdots \right)$$
$$- \frac{\mu}{2}\left(c_0^\dagger c_0 + c_1^\dagger c_1 + c_2^\dagger c_2 + \cdots \right)$$
$$+ \frac{\mu}{2}\left(c_0 c_0^\dagger + c_1 c_1^\dagger + c_2 c_2^\dagger + \cdots \right) + \text{const}$$

$$= \frac{1}{2}\begin{pmatrix} c_0^\dagger & c_1^\dagger & c_2^\dagger & \cdots & c_0 & c_1 & \cdots \end{pmatrix}$$

$$\begin{array}{c} c^\dagger \\ \\ \\ \\ \\ \\ c \end{array}\begin{bmatrix} -\mu & -t & 0 & \cdots & 0 & \Delta & 0 & \cdots \\ -t & -\mu & -t & 0 & -\Delta & 0 & \Delta & 0 \\ 0 & -t & -\mu & \ddots & 0 & -\Delta & 0 & \Delta \\ 0 & 0 & -t & \ddots & \ddots & 0 & \ddots & \ddots \\ 0 & -\Delta & 0 & \cdots & \mu & t & 0 & \cdots \\ \Delta & 0 & -\Delta & 0 & t & \mu & t & 0 \\ 0 & \Delta & 0 & -\Delta & 0 & t & \mu & t \\ \vdots & \ddots & \ddots & \ddots & \cdots & 0 & t & \mu \end{bmatrix}\begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_0^\dagger \\ c_1^\dagger \\ \vdots \end{bmatrix}$$

or we write more compactly

$$\hat{K} = \hat{H} - \mu \hat{N} = \frac{1}{2}(c_i^\dagger \; c_i) \begin{pmatrix} h & -\Delta \\ \Delta & -h \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

$s=\uparrow \quad \downarrow$

Here $h = \begin{matrix} \\ 0 \\ 1 \\ 2 \\ \vdots \end{matrix} \begin{matrix} \begin{matrix} 0 & 1 & 2 & 3 \end{matrix} \\ \begin{bmatrix} -\mu & -t & 0 & 0 & \cdots \\ -t & -\mu & -t & 0 & \\ 0 & -t & -\mu & -t & \\ 0 & 0 & -t & & \end{bmatrix} \end{matrix}$ $\quad \Delta = \begin{bmatrix} 0 & -\Delta & 0 & 0 \\ \Delta & 0 & -\Delta & 0 \\ 0 & \Delta & 0 & -\Delta \\ 0 & 0 & \Delta & \ddots \end{bmatrix}$

Instead of using this form let regroup according site index j first then s index, ie. use

$$\Psi = \begin{pmatrix} c_0 \\ c_0^\dagger \\ c_1 \\ c_1^\dagger \\ c_2 \\ c_2^\dagger \\ \vdots \end{pmatrix}$$

Then equivalently we can write

$$\hat{K} = \frac{1}{2}\Psi^\dagger \begin{matrix} \\ 0 \\ 1 \\ 2 \\ 3 \\ \vdots \end{matrix} \begin{matrix} \begin{matrix} 0 & 1 & 2 & 3 & \cdots \end{matrix} \\ \begin{bmatrix} A & B^T & 0 & 0 & \cdots \\ B & A & B^T & 0 & \\ 0 & B & A & B^T & 0 \\ 0 & 0 & B & A & B^T \\ \vdots & \ddots & \ddots & \ddots & \end{bmatrix} \end{matrix} \Psi \equiv \frac{1}{2}\Psi^\dagger K \Psi$$

here $\begin{matrix} & c & c^\dagger \end{matrix}$

$$A = \begin{matrix} c \\ c^\dagger \end{matrix} \begin{bmatrix} -\mu & 0 \\ 0 & \mu \end{bmatrix}$$

$$B = \begin{bmatrix} -t & -\Delta \\ \Delta & t \end{bmatrix}$$

The retarded Green's function is

$$(E^{+i\eta} I - \tilde{K}) G^r = I$$

See page 219. $\tilde{K}$ is the above matrix

To solve this equation, let focus on the 1st colm of G^r

$$G^r = \begin{bmatrix} g_{00} & g_{01} \\ g_{10} & \vdots \\ g_{20} & \\ \vdots & \end{bmatrix} \qquad g_{j0} = \begin{bmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{bmatrix} \text{ is } 2\times 2$$

We are only interested in g_{00} which is the surface Green's function. write out explicitly the equations for the 1st column (or $j=0$ column) we get

$$((E+i\eta)I - A)g_{00} + B^T g_{10} = I \quad \leftarrow 2\times 2 \qquad (1)$$

for $j = 1, 2, 3, \cdots$

$$-B g_{j-1,0} + ((E+i\eta)I - A) g_{j0} + B^T g_{j+1,0} = 0 \qquad (2)$$

We seek trial solution of the form

$$g_{j0} = C\lambda^j \quad \text{where } C \text{ is } 2\times 2 \text{ matrix}$$

So we get $-BC\frac{1}{\lambda} + ((E+i\eta)I - A)C + B^T \lambda C = 0$

?! How to solve the equations !! Need a non zero solution $C \neq \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

Try find λ by

$$\det\left(\frac{1}{\lambda}B + ((E+i\eta)I - A) + \lambda B^T\right) = 0 \quad \leftarrow 2\times 2$$

Since the matrix is 2×2 we'll find two λ λ_1, λ_2 take the one with $|\lambda_i| < 1$. Hopefully the other one if $|\lambda| > 1$. Since $g_{j0} \to 0$ as $j \to \infty$ we can use $|\lambda| > 1$ solution

Then $((E+i\eta)I - A)C + B^T C\lambda = I$

$$C = \left((E+i\eta)I - A + \lambda B^T\right)^{-1} \leftarrow 2\times 2$$

$$\det\left(\frac{1}{\lambda}B + \cdots\right) = 0$$

It seems to me the condition is too weak to satisfy Eq (2)!

The explicit form of the $\det(\cdots) = 0$ is

$$-\left((\lambda + \tfrac{1}{\lambda})t + \mu + E\right)\left((\lambda + \tfrac{1}{\lambda})t + \mu - E\right) + (\lambda - \tfrac{1}{\lambda})^2 \Delta^2 = 0$$

This is a 4-th order polynomial in λ and will give up 4 different solutions.

Use iterative algorithm to get g_{00}? But that will give up only a numerical one. We should have a analytic one.

Let $x = \lambda + \frac{1}{\lambda}$ then we can reduce the equation to quadratic

$$x^2(t^2-\Delta^2) + 2\mu t x + \mu^2 - E^2 - 4\Delta^2 = 0$$

Let x be find then

$$\lambda^2 - x\lambda + 1 = 0 \quad \text{so} \quad \lambda_1, \lambda_2 = ?$$

$$\lambda = \frac{x \pm \sqrt{x^2-4}}{2}$$ indeed we have 4 solutions as we have two x values x_1, x_2.

$$x = \frac{-2\mu t \pm \sqrt{4\mu^2 t^2 - 4(t^2-\Delta^2)(\mu^2 - E^2 - 4\Delta^2)}}{2(t^2-\Delta^2)}.$$

Does this mean we need to write our solution as

$$g_{j0} = C_1 \lambda_1^j + C_2 \lambda_2^j + C_3 \lambda_3^j + C_4 \lambda_4^j$$

I think we can get rid of two as $|\lambda_3| > 1$, $|\lambda_4| > 1$.

It seems to me then I have trouble to determine C_i! ??

?? How to determine g_{00} as 2×2 matrix analytically ?

For the determinant equation, instead of solving λ given E, let do the reverse, given λ, find E, which is mathematically simpler. So the equation is

$$(\xi_\lambda - E)(-\xi_\lambda - E) + \Delta_\lambda^2 = 0$$

Here we introduce the notation

$$\xi_\lambda = -t\left(\lambda + \frac{1}{\lambda}\right) - \mu \equiv \varepsilon_\lambda - \mu, \qquad \lambda = e^{iq}$$

$$\varepsilon_\lambda = -2t\cos q$$

we allow $q \in \mathbb{C}$ so that $\lambda \in \mathbb{C}$ is arbitrary complex number. And we have defined

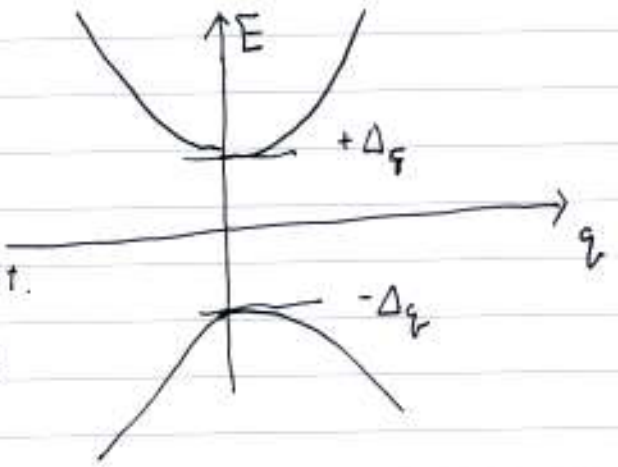
$$\Delta_\lambda^2 = -\left(\lambda - \frac{1}{\lambda}\right)^2 \Delta^2 = -\left(2i \sin q \cdot \Delta\right)^2 = 4\left(\sin^2 q\right)\Delta^2$$

is λ-dependent gap parameter, then $\Delta_\lambda = 2\Delta \sin q$

$$-\left(\xi_\lambda - E\right)\left(\xi_\lambda + E\right) - \Delta_\lambda^2 = 0$$

$$\rightarrow \quad E^2 - \xi_\lambda^2 - \Delta_\lambda^2 = 0 \quad \Rightarrow \quad E = \pm\sqrt{\xi_\lambda^2 + \Delta_\lambda^2}$$

This is nothing but the Bogoliubov superductor quasi-particle spectrum



Since $q = 0$ $\Delta_\lambda = 0$ it is gapless at Γ-point. otherwise gapped at $q \neq 0$.

