Time-dependent perturbation theory & Zero-temperature Green's functions

The need for time-dependent formalism

The Hamiltonian we are interested is time-independent (eq. (42) or (43)), then why do we need to use the time-dependent formalism?

There are several reasons for using time-dependent formalism:

(i) There are problems that involved quantities at different times.

For instance, the AC conductivity is defined as

$$\langle J_\alpha(r,t)\rangle = \int \sigma_{\alpha\beta}(r,t;r',t')\, E_\beta(r',t')\, dr'$$

↑ current (α-component)

$\sigma_{\alpha\beta}$ involves operators at different times t & t'.

In general, to characterize dynamics of the system completely, one needs to know

$$\langle \hat{O}(t)\,\hat{O}(t')\rangle \quad \text{for } t \neq t'$$

Hence one needs to have time-dependent formalism. The problem is non-equilibrium in nature.

(ii) Using time-dependant formalism can recover properties of time-independant problem.

In particle, it is more efficient if the formulation is appropriately designed.

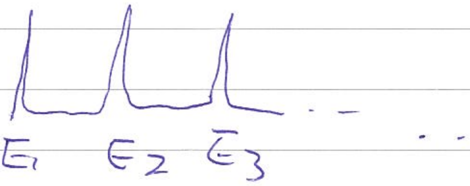
For example, in the time-independant approach, one tries to find the energy eigenvalues, say,

$$H|\psi\rangle = E|\psi\rangle \quad \cdots (95).$$

This is usually done one energy by one energy.

In the time-dependant approach, one starts from any typical $|\psi_0\rangle$, and solves the time-dependant Schrödinger eq. $i\hbar \frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$.

At time t, performing the Fourier transformation in time would give peaks at $\hbar\omega = E_n$ for all E_n!



Hence, $E_1, E_2, E_3, \ldots$ are obtained in one shot.

Note that unlike it is particularly chosen, $|\psi_0\rangle$

usually contains all possible E :

$$|\Psi_0\rangle = \sum_{E_n} |E_n\rangle \underbrace{\langle E_n|\Psi_0\rangle}_{a_{E_n} \neq 0 \text{ in general.}}$$

Adiabatic "Switching on"

The time-dependent approach allows one to reproduce results of time-independent perturbation theory.

This is achieved by adiabatic switching on, in which one changes $H = H_0 + U$

into $H = H_0 + e^{-\frac{\epsilon}{\hbar}|t|} U$. for $\epsilon \to 0^+$ --(96)

To see the approach based on (96) reproduces the time-independent approach, we consider

$-\infty < t \leq 0$. , at $t = -\infty$ $H = H_0$

$(e^{-\frac{\epsilon}{\hbar}|t|} \to e^{\frac{\epsilon}{\hbar}t})$

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar}Et}|\phi\rangle, \qquad H_0|\phi\rangle = E|\phi\rangle \quad \text{-(97)}$$

We shall adopt the interaction picture

$$|\Psi_I(t)\rangle \equiv e^{\frac{i}{\hbar}H_0 t}|\Psi\rangle$$

$\therefore$ at $t \to -\infty$, $|\Psi_I\rangle = |\phi\rangle$

$$\because \; i\hbar \frac{d|\Psi_I\rangle}{dt} = e^{\frac{\epsilon}{\hbar}t} \underbrace{e^{\frac{i}{\hbar}H_0 t} V e^{-\frac{i}{\hbar}H_0 t}}_{V_I(t)} |\Psi_I\rangle \quad \text{-(98)}$$

We shall show that

$\lim_{\varepsilon\to 0^+} |\Psi_I(t=0)\rangle$ is an eigenfunction

to $H = H_0 + U$ --- (99)

Pf: Eq. (98) can be rewritten as an integral eq. by integration from $t=-\infty$ to 0

$$|\Psi_I(0)\rangle = |\phi\rangle - \frac{i}{\hbar}\int_{-\infty}^{0} e^{\frac{\epsilon}{\hbar}t'} V_I(t')\,|\Psi_I(t')\rangle\, dt'$$

By iteration, the above equation becomes

$$|\Psi_I(0)\rangle = |\phi\rangle - \frac{i}{\hbar}\int_{-\infty}^{0} e^{\frac{\epsilon}{\hbar}t'} V_I(t')\,|\phi\rangle\, dt'$$

$$+\left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^{0} e^{\frac{\epsilon}{\hbar}t'} V_I(t')dt' \int_{-\infty}^{t'} e^{\frac{\epsilon}{\hbar}t''} V_I(t'')\,|\phi\rangle\, dt''$$
$(t'<0)$