Having worked on semi-infinite system for the Kitaev chain on surface Green's function we now consider bulk system, or finite system with $N \to +\infty$ and periodic boundary. Due to lattice periodicity, we can work in the momentum space, as in p-space the Hamilt is block diagonal. Our matrices will be small.

Take the model on page 51 with N site & periodic boundary condition

Here site N is equivalent to site 0

$$\hat{K} = \hat{N} - \mu \hat{N} = -t \sum_{j=0}^{N-1} \left(c_j^+ c_{j+1} + h.c. \right) - \mu \sum_{j=0}^{N-1} c_j^+ c_j$$

$$- \Delta \left(\sum_{j=0}^{N-1} c_j c_{j+1} + h.c. \right)$$

$$= -t \left(c_0^+ c_1 + c_1^+ c_2 + \cdots c_j^+ c_{j+1} + \cdots c_{N-1}^+ c_0 + h.c. \right)$$

$$- \mu \left(c_0^+ c_0 + c_1^+ c_1 + \cdots + c_{N-1}^+ c_{N-1} \right)$$

$$- \Delta \left(c_0 c_1 + c_1 c_2 + \cdots + c_{N-1} c_0 + h.c. \right)$$

For notational simplicity we set the lattice constant to $a = 1$, then the transform is

$$c_j = \frac{1}{\sqrt{N}} \sum_p \tilde{c}_p e^{ip \cdot j} \quad \rightarrow \quad c = U^\dagger \tilde{c} \quad \rightarrow \quad \tilde{c} = U c$$

$j = 0, 1, 2, \ldots N-1, \quad p = \frac{2\pi}{N} l \quad l = 0, 1, 2, \ldots N-1 \quad 0 \le p < 2\pi$

Going from c to $\tilde{c}$ is a unitary transform. One can check the commutation relation is the same in c or $\tilde{c}$.

i.e. $\tilde{c} \left(\tilde{c}^+ \right)^T + \text{permutation} = U c \left(c^+ \right)^T U^+ + \text{permutation}$

$$= U U^T = I$$

and $\tilde{c} \tilde{c}^T + \text{permutation} = 0$

$$\left(\tilde{c}^+ \right)^T \tilde{c}^+ + \text{permutation} = 0$$

Check this more carefully $\tilde{c}_i = \sum_k U_{ik} c_k$

$\tilde{C}(\tilde{C}^\dagger)^T$ + permutation really means $\begin{pmatrix} \tilde{C} \\ \vdots \end{pmatrix} (c_i^\dagger \cdots)$

$$\tilde{C}_i \tilde{C}_j^\dagger + \underbrace{\tilde{C}_j^\dagger \tilde{C}_i}_{\text{permute position of operators}} = \left(\sum_k U_{ik} c_k\right)\left(\sum_\ell U_{j\ell}^* c_\ell^\dagger\right) + \text{permutation}$$

$$= \sum_{k\ell} U_{ik} c_k c_\ell^\dagger U_{j\ell}^* + \sum_\ell U_{j\ell}^* c_\ell^\dagger \sum_k U_{ik} c_k$$

$$= \sum_{k\ell} U_{ik} \underbrace{\left(c_k c_\ell^\dagger + c_\ell^\dagger c_k\right)}_{=\delta_{k\ell}} U_{j\ell}^* = U \cdot I \cdot U^\dagger = U U^\dagger = I$$

$U_{j\ell}^* = (U^\dagger)_{\ell j}$

we see we have a correct MATMUL structure so the claim is valid.

similarly we can check $\tilde{C}_i \tilde{C}_j + \tilde{C}_j \tilde{C}_i = 0$ for all i, j

Conclusion — if we apply unitary transform to all annihilation operators $\tilde{c} = Uc$, new operators $\tilde{c}$ satisfy fermion operator definition. (This is not so if the transformation mixes c and $c^\dagger$.)??

Insert the Fourier transform, we find the particle number term is invariant in form

$$\sum_{j=0}^{N-1} c_j^\dagger c_j = \sum_{j=0}^{N-1} \frac{1}{N} \sum_p \tilde{c}_p^\dagger e^{-ipj} \sum_q \tilde{c}_q e^{iqj}$$

$$= \sum_{p,q} \tilde{c}_p^\dagger \tilde{c}_q \frac{1}{N} \sum_j e^{-i(q-p)j} = \sum_{pq} \tilde{c}_p^\dagger c_q \delta_{pq}$$

$$= \sum_p \tilde{c}_p^\dagger \tilde{c}_p$$

For the hopping term, we need shift by one lattice position, generate an extra phase

$$\sum_j c_j^\dagger c_{j+1} = \sum_{j=0}^{N-1} \frac{1}{N} \sum \tilde{c}_p^\dagger e^{-ipj} \sum_q \tilde{c}_q e^{iq(j+1)}$$

$$= \sum_p e^{ip} \tilde{c}_p^\dagger \tilde{c}_p$$

For the pairing interaction we get two c's not complex conjugate

$$\sum_j c_j c_{j+1} = \sum_j \frac{1}{N} \sum_p \tilde{c}_p e^{ipj} \sum_q \tilde{c}_q e^{iq(j+1)}$$

$$= \sum \tilde{c}_p \tilde{c}_q e^{iq} \underbrace{\delta(p+q)}_{\text{Kronecker } \delta} = \sum_p \tilde{c}_p \tilde{c}_{-p} e^{-ip}$$

$p+q=0$

Thus $$\hat{H} = -t \sum_p \left(e^{ip} + e^{-ip}\right) \tilde{c}_p^\dagger \tilde{c}_p - \mu \sum \tilde{c}_p^\dagger \tilde{c}_p$$

$$- \Delta \sum_p e^{-ip} \tilde{c}_p \tilde{c}_{-p} - \Delta \sum_p e^{ip} \tilde{c}_{-p}^\dagger \tilde{c}_p^\dagger$$

From now on we work in p-space so I will drop the tilde $\tilde{c} \to c$. It is in p-space as indicated by the subscript p.

We note the pairing interaction always couples p with $-p$ [Here $-p$ is the same as $-p+2\pi$, we'll work in the symmetric 1st BZ $-\pi \le p < \pi$]

It is then useful to look at p and $-p$ together. So we will do $\sum_{\text{all } p} = \sum_{p>0} + \sum_{p<0}$

We consider the Bogoliubov-de Gennes vector

$$\Psi_p = \begin{pmatrix} c_p \\ c_{-p}^+ \\ c_{-p} \\ c_p^+ \end{pmatrix}$$

here $p > 0$ only

so we have $\frac{N}{2} \cdot 4 = 2N$ operators of c and c^+.

this way, the sign of moment is made explicit c_p means $p > 0$ and c_{-p} means momenta less than 0.

We note

$$\Psi_p \left(\Psi_p^+\right)^T + \text{permutation} = \begin{pmatrix} c_p \\ c_{-p}^+ \\ c_{-p} \\ c_p^+ \end{pmatrix} \left(c_p^+ \; c_{-p} \; c_{-p}^+ \; c_p\right) + \text{permutation}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \qquad I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \text{ is } 2\times 2.$$

note $\{c_{-p}, c_p^+\} = 0$

similarly we find

$$\Psi_p \Psi_p^T + \text{permutation} = \begin{pmatrix} c_p \\ c_{-p}^+ \\ c_{-p} \\ c_{+p}^+ \end{pmatrix} \left(c_p \; c_{-p}^+ \; c_{-p} \; c_p^+\right) + \text{permutation}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} = \mathbb{1}_x \otimes \sigma_x$$

similarly for $\left(\Psi_p^+\right)^T \Psi_p^+ + \text{permutation} = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}$

I will call the anti-commutation relation

$$\{\psi, \psi^\dagger\} = I^{4\times 4} \qquad \{\psi, \psi\} = \{\psi, \psi^\dagger\} = \sigma_x \otimes \sigma_x$$

The fermionic structure as it is really a direct consequence of the c commutation relation $\{c, c^\dagger\} = I$

$$\{c, c\} = \{c^\dagger, c^\dagger\} = 0$$

Hamiltonian in p space is

$$\hat{H} = \sum_{\text{all } p} \xi_p c_p^\dagger c_p - \Delta \sum_{\text{all } p} e^{-ip} c_p c_{-p} - \Delta \sum_{\text{all } p} e^{ip} c_{-p}^\dagger c_p^\dagger$$

split $\sum_{\text{all } p} = \sum_{p>0} + \sum_{p<0}$ and for the 2nd sum we do $p \to -p$

then $\sum_{p>0} \xi_p c_p^\dagger c_p + \xi_{-p} c_{-p}^\dagger c_{-p} - \Delta \sum_{p>0} \left(e^{-ip} c_p c_{-p} + e^{ip} c_{-p} c_p \right)$

$$- \Delta \sum_{p>0} \left(e^{ip} c_{-p}^\dagger c_p^\dagger + e^{-ip} c_p^\dagger c_{-p}^\dagger \right)$$

use $\xi_p = \xi_{-p} = -2t\cos(p) - \mu$

= and define $\Delta_p = [2\sin(p)] \cdot \Delta$

$$\hat{H} = \sum_{p>0} \xi_p \left(c_p^\dagger c_p + c_{-p}^\dagger c_{-p} \right) + i \sum_{p>0} \Delta_p c_p c_{-p} - i \sum_{p>0} \Delta_p c_{-p}^\dagger c_p^\dagger$$

[Here we split half into a more symmetric form so

$$c_p^\dagger c_p = \tfrac{1}{2} c_p^\dagger c_p - \tfrac{1}{2} c_p c_p^\dagger + \text{const}$$

similarly $c_p c_{-p} = \tfrac{1}{2} c_p c_{-p} - \tfrac{1}{2} c_{-p} c_p$]

we could get rid of the "i" here if we perform a gauge transform $c_p \to e^{i\frac{\pi}{4}} c_p$ + const

we can then express as

$$\hat{H} = \sum_{p>0} \begin{pmatrix} c_p^\dagger & c_{-p} \end{pmatrix} \begin{pmatrix} \xi_p & i\Delta_p \\ -i\Delta_p & -\xi_p \end{pmatrix} \begin{pmatrix} c_p \\ c_{-p}^\dagger \end{pmatrix}$$

$$\phi \equiv \begin{pmatrix} c_p \\ c_{-p}^\dagger \end{pmatrix}, \quad \{\phi, \phi^\dagger\} = I \quad \{\phi, \phi\} = 0$$

It is tempting to diagonalize this matrix of 2×2

we get

$$\phi^\dagger H \phi = \phi^\dagger S^\dagger H S S^\dagger \phi = \gamma^\dagger \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \gamma$$

Here $H = \begin{bmatrix} \xi_k & i\Delta_k \\ -i\Delta_k & -\xi_k \end{bmatrix}$ with eigen values $\det(EI - H) = 0$

omit k

or $\det \begin{pmatrix} E-\xi & -i\Delta \\ i\Delta & E+\xi \end{pmatrix} = 0 \Rightarrow (E-\xi)(E+\xi) - \Delta^2 = 0$

or $E^2 - \xi^2 - \Delta^2 = 0 \Rightarrow E = \pm\sqrt{\xi^2+\Delta^2}$

with the unitary matrix [See page 77 later for S]

$$S = \begin{bmatrix} ia\Delta & ib\Delta \\ a(E-\xi) & -b(E+\xi) \end{bmatrix} \qquad \Delta \equiv \Delta_k \quad E \equiv E_k \quad \xi \equiv \xi_k$$

$$a = \frac{1}{\sqrt{\Delta^2 + (E-\xi)^2}}$$

The trouble with this is that γ is NOT fermion.

$$\begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} \equiv \begin{bmatrix} \gamma_p \\ \gamma_{-p}^\dagger \end{bmatrix} = S \begin{bmatrix} c_p \\ c_{-p}^\dagger \end{bmatrix}$$

This is because p and $-p$ are thoroughly mixed.

WRONG!

Check $\gamma_p = ia\Delta\, c_p + ib\Delta\, c_{-p}^\dagger$

we have $\{c_p, c_{-p}\} = c_p c_{-p} + c_{-p} c_p = 0$

but $\{\gamma_p, \gamma_{-p}\} = \gamma_p \gamma_{-p} + \gamma_{-p}\gamma_p$

$= 2ab\Delta^2 \neq 0.$

So, a unitary transform with mixing c_i and $c_i^\dagger$ and p and $-p$ do not lead to a fermi operator.

Alternatively, we can use $\Psi_p = \begin{pmatrix} c_p \\ c_{-p}^+ \\ c_{-p} \\ c_p^+ \end{pmatrix}$

Then we can write the Hamiltn as

$$\hat{H} = \sum_{p>0} \frac{1}{2} \Psi_p^+ \left(\begin{array}{cc|cc} \xi_k & i\Delta_k & 0 & 0 \\ -i\Delta_k & -\xi_k & 0 & 0 \\ \hline 0 & 0 & \xi_k & -i\Delta_k \\ 0 & 0 & i\Delta_k & -\xi_k \end{array}\right) \Psi_p$$

$$= \sum_{p>0} \frac{1}{2} \Psi_p^+ \begin{pmatrix} H_{11} & 0 \\ 0 & H_{11}^T \end{pmatrix} \Psi_p$$

Since $H_{11} \neq H_{11}^T$ we have to do Hamiltn to diagonalise

But clearly H_{11} and H_{11}^T are trivially related!

so let consider $\begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \gamma_4 \end{pmatrix} = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{22} \end{pmatrix} \Psi_p$

Here $S_{11} S_{11}^+ = I$

$S_{22} S_{22}^+ = I$

which diagonalise the matrix as

$\begin{pmatrix} E & 0 & 0 & 0 \\ 0 & -E & 0 & 0 \\ 0 & 0 & E & 0 \\ 0 & 0 & 0 & -E \end{pmatrix}$

But $S_{11} S_{22}^+ \neq I$ as a result γ is not fermion in the sense

WRONG!

$\{\gamma, \gamma^+\} = I, \quad \{\gamma, \gamma\} = \sigma_x \otimes \sigma_x$

This leads up to the conclusion that we must use Bogoliubov transform. i.e. $S S^+ = I$ also

$p>0$, $\begin{pmatrix} \gamma_p \\ \gamma_{-p}^+ \\ \gamma_{-p} \\ \gamma_p^+ \end{pmatrix} = \begin{pmatrix} u_p & -v_p & 0 & 0 \\ +v_p & u_p & 0 & 0 \\ 0 & 0 & u_p & +v_p \\ 0 & 0 & -v_p & u_p \end{pmatrix} \begin{pmatrix} c_p \\ c_{-p}^+ \\ c_{-p} \\ c_p^+ \end{pmatrix} = \begin{pmatrix} S & 0 \\ 0 & S^+ \end{pmatrix} \Psi_p$

$\downarrow$ $u_p = u_p$, $v_p = -v_{-p}$

take minus sign

The claim here is with the Bogoliubov transform

$$\gamma_p = u_p c_p \underline{+} v_p c_{-p}^+$$

as well other γ_{-p}, γ_p^+, γ_{-p}^+, which is already implied by this equation if we assume u_p symmetric
v_p anti symmetric in p.

Then γ is fermionic!

please check this. However with $\gamma = U^\dagger \psi$

$$U = \begin{bmatrix} S & 0 \\ 0 & S^T \end{bmatrix} \qquad U^\dagger H U \text{ is not diagonal.}$$

$u^2 + v^2 = 1$ since $SS^+ = 1$, we choose u & v such that the offdiagonal terms is set to 0.

check anti-commutation relation. focus on $|\vec{p}|$ of a given value Let $c = c_p$ $d^+ = c_{-p}^+$

$$\begin{pmatrix} \gamma_p \\ \gamma_{-p}^+ \end{pmatrix} = \begin{pmatrix} \gamma \\ \delta^+ \end{pmatrix} = \begin{pmatrix} u & -v \\ +v & u \end{pmatrix} \begin{pmatrix} c \\ d^+ \end{pmatrix} \rightarrow \qquad \begin{pmatrix} c \\ d^+ \end{pmatrix} = \begin{pmatrix} u & v \\ -v & u \end{pmatrix} \begin{pmatrix} \gamma \\ \delta^+ \end{pmatrix}$$

and $$\begin{pmatrix} \gamma^+ \\ \delta \end{pmatrix} = \begin{pmatrix} u & -v \\ +v & u \end{pmatrix} \begin{pmatrix} c^+ \\ d \end{pmatrix}$$

With some patience, it can be checked that all required commutation rules is valid. i.e.

$$\gamma^2 = \delta^2 = (\delta^+)^2 = (\delta^+)^2 = 0$$

$$\gamma\gamma^+ + \gamma^+\gamma = 1, \qquad \delta\delta^+ + \delta^+\delta = 1$$

$$\gamma\delta + \delta\gamma = 0, \qquad \gamma\delta^+ + \delta^+\gamma = 0, \quad \text{etc.}$$

Fellow Tinkham Eq (3.63) & (3.42) we use a minus sign here

$$\gamma_p = u_p c_p - v_p c_{-p}^+$$

$\gamma_{p0} = \gamma_p$

$\gamma_{p1} = +\gamma_{-p}$ $p > 0$

so $$c_p = u_p \gamma_p + v_p \gamma_{-p}^+$$

14 Nov 2018

Diagonalize the superconductor BdG Hamiltonian

$$H = \begin{bmatrix} \xi & \Delta^* \\ \Delta & -\xi \end{bmatrix}$$

both $\xi \equiv \xi_p$ $\Delta \equiv \Delta_p$ depends on $p > 0$ and Δ is complex

ξ is even in p $E \equiv E_p$ as well

Δ is odd in p

$\Delta \equiv -i\,\Delta_p = -i\,\Delta\, 2\sin(p)$

Eigenvalue problem is $\begin{bmatrix} \xi & \Delta^* \\ \Delta & -\xi \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \pm E \begin{bmatrix} a \\ b \end{bmatrix}$ or $H\begin{bmatrix} a \\ b \end{bmatrix} = \pm E \begin{bmatrix} a \\ b \end{bmatrix}$

$E = \sqrt{\xi^2 + |\Delta|^2} \geq 0$

For the positive eigenvalue $\begin{bmatrix} \xi & \Delta^* \\ \Delta & -\xi \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = E\begin{bmatrix} a \\ b \end{bmatrix}$

or $\begin{bmatrix} \xi - E & \Delta^* \\ \Delta & -(\xi + E) \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ we take $\begin{bmatrix} a \\ b \end{bmatrix} = \begin{pmatrix} \Delta^* \\ E - \xi \end{pmatrix}\frac{1}{\sqrt{\cdots}}$

for $-E$ $\begin{bmatrix} \xi & \Delta^* \\ \Delta & -\xi \end{bmatrix}\begin{bmatrix} a' \\ b' \end{bmatrix} = -E\begin{bmatrix} a \\ b \end{bmatrix}$ or $\begin{bmatrix} \xi + E & \Delta^* \\ \Delta & E - \xi \end{bmatrix}\begin{bmatrix} a' \\ b' \end{bmatrix} = \begin{bmatrix} a \\ 0 \end{bmatrix}$

we take $\begin{bmatrix} a' \\ b' \end{bmatrix} = \begin{bmatrix} \xi - E \\ \Delta \end{bmatrix}\frac{1}{\sqrt{|\Delta|^2 + (E-\xi)^2}}$