$+ \cdots$

$$\because\ V_I(t')|\phi\rangle = e^{\frac{i}{\hbar}H_0 t'}\, U\, e^{-\frac{i}{\hbar}H_0 t'}|\phi\rangle$$

$$= e^{\frac{i}{\hbar}H_0 t'}\, U\, e^{-\frac{i}{\hbar}E t'}, \quad H_0|\phi\rangle = E|\phi\rangle$$

$$\therefore\ \frac{-i}{\hbar}\int_{-\infty}^{0} e^{\frac{\epsilon}{\hbar}t'} V_I(t')\,|\phi\rangle\, dt'$$

$$= \frac{-i}{\hbar}\int_{-\infty}^{0} e^{-\frac{i}{\hbar}(E-H_0+i\epsilon)t'}\, dt'\, \hat{U}\,|\phi\rangle$$

$$= \frac{1}{E-H_0+i\varepsilon}\,\hat{U}\,|\phi\rangle$$

Performing similar integral for the 2nd term and noting that $e^{\frac{i}{\hbar}H_0 t'}$ gets cancelled in the middle, one finds

$$|\Psi_I(0)\rangle = |\phi\rangle + \frac{1}{E-H_0+i\varepsilon}V|\phi\rangle + \frac{1}{E-H_0+i\varepsilon}V\frac{1}{E-H_0+i\varepsilon}V|\phi\rangle$$

$+ \cdots$ (100)

Clearly, one sees that eq. (100) reproduces time-independent perturbation theory.

Eq. (100) can be rewritten as

$$|\Psi_I(0)\rangle = |\phi\rangle + \frac{1}{E-H_0+i\varepsilon}V|\Psi_I^{(0)}\rangle$$

$\therefore |\Psi_I(0)\rangle = |\psi^+\rangle$ in the Lippman-Schwinger equation.

Hence $H|\Psi_I(0)\rangle = E|\Psi_I(0)\rangle$

$\therefore |\Psi_I(0)\rangle$ is an eigenstate to $\hat{H}$

Gell-mann & Low theorem

We have seen that by starting from the eigenstate of H_0 and turning on U adiabatically, one can get the eigenstate of $H = H_0 + U$ at $t=0$

Now, just as the usual time-independent perturbation, eq. (100) is not appropriately normalized:

Let the eigenstate of H_0 be $|n^0\rangle$, (eigenvalue $= E_n^0$)

The eigenstate of H is $|n\rangle = \alpha|n^0\rangle + |n'\rangle + \cdots$ ($|n^k\rangle = O(V^k)$)

In the usual perturbation theory, one sets $\alpha = 1$ so that $E_n - E_n^0 = \langle n^0 | V | n \rangle$ & $\langle n^0 | n^k \rangle = 0$. ⟵ (101)

This is what eq. (60) states! $\therefore |n\rangle = |n^0\rangle + \cdots$

(because in principle, there can be an coefficient of α in front of $|\phi\rangle$)

Now, to normalized $|n\rangle$ appropriately, we note that $|n_R\rangle = \alpha |n^0\rangle + |n_\perp\rangle$ and requiring $\langle n_R | n_R \rangle = 1$ to find α.

$$\because \langle n^0 | n_\perp \rangle = 0 \quad \therefore \alpha = \langle n^0 | n_R \rangle$$

Clearly, in the usually normalization. $\langle n | n^0 \rangle = 1$

$$|n\rangle = \frac{1}{\alpha} |n_R\rangle$$

$\therefore$ (101) becomes
$$E_n - E_n^0 = \frac{\langle n^0 | V | n^R \rangle}{\langle n^0 | n^R \rangle} \quad \cdots \quad (102)$$

Eq (102) is essentially the Gell-man & Low theorem if one writes it as
$$E_n = \frac{\langle n^0 | \overbrace{H_0 + V}^{H} | n^R \rangle}{\langle n^0 | n^R \rangle}$$
and conclude
$$H \frac{|n^R\rangle}{\langle n^0 | n^R \rangle} = E \frac{|n^R\rangle}{\langle n^0 | n^R \rangle} \quad \cdots \quad (103)$$

Since $|n^R\rangle = \hat{S}_\epsilon(0, -\infty) |\phi\rangle$, S_ϵ = evolution operator, (interaction picture) ↳ from $-\infty$ to 0 usually called S-matrix

one gets the Gell-man & Low theorem:

If $\lim_{\varepsilon\to 0^+} \dfrac{\hat{S}_\varepsilon(0,-\infty)|\phi\rangle}{\langle\phi|\hat{S}_\varepsilon(0,-\infty)|\phi\rangle} \equiv \dfrac{|\Psi\rangle}{\langle\phi|\Psi\rangle}$ exists

$$\hat{H}\frac{|\Psi\rangle}{\langle\phi|\Psi\rangle} = E\frac{|\Psi\rangle}{\langle\phi|\Psi\rangle} \qquad \cdots (104)$$

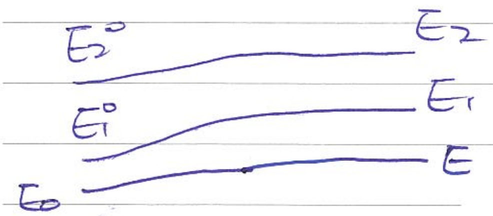
(see Fetter & Waleca for another proof.)

Note that the above proof applies well if one replace $\hat{S}_\varepsilon(0,-\infty)$ (retarded) by $\hat{S}_\varepsilon(0,\infty)$ (advanced) (see over)

Green's function at zero temperature

The Gell-man & Low theorem is a fundamental theorem to connect eigenstates of H $|\Psi\rangle$ to eigenstates of H_0, $|\phi\rangle$. This connection does not guarantee $|\phi_0\rangle$ (ground state of H_0) is connected to the ground state of $|\Psi_0\rangle$.

However, if during the adiabatic switching on, there is no level-crossing (or phase transition), $\dfrac{|\Psi_0\rangle}{\langle\phi_0|\Psi_0\rangle}$ is the ground state to H.



(no level crossing.)

Average in different pictures

There are different representations in describing quantum dynamics

Schrödinger picture

The elementary Quantum mechanics is expressed in the Schrödinger picture where

$$\hbar i \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

with time-dependance carried by $|\psi\rangle$ fully.

Even if $\hat{H}$ is time-independent, $|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle$ is time-dependent. $\therefore \langle\hat{O}\rangle = \langle\psi(t)|\hat{O}|\psi(t)\rangle$ for any time-independent operator

Heisenberg picture

In the representation, one defines $|\psi_H\rangle \equiv |\psi(0)\rangle = e^{\frac{i}{\hbar}Ht}|\psi(t)\rangle$. Since the average $\langle\hat{O}\rangle$ is independent of representation,

$$\langle\hat{O}\rangle = \langle\psi(t)|\hat{O}|\psi(t)\rangle$$
$$= \langle\psi(0)|e^{\frac{i}{\hbar}Ht}\hat{O}e^{-\frac{i}{\hbar}Ht}|\psi(0)\rangle$$

$\therefore$ In the Heisenberg picture, one shifts time-dependence to the operator

$$\hat{O}_H \equiv e^{\frac{i}{\hbar}Ht}\hat{O}e^{-\frac{i}{\hbar}Ht} \quad \text{--- (105)}$$

Hence, the operator $\hat{O}_H$ becomes time-dependent.

$$i\hbar\frac{d\hat{O}_H}{dt} = [\hat{O}_H(t), \hat{H}] + i\hbar\frac{\partial\hat{O}_H}{\partial t} \quad \text{--- (106)}$$

↑ differentiation for explicit t-time-dependence

Interaction picture

In the interaction picture as we have already used, it is aimed to deal with the situation when we know how to solve H_0 but do not know how to solve $H=H_0+U$.

In this picture, one removes the dynamics we know,

$$\therefore \quad |\Psi_I(t)\rangle = e^{\frac{i}{\hbar}H_0 t}|\Psi(t)\rangle$$

$$= e^{\frac{i}{\hbar}H_0 t}\, e^{-\frac{i}{\hbar}Ht}|\Psi(0)\rangle \quad \cdots (107)$$

$$\therefore \langle\hat{O}\rangle = \langle\Psi(0)|e^{\frac{i}{\hbar}Ht}\,\hat{O}\,e^{-\frac{i}{\hbar}Ht}|\Psi(0)\rangle$$

$$= \langle\Psi_I(t)|\,e^{\frac{i}{\hbar}H_0 t}\,\hat{O}\,e^{-\frac{i}{\hbar}H_0 t}\,|\Psi_I(t)\rangle$$

$$\therefore \hat{O}_I(t) = e^{\frac{i}{\hbar}H_0 t}\,\hat{O}\,e^{-\frac{i}{\hbar}H_0 t} \quad \cdots (108)$$