$\rightarrow |\Delta|^2 + E^2 - 2\xi E + \xi^2$

$= |\Delta|^2 + \xi^2 + |\Delta|^2 - 2\xi E + \xi^2$

$= 2(|\Delta|^2 + \xi^2 - \xi E)$

$= 2(E - \xi)E$

So $S = \begin{pmatrix} \Delta^* & -(E-\xi) \\ E - \xi & \Delta \end{pmatrix}\frac{1}{\sqrt{2E(E-\xi)}}$

$= \begin{pmatrix} u^* & v \\ -v & u \end{pmatrix}$ we identify the unitary transformation

with $u = \dfrac{\Delta}{\sqrt{2E(E-\xi)}}$ $v = \dfrac{-(E-\xi)}{\sqrt{2E(E-\xi)}}$ $u_p = -u_p$ $v_p = v_{-p}$

note v is real but u is complex so

$v^2 = |v|^2 = \dfrac{(E-\xi)^2}{2E(E-\xi)} = \dfrac{E-\xi}{2E} = \frac{1}{2}\left(1 - \frac{\xi}{E}\right)$

since $|u|^2 + |v|^2 = 1$

$|u|^2 = \frac{1}{2}\left(1 + \frac{\xi}{E}\right)$

$u v = \frac{\Delta^*}{2E}$ with S find such that the diagonalization is accomplished

$$S^\dagger H S = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$$

Let $$\gamma = \begin{pmatrix} \gamma_p \\ \gamma_{-p}^\dagger \end{pmatrix} = S^\dagger \begin{pmatrix} c_p \\ c_{-p}^\dagger \end{pmatrix} = \begin{pmatrix} u & -v \\ v & u^* \end{pmatrix} \begin{pmatrix} c_p \\ c_{-p}^\dagger \end{pmatrix} = S^\dagger \phi$$

$S S^\dagger = I$
so $|u|^2 + |v|^2 = 1$

So that

$$\hat{H} = \sum_{p>0} \phi_p^\dagger H_p \phi_p = \sum_{p>0} \phi_p^\dagger S S^\dagger H S \underbrace{S^\dagger \phi_p}_{\gamma}$$

$$= \sum_{p>0} \gamma_p^\dagger \begin{pmatrix} E_p & 0 \\ 0 & -E_p \end{pmatrix} \gamma_p = \sum_{p>0} (\gamma_p^\dagger \ \gamma_{-p}) \begin{pmatrix} E_p & 0 \\ 0 & E_{-p} \end{pmatrix} \begin{pmatrix} \gamma_p \\ \gamma_{-p}^\dagger \end{pmatrix}$$

$$= \sum_{p>0} \left(E_p \gamma_p^\dagger \gamma_p - E_p \gamma_{-p} \gamma_{-p}^\dagger \right)$$

Here we have defined $E_{-p} = +E_p = \sqrt{\xi_p^2 + \Delta_p^2}$. We need to check γ has correct commutation relation

$$\gamma_p \gamma_{-p} + \gamma_{-p} \gamma_p = (u_p c_p - v_p c_{-p}^\dagger)(u_{-p} c_{-p} - v_{-p} c_p^\dagger) + \ldots$$

$$= u_p u_{-p} \underbrace{(c_p c_{-p} + c_{-p} c_p)}_{=0} + v_p v_{-p} (c_{-p}^\dagger c_p^\dagger + c_p^\dagger c_{-p}^\dagger)_{=0}$$

$$- u_p v_{-p} \underbrace{(c_p c_p^\dagger + c_p^\dagger c_p)}_{=1} - v_p u_{-p} \underbrace{(c_{-p}^\dagger c_{-p} + c_{-p} c_{-p}^\dagger)}_{=1}$$

$$= -(u_p v_{-p} + u_{-p} v_p) \qquad \begin{matrix} u \text{ is odd} \\ v \text{ is even} \end{matrix} \Big\} \text{in } p$$

$$= -(+u_p v_p - u_p v_p) = 0 \quad \text{checked!}$$

2nd term is $-E_p \gamma_{-p} \gamma_{-p}^\dagger = E_p \gamma_{-p}^\dagger \gamma_{-p} + \text{const}$

Use $$\sum_{p>0} (E_p \gamma_p^\dagger \gamma_p + E_p \gamma_{-p}^\dagger \gamma_{-p}) = \sum_{\text{all } p} E_p \gamma_p^\dagger \gamma_p$$

This is standard free particle form.

The BCS ground state $|BCS\rangle$

we define $|BCS\rangle$ the vacuum state of operator γ

i.e. $\gamma_p |BCS\rangle = 0$ for all p ($p>0$ and $p<0$)

How we express $|BCS\rangle$ in terms of vacuum of C operator?

$$C_p |0\rangle = 0 \quad \text{for all } p$$

It turns out there is an explicit expression, which is given by Barden, Cooper, Schrieffer

$$|BCS\rangle = \prod_{p>0} (u_p + v_p C_p^+ C_{-p}^+) |0\rangle$$

Here we need the restriction $p>0$ as $C_p^+ C_{-p}^+ = -C_{-p}^+ C_p^+$ is creating the same states. Since $V_p = +V_{-p}$ without this restriction we get a 0.

$$(V_p C_p^+ C_{-p}^+ + V_{-p} C_{-p}^+ C_p^+) |0\rangle = 0$$

as $V_{-p} = V_p$

Thus the eigenvalue problem of Hamiltonian $\hat{K}$ on page 61, 65, ... is solved. The set of all $2^{|N|}$ states (eigenstates of $\hat{K}$ which are orthonormal) is

$$|\psi\rangle = (\gamma_0^+)^{n_0} (\gamma_1^+)^{n_1} \cdots (\gamma_p^+)^{n_p} \cdots (\gamma_{-p}^+)^{n_{-p}} \cdots |BCS\rangle$$

here $n_p = 0$ or 1

Its energy is $E = \sum_{\text{all } p} n_p E_p$. In this notation or convention, the ground state energy for $|BCS\rangle$ is 0.

$$\hat{H} |BCS\rangle = 0$$

A quantum dots model

$$\hat{H} = \epsilon\left(c_1^+ c_1 + c_2^+ c_2\right) + \Delta\left(c_1 c_2 + c_2^+ c_1^+\right)$$

This Hamiltonian acts on the 4-dimensional Fock space spanned by

$|\varphi_0\rangle = |0\rangle$ no particle

$|\varphi_1\rangle = c_1^+|0\rangle$, $|\varphi_2\rangle = c_2^+|0\rangle$ } 1 particle

$|\varphi_3\rangle = c_1^+ c_2^+|0\rangle$ } two particles

So $\hat{H}$ can be represented as 4×4 matrix

$$H_{ij} = \langle\varphi_i|\hat{H}|\varphi_j\rangle \qquad i,j = 0,1,2,3$$

$$\hat{H} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \end{array}\begin{array}{c} \begin{array}{cccc} 0 & 1 & 2 & 3 \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & -\Delta \\ 0 & \epsilon & 0 & 0 \\ 0 & 0 & \epsilon & 0 \\ -\Delta & 0 & 0 & 2\epsilon \end{bmatrix} \end{array}$$

Note the Δ term mixes vacuum $|0\rangle$ and two particle state $|\varphi_3\rangle$

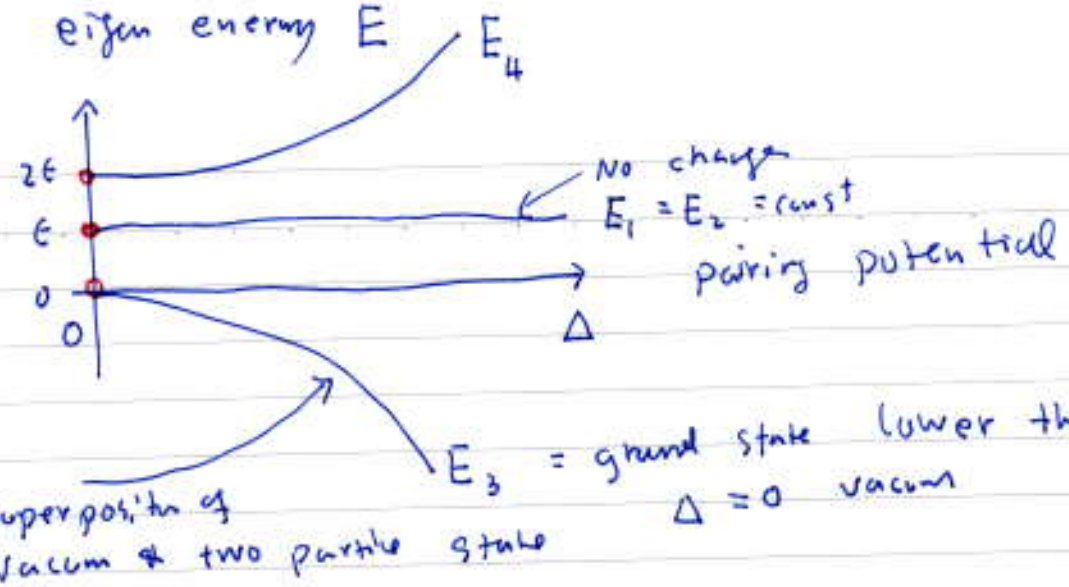
The 4 eigenvalues & vectors are

$$E_1 = \epsilon, \quad \psi_1 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \qquad E_2 = \epsilon, \quad \psi_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

$$E_3 = \epsilon - \sqrt{\epsilon^2+\Delta^2}, \quad \psi_3 = \begin{bmatrix} \Delta \\ 0 \\ 0 \\ \sqrt{\epsilon^2+\Delta^2} - \epsilon \end{bmatrix} \frac{1}{\sqrt{2\left(\Delta^2+\epsilon^2-2\epsilon\sqrt{\epsilon^2+\Delta^2}\right)}}$$

$$E_4 = \epsilon + \sqrt{\epsilon^2+\Delta^2}, \quad \psi_4 = \begin{bmatrix} \epsilon - \sqrt{\epsilon^2+\Delta^2} \\ 0 \\ 0 \\ \Delta \end{bmatrix} \frac{1}{\sqrt{\cdots}}$$

We see $|0\rangle$ is not an eigenstate, and superposition of $|0\rangle$ and $|\varphi_3\rangle$ produced lower energy. Very much like BCS state.