The evolution operator in the interaction picture

$$\hat{U}(t) = e^{iH_0 t/\hbar}\,e^{-\frac{i}{\hbar}Ht}$$

$$\frac{d\hat{U}(t)}{dt} = \frac{i}{\hbar}\,e^{i\frac{H_0 t}{\hbar}}\,[H_0 - H]\,e^{-\frac{i}{\hbar}Ht}$$

$$= -\frac{i}{\hbar}e^{\frac{i}{\hbar}H_0 t}\,V\,e^{-\frac{i}{\hbar}H_0 t}\,e^{\frac{i}{\hbar}H_0 t}\,e^{-\frac{i}{\hbar}Ht}$$

$$= -\frac{i}{\hbar}\hat{V}_I(t)\,\hat{U}(t)$$

$$\therefore \hat{U}(t) - \underbrace{\hat{U}(0)}_{I} = -\frac{i}{\hbar}\int_0^t dt_1\,\hat{V}_I(t_1)\,\hat{U}(t_1) \quad \cdots (109)$$

Eq. (109) can be iterated and we find

$$U(t) = 1 - i\int_0^t dt_1\, \hat{V}_I(t_1) + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2\, \hat{V}_I(t_1)\hat{V}_I(t_2)$$

$$+ \cdots + (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, \hat{V}_I(t_1)\hat{V}_I(t_2)\cdots\hat{V}_I(t_n)$$

$$+ \cdots\cdots \qquad (110)$$

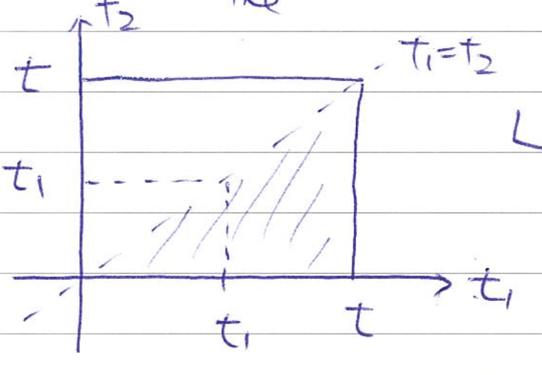
Eq. (110) can be put into more compact form by using the time-ordering operator T, which always puts lastest time in the left:

For example: $T[\hat{V}_I(t_1)\hat{V}_I(t_2)\hat{V}_I(t_3)] = \hat{V}_I(t_3)\hat{V}_I(t_1)\hat{V}_I(t_2)$, if $t_3 > t_1 > t_2$

If we define $\theta(x) = 1$, $x > 0$
$= 0$ $x < 0$
$= \frac{1}{2}$ $x = 0$, we have

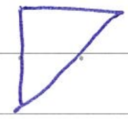
$$T[\hat{V}_I(t_1)\hat{V}_I(t_2)] = \theta(t_1 - t_2)\hat{V}_I(t_1)\hat{V}_I(t_2) + \theta(t_2 - t_1)\hat{V}_I(t_2)\hat{V}_I(t_1)$$

$\therefore$ For the $O(V^2)$ term, as indicated in the following figure,



$$I_2 = \int_0^t dt_1 \int_0^{t_1} dt_2\, \hat{V}_I(t_1)\hat{V}_I(t_2)$$

is the integration in the dash line area, in which $\underline{t_1 > t_2}$ $\therefore \hat{V}_I(t_1)\hat{V}_I(t_2) = T[\hat{V}_I(t_1)\hat{V}_I(t_2)]$ --- (111)

One can also include the other triangle 

by noting that if we change notation:

$t_1 \leftrightarrow t_2$, $U_2 = \int_0^t dt_2 \int_0^{t_2} dt_1 \, \hat{V}_I(t_2) \hat{V}_I(t_1)$

$= \int_0^t dt_2 \int_0^{t_2} dt \; T[V_I(t_1) V_I(t_2)]$ --(112)

Combing eqs. (111) & (112), one gets

$$U_2 = \frac{1}{2!} \int_0^t dt_1 \int_0^t dt_2 \; T[V_I(t_1) V_I(t_2)]$$

Similarly, for general term

$$U_n = (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \; \hat{V}_I(t_1) \hat{V}_I(t_2) \cdots \hat{V}_I(t_n)$$

$$= (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \; T[\hat{V}_I(t_1) \hat{V}_I(t_2) \cdots \hat{V}_I(t_n)]$$