$\Psi_3 = \alpha|0\rangle + \beta|1,1\rangle$

London penetration depth $\lambda = \sqrt{\frac{m}{ne^2\mu_0}}$, plasma frequency $\omega_p = \sqrt{\frac{ne^2}{m\varepsilon_0}}$

So $\lambda\omega_p = c$ is speed of light.

London equation $\vec{j} = -\frac{ne^2}{m}\vec{A}$ $(\vec{\nabla}\cdot\vec{A}=0)$

correlation length $\xi_0 \approx \frac{\hbar v_F}{\Delta}$

BCS theory – gap equation

The BdG Hamiltonian, in the bilinear Hamiltonian of general form containing cc & c^+c^+ are considered not a fundamental Hamiltn, rather, they are a result of mean-field approximation. To motivate the Coulomb interaction with a negative interaction, we introduce the Cooper operator $b_p^+ = c_p^+ c_{-p}^+$

thus $b_p = c_{-p} c_p$

If $p \neq q$ they all commute so they behave like bosons

$$[b_p, b_q^+] = 0$$

$$[b_p, b_q] = 0$$

$$[b_p^+, b_q^+] = 0$$

For $p = q$ it does not follow bosonic operator

$[b_p, b_p^+] \neq 1$, they are more like fermion

in the sense $b_p^2 = 0 \quad (b_p^+)^2 = 0$

sense $b_p^2 = c_{-p} c_p c_{-p} c_p = -c_{-p} c_{-p} c_p c_p = 0$

Never theless $b_p^+ b_p = c_p^+ c_{-p}^+ c_{-p} c_p = c_p^+ (-c_{-p} c_{-p}^+ + 1) c_p$

$= - c_p^+ c_{-p} c_{-p}^+ c_p + c_p^+ c_p$

take $p \to -p$ $\quad b_{-p}^+ b_{-p} = - c_p^+ c_p \, c_{-p} c_{-p}^+ + c_{-p}^+ c_{-p}$

$b_{-p} = c_p c_{-p} = - c_{-p} c_p = - b_p$ is anti symmetric

$c_p^+ c_p$

we have instead $\quad //$

$[b_p, b_p^+] = b_p b_p^+ - b_p^+ b_p = 1 - n_p - n_{-p}$

ie. $b_p^+ b_p = c_{+p}^+ c_{+p} - c_p^+ c_p \, c_{-p} c_{-p}^+$

Similarly $b_p b_p^+ = c_{-p} c_p \, c_p^+ c_{-p}^+ = c_{-p} (- c_p^+ c_p + 1) c_{-p}^+$

$= c_{-p} c_{-p}^+ - c_{-p} c_p^+ c_p c_{-p}^+$

$= - c_{-p}^+ c_{-p} + 1 - c_p^+ c_p \, c_{-p} c_{-p}^+$

The above commutation relation can be proved.

Consider subspace of the Fock space which is always in pair of electron of p and $-p$ i.e. state of the form $\quad \prod_p (b_p^+)^{n_p} |0\rangle \qquad n_p = 0, 1$

then $b_p b_p^+$ action on it is 0. ??

then we can say $\quad n_p + n_{-p} \simeq 2 b_p^+ b_p$?

The BCS reduced Hamilton is then

$$H_{BCS}^{red} = \underbrace{\sum_{p>0} 2\xi_p b_p^+ b_p}_{\text{free pair}} + \sum_{pq} V_{pq} b_p^+ b_q$$

The second term is the BCS interaction which represents a scattering from state p into q, But we'll not use the first term as consider only

$$H^{BCS} = \sum_{\text{all } p} \xi_p c_p^+ c_p + \sum_{p,q>0} V_{pq} c_p^+ c_{-p}^+ c_{-q} c_q$$

$$\| \quad K$$

Now we see H^{BCS} is particle number conserving. The Hamilton is diagonal (Block diagonal) in the particle number N. However the mean-field approximation break the particle number conservation

Mean-field approximation

$$c_p^+ c_{-p}^+ c_{-q} c_q \to \langle c_p^+ c_{-p}^+ \rangle c_{-q} c_{+q} + c_p^+ c_{-p}^+ \langle c_{-q} c_q \rangle$$

We ignore the usual "Hartree" and "Fock" terms.

i.e. $c_p^+ \langle c_{-p}^+ c_{-q} \rangle c_q$ or $c_{-p}^+ \langle c_p^+ c_{-q} \rangle c_q$

Compare this mean-field approximation with that on page 69, we get

$$i \sum_{p>0} \Delta_p c_p c_{-p} \sim \sum_{pq>0} V_{pq} \langle c_p^+ c_{-p}^+ \rangle c_{-q} c_q$$

swap $p \leftrightarrow q$

$$= \sum_{qp>0} V_{qp} \langle c_q^+ c_{-q}^+ \rangle \underbrace{c_{-p} c_p}_{-c_p c_{-p}}$$

$$= \sum \left(-\sum V_{qp} \langle c_q^+ c_{-q}^+ \rangle \right) c_p c_{-p}$$

Thus we find $i\Delta_p = -\sum_q V_{qp} \langle C_q^+ C_{-q}^+ \rangle$ $\quad p>0,\ q>0$

To calculate the average $\langle \dots \rangle$ we can use the Green's function, but since it is at equal time, we don't really need the machinery. Using γ variables which is diagonal we find

$$\gamma_p = u_p C_p - V_p C_{-p}^+$$

$$\gamma_{-p}^+ = u_{-p}^* C_{-p}^+ - V_{-p}^* C_p = -u_p^* - V_p C_p$$

$$\text{So} \quad \begin{pmatrix} \gamma_p \\ \gamma_{-p}^+ \end{pmatrix} = \begin{pmatrix} u & -V \\ -V & -u^* \end{pmatrix} \begin{pmatrix} C_p \\ C_p^+ \end{pmatrix}$$

According to the expression for u & V, V is real and symmetric in p and u is complex and antisymmetric in p. see page 77. Then

$$\begin{pmatrix} C_p \\ C_{-p}^+ \end{pmatrix} = \begin{pmatrix} u^* & -V \\ -V & -u \end{pmatrix} \begin{pmatrix} \gamma_p \\ \gamma_{-p}^+ \end{pmatrix}$$

This differ from standard convention because of i in the pair term.

or $\quad C_{-q}^+ = -V_q \gamma_q - u_q \gamma_{-q}^+ \qquad u_q \equiv -u_{-q}$

$\qquad C_q^+ = -V_q \gamma_{-q} + u_q \gamma_q^+ \qquad V_q = V_q$

$$\langle C_q^+ C_{-q}^+ \rangle = \langle (-V_q \gamma_{-q} + u_q \gamma_q^+)(-V_q \gamma_q - u_q \gamma_q^+) \rangle$$

$$= +V_q u_q \langle \gamma_{-q} \gamma_{-q}^+ \rangle - V_q u_q \langle \gamma_q^+ \gamma_q \rangle$$

$$= V_q u_q [1 - f_{q_r} - f_q]$$

Note $\langle \gamma\gamma \rangle = \langle \gamma^+ \gamma^+ \rangle = 0$

$$= V_q u_q (1 - 2 f_q)$$

$$f_q \equiv \frac{1}{e^{\beta E_q} + 1} \qquad E_q = \sqrt{\xi_q^2 + \Delta_q^2}$$

on page we find $uv = \frac{\Delta^*}{2E} = \frac{(-i\Delta_q)^*}{2E_q} = \frac{i\Delta_q}{2E_q}$

so we obtain (cancel the i)

$$\Delta_p = -\sum_{q>0} V_{qp} \frac{\Delta_q}{2E_q}(1-2f_q)$$

$$1-2f = 1 - \frac{2}{e^{\beta E_q}+1} = \frac{e^{\beta E_q}+1-2}{e^{\beta E_q}+1} = \frac{e^{\beta E_q}-1}{e^{\beta E_q}+1}$$

$$= \frac{e^{\beta E_q/2} - e^{-\beta E_q/2}}{e^{\beta E_q/2} + e^{-\beta E_q/2}} = \tanh\left(\beta \frac{E_q}{2}\right).$$

or $$\Delta_p = -\sum_q V_{qp} \frac{\Delta_q}{2E_q} \cdot \tanh\left(\beta \frac{E_q}{2}\right)$$

This is the famous BCS theory gap equation to determine Δ_p assuming scattering potential V_{qp} is known (usually assumed a constant $V_{qp} = V^0$)

BCS variational determination of superconductor ground state $|BCS\rangle$.

The BCS form, $|BCS\rangle = \prod_{p>0} (u_p + v_p b_p^+)|0\rangle$,

where $b_p^+ = c_p^+ c_{-p}^+$ is considered a trial wave function with variational parameters u & v.

It is clear since b_p^+ is Bosonic like if p values are distinct all the factors $u + v b_p^+$ commute with each other, the order does not matter. Focusing on a particular value p

$b^\dagger = c_p^\dagger c_{-p}^\dagger$

we see

$\langle BCS|BCS\rangle = 1 = \langle 0|\ldots\ldots(u^* + v^* b)(u + v b^\dagger)\ldots|0\rangle$

so the p term is $|u|^2 + v^* u\, b + u^* v\, b^\dagger + |v|^2 b\, b^\dagger$

move b to the right most annihilate the vacuum (since b commute with all other factors which has a different p.)

$b|0\rangle = c_{-p} c_p |0\rangle = 0$

similarly move $b^\dagger$ to left-most $\langle 0|b^\dagger = 0$

$|v|^2$ is $\langle 0|\, c_{-p} c_p\, c_p^\dagger c_{-p}^\dagger |0\rangle = \| b^\dagger|0\rangle \|^2 = 1$

or $\langle 0|\, c_{-p}\left[-c_p^\dagger c_p + 1\right] c_{-p}^\dagger |0\rangle$

$= \langle 0| c_{-p} c_{-p}^\dagger |0\rangle - \langle 0|\, c_{-p} c_p^\dagger c_p c_{-p}^\dagger |0\rangle$ $= 1$

$= \langle 0|\left(-c_p^\dagger c_p + 1\right)|0\rangle + \langle 0|\, c_{-p} c_p^\dagger c_{-p}^\dagger c_p |0\rangle$ $\to 0$

$\langle 0|\left(-c_p^\dagger c_p + 1\right)|0\rangle = 0$

we find $\langle BCS|BCS\rangle = \prod_{p>0}\left(|u_p|^2 + |v_p|^2\right)$

For a normalized wave function, we demand

$|u_p|^2 + |v_p|^2 = 1$

Since $|BCS\rangle$ and $e^{i\phi}|BCS\rangle$ ϕ real is equivalent, we can make u or v real. Let's assume we take v to be real. Why is BCS theory we can also make both real simultaneously?

Given the form of $|BCS\rangle$, we compute

$K^{BCS} = \sum_p{}^{\text{all } p \text{ or } p<0}_{p>0}\, \xi_p c_p^\dagger c_p + \sum_{p,q \text{ restricted to } p>0,\ q>0} V_{pq}\, c_p^\dagger c_{-p}^\dagger c_{-q} c_q$

or NOT?

the expectation value $\langle BCS|\, K^{BCS}\, |BCS\rangle$ and then

$b_p^+ = c_p^+ c_{-p}^+$

minimize the energy with respect to u and v.

Kinetic energy term

$$\langle 0| \cdots (u_p^* + v_p^* b_p) c_p^+ c_p (u_p + v_p b_p^+) \cdots |0\rangle \quad p>0$$

$$\langle 0| \cdots \left(|u|^2 c_p^+ c_p + |v|^2 \underbrace{b_p b_p^+}_{c_p^+ c_p} + u_p^* v_p c_p^+ c_p b_p^+ + v_p^* u_p b_p c_p^+ c_p\right) \cdots |0\rangle$$

$$= \langle 0| \cdots |u^2| \overset{=0}{c_p^+ c_p |0\rangle} + |v|^2 \langle 0| b_p (-c_p c_p^+ + 1) b_p^+ |0\rangle$$

// $c_p^+ b_p^+ = 0$ $\quad b_p = c_p c_p$

$|v|^2$

$$\langle 0| u_p^* v_p [-c_p c_p^+ + 1] b_p^+ |0\rangle \quad v_p^* u_p b_p (-c_p c_p^+ + 1) |0\rangle = 0$$

$\searrow 0$ $\quad b_p c_p = 0$

so $\langle BCS| \sum_p \xi_p c_p^+ c_p |BCS\rangle = \sum_{\text{all } p} \xi_p |v_p|^2 = \sum_{p>0} 2\xi_p |v_p|^2$ Note for $-p<0$ $b_{-p} = -b_p$

Unlike the usual BCS which has $\prod_{\text{all } p} (u + v b^+)$ the result is the same. We don't have a factor of 2 here. The 2 due to spin degeneracy and we don't have a spin here.

The interaction term

$$\langle 0| \cdots (u_p^* + v_p^* b_p) \cdots (u_q^* + v_q^* b_q) b_p^+ b_q (u_q + v_q b_q^+) (u_p + v_p b_p^+)$$

Since p & q commute we group p & q separately

$$\underbrace{(u^* + v^* b) b^+ (u + v b^+)}_{p \text{ term}} \cdots \underbrace{(u^* + v^* b) b (u + v b^+)}_{q \text{ term}}$$

$(b^+) = 0$ $\quad b^2 = 0$

$$|u|^2 b^+ + (v^* u) \underset{\sim}{b b^+} \qquad \langle 0| u^* (u b + v b b^+) |0\rangle$$

Note $\langle 0|\, b\, b^\dagger |0\rangle = \| b^\dagger|0\rangle \| = 1$ $\quad$ use $(b^\dagger) = 0$

so we find

$$\langle BCS|\, b_p^\dagger b_q \,|BCS\rangle = \langle BCS|\, C_p^\dagger C_{-p}^\dagger C_{-q} C_q \,|BCS\rangle$$

$$= (V_p^* u_p)(v_q u_q^*) \;\rightsquigarrow\; \bar{r}\cdot \quad u_p v_p^* u_q^* v_q$$

$p>0$ & $p<0$ have same energy

Putting together we get

$$\langle BCS|\, \hat{K}^{BCS} \,|BCS\rangle = 2\sum_{p>0} \xi_p^p |v_p|^2 + \sum_{pq>0} V_{pq}\, u_p v_p^*\, u_q^* v_q$$

Let choose V and u all real (why possible)

$$\bar{E} = 2\sum_{p>0} \xi_p v_p^2 + \sum_{pq>0} V_{pq}\, u_p v_p\, u_q v_q$$

let vary δu δv, subject to $u^2+v^2 = 1$ $\quad V_{pq}$ real

$$\delta(u^2+v^2) = 0$$

$$\delta\tilde{E} = 2\sum_p \xi_p 2v_p \delta v_p + \sum_{pq} V_{pq}\big[\delta u_p v_p u_q v_q + u_p \delta v_p u_q v_q + u_p v_p \delta u_q v_q + u_p v_p u_q \delta v_q\big] + \lambda(2u_p\delta u_p + 2v_q \delta v_q) = 0$$

↑ Lagrange multiplier.

For the 2nd term we permute $p \leftrightarrow q$

$$\delta\tilde{E} = 2\sum_p \xi_p (2v_p)\delta v_p + \sum V_{pq}\big[v_p u_q v_q \delta u_p + u_q v_q u_p \delta v_p\big] + \sum V_{qp}\big[u_q v_q v_p \delta u_p + u_q v_q u_p \delta v_p\big] + \lambda\sum_p(2u_p\delta u_p + 2v_p\delta v_p) = 0$$

So $\quad \sum_q (V_{pq} + V_{qp})\, u_q v_q v_p + \lambda 2u_p = 0$

and $\quad 4\xi_p v_p + \sum_q (V_{pq} + V_{qp})\, u_q v_q u_p + \lambda 2v_p = 0$

We assume $V_{pq} = V_{qp}$ is symmetric (OK ?)

and define the gap

put 2 here → $\Delta_p \equiv -\sum_{q>0} V_{pq} u_q v_q$? all q or $q>0$ $q>0$

$\delta \vec{E} = 0$ implies $\begin{cases} -\Delta_p v_p + \lambda u_p = 0 \\ 2\xi_p v_p - \Delta_p u_p + \lambda v_p = 0 \end{cases}$

so $\lambda = \Delta_p$ $\quad \xi_p v_p - \Delta_p u_p + \Delta_p v_p = 0$

$\xi v_p = \Delta_p (u_p - v_p)$ $\quad u^2 + v^2 = 1$

or $(\xi v)^2 = \Delta^2 (u-v)^2 = \Delta^2 (u^2 + v^2 - 2uv)$

$= \Delta^2 (1 - 2uv)$??

$\begin{cases} -\Delta \cdot v + \lambda u = 0 \\ (2\xi + \lambda) v - \Delta u = 0 \end{cases}$ $\quad \lambda = \frac{v}{u} \cdot \Delta$

$\left(\xi + \frac{v}{u} \cdot \Delta\right) v - \Delta u = 0$

$2\xi v + \frac{v^2}{u} \cdot \Delta - \Delta u = 0$ $\quad u^2 + v^2 = 1$

or $\xi uv + v^2 \cdot \Delta - \Delta u^2 = 0$

or $2\xi u \cdot v + (v^2 - u^2) \cdot \Delta = 0$

... the fo... ... ξ ... by in f...

$2\xi u \cdot v + (v^2 - u^2) \cdot \Delta = 0$

consider ansatz $u^2 = \frac{1}{2}(1 + x)$ $\quad uv = \frac{1}{4}(1 - x^2)$

$v^2 = \frac{1}{2}(1 - x)$ $\quad u^2 = \frac{1}{4}(1 + 2x + x^2)$

$v^2 = \frac{1}{4}(1 - 2x + x^2)$

so $2\xi \frac{1}{4}(1 - x^2) + \left(\frac{1}{4}\right)(-4x)\Delta = 0$ $\quad v^2 - u^2 = -x$

$-2\xi x^2 - \Delta x - \frac{1}{2}\xi = 0$ $\quad \boxed{2\xi uv = -x\Delta}$

So $4\zeta^2 (uv)^2 = x^2\Delta^2 \Rightarrow 4\zeta^2(1-x^2)\frac{1}{4} = x^2\Delta^2$

$\zeta^2 q - \zeta^2 x^2 = \Delta^2 x^2$ or $\zeta^2 = (\zeta^2 + \Delta^2)x^2$

so $x = \frac{\zeta}{\sqrt{\zeta^2+\Delta^2}}$ or $u^2 = \frac{1}{2}\left(1 + \frac{\zeta}{E}\right)$ $E = \sqrt{\zeta^2+\Delta^2}$

$v^2 = \frac{1}{2}\left(1 - \frac{\zeta}{E}\right)$

This is the correct solution for u & v! It is the same as via Bogaliubov transform on page 77.

It has been shown on page 225 – 255 and 3-9 that we do have a Dyson equation

$$G_n = G + G\Sigma G_n$$ ← 2x2 matrix in Nambu space

in Nambu space as a proper matrix structure. Here it is shown we have (Fock term)

$$\Sigma = e^2 i\hbar\, G\, \mathbb{D} \quad \text{or} \quad \Sigma(1,2) = e^2 i\hbar\, \mathbb{D}(1,2)\, G(1,2)$$

Here $1 \equiv (j, \tau_1, s_1)$

$2 \equiv (j, \tau_2, s_2)$

And $\mathbb{D}$ in Nambu space take the form $\mathbb{D} = \begin{bmatrix} D & -D \\ -D & D \end{bmatrix}$

However, we also know D is in orbital charge space which does not have a Nambu structure i.e. for D we have

$$D = V + V \Pi D$$ where D is 1×1 not 2×2

and here D do not have a Nambu index s.

Although we don't have a Nambu index structure for $\mathbb{D}$, we can take one as follows.

$$\mathbb{D} = \mathbb{V} + \mathbb{V}\,\mathbb{\Pi}\,\mathbb{D}$$

$\mathbb{\Pi} = \frac{\Pi}{2} \mathbf{I}$

Let's define $\mathbb{D} = \begin{bmatrix} V & -V \\ -V & V \end{bmatrix}$ (2×2) $= \begin{bmatrix} V & -V \\ -V & V \end{bmatrix} \begin{bmatrix} \Pi/2 & 0 \\ 0 & \frac{\Pi}{2} \end{bmatrix} \mathbb{D}$

Here $\Pi = \Pi^{11} + \Pi^{12}$ as defined on page 3, page 9.

Multiply out for each components we get

$$\begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix} = \begin{bmatrix} V & -V \\ -V & V \end{bmatrix} + \begin{bmatrix} V & -V \\ -V & V \end{bmatrix} \frac{\Pi}{2} \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix}$$

Now $\mathbb{\Pi} \propto \mathbf{I}$ is proportional to the 2×2 identity matrix

$$\begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix} = \begin{bmatrix} V + \frac{1}{2} V\frac{\Pi}{2}(D_{11} - D_{21}) & -\left(V + \frac{1}{2} V\Pi(D_{22} - D_{12})\right) \\ -\left(V + V\frac{\Pi}{2}(D_{21} - D_{11})\right) & V + \frac{1}{2} V\Pi(D_{22} - D_{12}) \end{bmatrix}$$

It is not clear that $D_{11} = D_{22} = -D_{12} = -D_{21} = D$ is the only solution but if so then the above matrix became

$$\begin{bmatrix} D & -D \\ -D & D \end{bmatrix} = \begin{bmatrix} V + V\Pi D & -(V + V\Pi D) \\ -(V + V\Pi D) & V + V\Pi D \end{bmatrix}$$

i.e. $\mathbb{D} = V + V\mathbb{\Pi}\mathbb{D}$ is then equivalent to

$D = V + V\Pi D \rightarrow 1\times 1$ } in Nambu space

Need careful about the order as V is still $N \times N$ matrix

Alternatively try to solve

$$(I - V\mathbb{\Pi})\mathbb{D} = \begin{bmatrix} V & -V \\ -V & V \end{bmatrix}$$

or $$\begin{pmatrix} 1 & 0 \\ 0 & I \end{pmatrix} - \begin{pmatrix} V & -V \\ -V & V \end{pmatrix} \begin{pmatrix} \frac{\Pi}{2} & 0 \\ 0 & \frac{\Pi}{2} \end{pmatrix} = \begin{pmatrix} I - V\frac{\Pi}{2} & V\frac{\Pi}{2} \\ V\frac{\Pi}{2} & I - V\Pi/2 \end{pmatrix}$$

$$\begin{pmatrix} I & -\frac{1}{2}V\Pi & \frac{1}{2}V\Pi \\ \frac{1}{2}V\Pi & I - \frac{1}{2}V\Pi \end{pmatrix} \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} = \begin{pmatrix} V & -V \\ -V & V \end{pmatrix}$$

Since the matrix is symmetric we conclude $D_{12} = D_{21}$.

Focus on 1st column

$$(I - \tfrac{1}{2}V\Pi)D_{11} + \tfrac{1}{2}V\Pi D_{21} = V \qquad (1)$$

$$\tfrac{1}{2}V\Pi D_{11} + (I - \tfrac{1}{2}V\Pi)D_{21} = -V \qquad (2)$$

add the two equations we find

$$(I - V\Pi)D_{11} + (I - V\Pi)D_{21} = 0$$

As $I - V\Pi$ is diagonal dominate $(I - V\Pi)^{-1}$ exists generically. so this implies

$$(I - V\Pi)(D_{11} + D_{21}) = 0 \quad \text{or} \quad D_{11} = -D_{21}$$

similarly we can show by working on second column of $\mathbb{D}$

$D_{22} = -D_{12}$ as a result if we define

$D = D_{11} = -D_{21}$ we get from (1)

$$(I - \tfrac{1}{2}V\Pi)D - \tfrac{1}{2}V\Pi D = V \Rightarrow \text{or} \quad (I - V\Pi)D = V$$

or $D = V + V\Pi D$

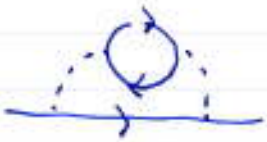
the usual Dyson equation is recovered in 1x1 matrix in Nambu space

We have successful "faked" a Dyson structure for $\mathbb{D}$ in Nambu space as ← diagonal and ∝ I

$$\mathbb{D} = \begin{bmatrix} V & -V \\ -V & V \end{bmatrix} + \begin{bmatrix} V & -V \\ -V & V \end{bmatrix} \begin{bmatrix} \frac{\Pi}{2} & 0 \\ 0 & \frac{\Pi}{2} \end{bmatrix} \mathbb{D}$$

In this new Nambu structure, we can associate each point in the Feynman diagram a triplet label (j, τ, β) j site, τ contour time, β Nambu index

The diagrams built from  and  should work as expected. Such as



So I expect my failed rule for $\mathbb{D}$ worked at the level of RPA. However, there is no reason to believe that the rule will work beyond RPA. For example, will the rule work for

 ? [This graph is needed for Coulomb drag]

I think not. or graphs like  ?

At least under RPA we get a pair of Dyson equations

$$\left.\begin{aligned} G_n &= G + G\Sigma G_n \\ \mathbb{D} &= V + V\Pi\mathbb{D} \end{aligned}\right\} \text{ now all in } 2\times 2 \text{ Nambu space } \mathbb{D} \to \begin{bmatrix} D & -D \\ -D & +D \end{bmatrix}$$

$$\mathbb{\Pi} = \frac{1}{2}\begin{bmatrix} \Pi_1 & -\Pi_2 \\ -\Pi_2 & \Pi_1 \end{bmatrix} \qquad \underbrace{\Pi_1}_{\text{normal}} + \underbrace{\Pi_2}_{\text{super. response}} = \Pi$$

$$\mathbb{\Pi} = \begin{bmatrix} \frac{\Pi}{2} & 0 \\ 0 & \frac{\Pi}{2} \end{bmatrix}$$

The Caroli formula can then be derived exactly the same way as in arXiv:1805.09493 by J Peng & J-S Wang. in suppl materials Eq (S15) – (S26)

Except now everything is in Nambu space. The Caroli/Landauer formula is now $\int_0^\infty$?? $\frac{1}{2}$ or not, probably, not !!

no $\frac{1}{2}$ here $\quad I_L = \int_0^\infty \frac{d\omega}{2\pi}\, \hbar\omega\, T(\omega)\left(N_L(\omega) - N_R(\omega)\right)$

$$N_\alpha(\omega) = \frac{1}{e^{\beta_\alpha \hbar\omega} - 1} \quad \text{is the Bose function}$$

and the Caroli formula for the transmission is

$$T(\omega) = \mathrm{Tr}_{js}\left[\mathbb{D}^r \mathbb{\Gamma}_L \mathbb{D}^a \mathbb{\Gamma}_R\right] \qquad \mathbb{\Gamma}_\alpha = i\left(\mathbb{\Pi}_\alpha^r - \mathbb{\Pi}_\alpha^a\right) = -2\,\mathrm{Im}\,\mathbb{\Pi}_\alpha^r$$

Here the trace is over space index j as well as Nambu index s. $\mathbb{\Pi}$ is diagnl in Nambu spc so

$$\mathrm{Tr}\left(\mathbb{D}^r \mathbb{\Gamma}_L \mathbb{D}^a \mathbb{\Gamma}_R\right) = \text{sum of diagonals of}$$

we have redefined $\mathbb{\Pi}$. See page 117

$$\begin{pmatrix} D^r & -D^r \\ -D^r & D^r \end{pmatrix}\begin{pmatrix} \Gamma_L/2 & 0 \\ 0 & \Gamma_L/2 \end{pmatrix}\begin{pmatrix} D^a & -D^a \\ -D^a & D^a \end{pmatrix}\begin{pmatrix} \Gamma_R/2 & 0 \\ 0 & \Gamma_R/2 \end{pmatrix}$$

Note we need to divide by 2 as $\mathbb{\Pi} = \frac{1}{2}\begin{pmatrix} \Pi & 0 \\ 0 & \Pi \end{pmatrix}$

$\Gamma_L = i(\Pi_L^r - \Pi_L^a)$ as usual.

Multiply out we get

$$\begin{pmatrix} D^r\frac{\Gamma_L}{2} & -D^r\frac{\Gamma_L}{2} \\ -D^r\frac{\Gamma_L}{2} & D^r\frac{\Gamma_L}{2} \end{pmatrix}\begin{pmatrix} D^a\frac{\Gamma_R}{2} & -D^a\frac{\Gamma_R}{2} \\ -D^a\frac{\Gamma_R}{2} & D^a\frac{\Gamma_R}{2} \end{pmatrix}$$

$$= \mathrm{Tr}_s\begin{pmatrix} D^r\Gamma_L D^a\Gamma_R\left(\frac{1}{4}+\frac{1}{4}\right) & \cdots \\ \cdots & \frac{1}{2} D^r\Gamma_L D^a\Gamma_R \end{pmatrix} = \underbrace{D^r\Gamma_L D^a\Gamma_R}$$

not in Nambu space any more

So we obtain

$$T(\omega) = \mathrm{Tr}_j\left[D^r\Gamma_L D^a\Gamma_R\right]$$ Here the trace is in space index j only. No Nambu index. This formula, of ~~course~~ course, is the one we naively should expect! I have $\frac{1}{2}$ factor problem, Meir-Wingreen on page 31. So should also have $\frac{1}{2}$ here in Caroli formula!

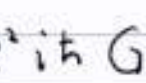
Condition to derive the Caroli formula

In order to show the equivalence of Meir-Wingreen formula, integral of E times $\frac{1}{2}\mathrm{Tr}(G^{>}\Sigma_L^{<} - G^{<}\Sigma_L^{>})$, to is the Caroli formula we need the following conditions

1) Take lowest order expansion approximation

i.e. $G_n \approx G + G\Sigma G$ still in contour variable τ

This is valid when V is small $\Sigma \propto V$ $G \to$ free electrons!

2) Use RPA $\Sigma = e^2 i\hbar G D$, $\Pi =$  $= G \cdot G$.

3) use local equilibrium approximation. i.e.

$G = \begin{bmatrix} G_L & 0 \\ 0 & G_R \end{bmatrix}$ each one we can apply fluctuation-dissipation theorem locally. e.g. $G_L^{<}(E) = \frac{-1}{e^{\beta_L E}+1}(G_L^{r} - G_L^{a})$

Note for superconductor no chemical potential μ here. Use $\frac{1}{e^{\beta(E-\mu)}+1}$ is wrong!

With these approximations to the Green's functions then

Meir-Wingreen = Caroli exactly.

this could be verified numerically.

Check where I made mistake for the extra $\frac{1}{2}$ or missing one!

18 Nov 2018

Alternative derivation of Feynman rules.

Since Green's function is expressed in Ψ $\quad \Psi = \begin{pmatrix} c \\ c^+ \end{pmatrix}$

$$G_{jsks'}(\tau, \tau') = -\frac{i}{\hbar} \langle T\, \Psi_{js}(\tau)\, \Psi^+_{ks'}(\tau') \rangle$$ see page 209

We also express the Coulomb interaction in term of Ψ $\quad \Psi^+ = (c^+, c)$

$$V_{int} = \frac{e^2}{2} \sum_{ij} c_i^+ c_j^+ V_{ij} c_j c_i \qquad c_j c_j^+ + c_j^+ c_j = 1$$

$$= \frac{e}{2} \sum_{ij} c_i^+ c_j^+ c_j c_i V_{ij} \quad (-1)$$

$$(-c_i c_j^+ + \delta_{ij})$$

we set $V_{ii} = 0$ or shift on site

$$= \frac{e}{2} \sum_{ij} \left[c_i^+ c_i c_j^+ c_j V_{ij} - c_i^+ c_i V_{ii} \right]$$

$$= \frac{1}{2} \sum_{ij} \Big[\Big(\tfrac{1}{2} c_i^+ c_i + \tfrac{1}{2} c_i^+ c_i \Big) c_j^+ c_j V_{ij} - \tfrac{1}{2} c_i c_i^+ + \tfrac{1}{2} \Big) \Big[\tfrac{1}{2} c_j^+ c_j - \tfrac{1}{2} c_j c_j^+ + \tfrac{1}{2} \Big] V_{ij}$$

If we shift / redine the onsite which contribution to a hartree term, we get

$$= \frac{1}{2} \frac{1}{4} \sum_{ij} \left(c_i^+ c_i - c_i c_i^+ \right) V_{ij} \left(c_j^+ c_j - c_j c_j^+ \right) + \text{hartree term}$$

$\Psi_1 = c$

$\Psi_2 = c^+$

ignore hartree term $\quad \Psi^+_{i1} \Psi_{i1} \qquad \Psi^+_{i2} \Psi_{i2}$

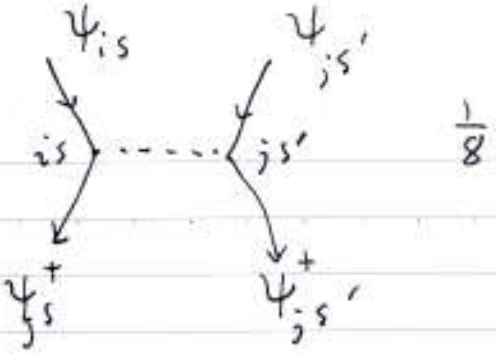
$$= \frac{1}{2} \frac{1}{4} \sum_{is\, js'} V_{ij}^{ss'} \Psi^+_{is} \Psi_{js'} \qquad s = 1, 2$$

$$\hookrightarrow \frac{1}{2} \frac{1}{4} \cdot \sum_{ij\, ss'} \Psi^+_{is} \Psi_{is} V_{ij}^{ss'} \Psi^+_{js'} \Psi_{js'}$$

$$= \frac{1}{8} (\Psi_1^+ \; \Psi_2^+) \begin{pmatrix} V & -V \\ V & -V \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}$$

$$\mathbb{V} = \begin{pmatrix} V & -V \\ -V & V \end{pmatrix}$$

Diagrammatically we have



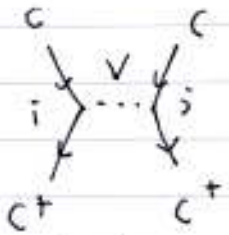
$\frac{1}{8}$

Note: s scattering does not change location and Matsubara index i, s.

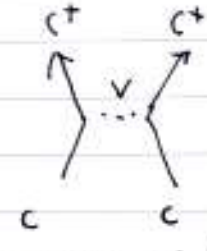
We need a factor $\frac{1}{8}$ instead of the original $\frac{1}{2}$.

when s, s' runs over 1 & 2 we get 4 cases

$s = s' = 1$

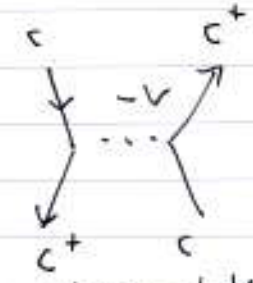


scatter of electrons



scatter of holes

$s = s' = 2$



electron-hole scattering

$s = 1, s' = 2$

$s = 2 \quad s' = 1$

electron & hole are attractive, thus $-V$.

Can we set $M^{ks''}_{is,\,js'} = \delta_{ij}\,\delta_{ks}\,\delta_{ss'}\,(-1)^{s+s''}\,(-e)\,\frac{1}{2}$?

since $\langle \psi\psi \rangle$, $\langle \psi^+\psi^+ \rangle$, $\langle \psi\,\psi^+ \rangle$ $\langle \psi^+\psi \rangle$ all non vanishing there is a little trouble to work this out!

But the final results must equivalent to before !!

Still missing factor of 2 !!

should we take $\Pi\Pi = \frac{1}{4}\begin{pmatrix} \Pi & -\Pi \\ -\Pi & \Pi \end{pmatrix}$??

---

where is the missing factor of $\frac{1}{2}$?

We define $\Pi^{(\tau,\tau')}_{js\,ks'} = \frac{1}{2}(-ie^2)\,G^{(\tau,\tau')}_{js\,ks'}\,G^{(\tau',\tau)}_{ks'\,js}$

so $\Pi\Pi = \frac{1}{2}\begin{pmatrix} \Pi_1 & -\Pi_2 \\ -\Pi_2 & \Pi_1 \end{pmatrix}$

$\Pi_1 = \Pi^N = -ie^2 G_{11}\,G_{11}$

$\Pi_2 = \Pi^S = ie^2 G_{12}\,G_{21}$

such that $\Pi = \Pi^N + \Pi^S$

See page 9 to understand

Then $\mathbb{D} = \begin{bmatrix} v & -v \\ -v & v \end{bmatrix} + \begin{bmatrix} v & -v \\ -v & v \end{bmatrix} \frac{1}{2} \begin{bmatrix} \Pi_1 & -\Pi_2 \\ -\Pi_2 & \Pi_1 \end{bmatrix} \mathbb{D}$

is consistent with $D_{11} = D = v + v\Pi D$

$\Pi = \Pi_1 + \Pi_2$

The derivation from Meir-Wingreen to Caroli goes like that

$$G^> \to G^r \Sigma_n^> G^a$$

so $G^> \Sigma_L^< \to G^r \Sigma_n^> G^a \Sigma_L^<$ this Π is from Dyson equation $D = v + v\Pi D$

The self energy we use RPA for Π

$$\Sigma_n^> = G^> D^> \qquad D^> = D^r \Pi^> D^a$$

so $G^> \Sigma_L^< \to \underbrace{G^r \Sigma_n^> G^a}_{\Sigma_n^>} \Sigma_L^< \to G^r \underbrace{G^> D^>}_{\Sigma_n^>} G^a \Sigma_L^<$

$\to G^r G^> (D^r \Pi^> D^a) G^a \Sigma_L^<$

cyclic permutation and time reversal symmetry

$\to G^> D^r \Pi^> D^a \underbrace{G^r \Sigma_L^< G^a}_{G^<}$ we use fluctuation-dissipation theorem for $\Pi^{>,<}$.

$\to D^r \Pi^> D^a \underbrace{(G^< G^>)}_{2\Pi^<}$ because our definition of Π is half of the usual one

$\Pi\Pi = \frac{1}{2} GG$ as a result, we get extra factor of 2 here. This cancel the $\frac{1}{2}$ factor in Meir-Wingreen. Caroli formula thus has no $\frac{1}{2}$ in front

$$\int_0^\infty \frac{d\omega}{2\pi} \cdot \hbar\omega \, \mathrm{Tr}(\mathbb{D}^r \Gamma_L \mathbb{D}^a \Gamma_R)(N_L - N_R)$$