Any change of notation is a permutation of

$t_1, t_2, \ldots, t_n$ which fills one of $\frac{1}{n!} \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n$

$$\therefore \; n! \, U_n = (-i)^n \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \; T[\hat{V}_I(t_1) \cdots \hat{V}_I(t_n)]$$

$$\therefore \; U_n = \frac{(-i)^n}{n!} \int_0^t dt_1 \int_0^t dt_2 \cdots \int_0^t dt_n \; T[\hat{V}_I(t_1) \cdots \hat{V}_I(t_n)]$$

$$\therefore \; U(t) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_1 \cdots \int_0^t dt_n \; T[\hat{V}_I(t_1) \cdots \hat{V}_I(t_n)]$$

$= T e^{-i \int_0^t dt_1 \hat{V}_I(t_1)}$ is a formal expression for $U(t)$. ← --(113)

The above $\hat{U}(t)$ connects the Schrödinger wavefunction $|\Psi(0)\rangle$ to $|\Psi_I(t)\rangle$. The connection of $|\Psi_I(t')\rangle$ to $|\Psi_I(t)\rangle$ is defined as the S-matrix $\quad |\Psi_I(t)\rangle = S(t,t')\,|\Psi_I(t')\rangle \cdots$ (114)

$\because\ |\Psi_I(t')\rangle = e^{\frac{i}{\hbar}H_0t'}\,e^{-\frac{i}{\hbar}Ht'}\,|\Psi(0)\rangle$, eq. (107)

implies $\quad |\Psi_I(t)\rangle = e^{\frac{i}{\hbar}H_0t}\,e^{-\frac{i}{\hbar}Ht}\,e^{\frac{i}{\hbar}Ht'}\,e^{-\frac{i}{\hbar}H_0t'}\,|\Psi_I(t')\rangle$

$$= e^{\frac{i}{\hbar}H_0t}\,e^{-\frac{i}{\hbar}H(t-t')}\,e^{-\frac{i}{\hbar}H_0t'}\,|\Psi_I(t')\rangle$$

$\therefore\ S(t,t') = U(t)\,U^+(t') = e^{\frac{i}{\hbar}H_0t}\,e^{-\frac{i}{\hbar}H(t-t')}\,e^{-\frac{i}{\hbar}H_0t'} \cdots$ (115)

$$\frac{\partial S(t,t')}{\partial t} = \frac{\partial U(t)}{\partial t}\,U^+(t') = -\frac{i}{\hbar}\hat{V}_I(t)\,U(t)\,U^+(t')$$

$$= -\frac{i}{\hbar}\hat{V}_I(t)\,S(t,t')$$

$$\therefore\ S(t,t') = 1 - \frac{i}{\hbar}\int_{t'}^{t} dt_1\,\hat{V}_I(t_1)\,S(t_1,t')$$

$$= T e^{-\frac{i}{\hbar}\int_{t'}^{t} dt_1\,\hat{V}(t_1)} \cdots \text{(116)}$$

In the adiabatic turning on process, one replaces $V_I(t) = e^{-\frac{|\epsilon|}{\hbar}t}\,V_I(t)$, one gets

$$S_\epsilon(0,-\infty) = T e^{-\frac{i}{\hbar}\int_{-\infty}^{0} e^{\frac{|\epsilon|}{\hbar}t_1} dt_1\,\hat{V}_I(t_1)} \cdots \text{(117)}$$

$$\because\ S^+(t,t') = U(t')\,U^+(t) = S(t',t)$$

$$\therefore\ S_\epsilon^+(0,-\infty) = S_\epsilon(-\infty,0) = T e^{\frac{i}{\hbar}\int_0^{\infty} dt_1\,e^{-\frac{|\epsilon|}{\hbar}t_1}\,\hat{U}(t_1)} \cdots \text{(118)}$$

Using eq. (104) (combined with eq. (118)), one finds the expectation value with respect to the ground state $|\Psi_0\rangle$ of H can be expressed in terms of the ground state $|\Phi_0\rangle$ of H_0:

First, $|\Psi_0\rangle$ has no time dependence, one can use the Heisenberg picture to write

$$\langle \hat{O}(t)\rangle = \frac{\langle\Psi_0|\hat{O}_H(t)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \quad \cdots (119)$$

To express eq. (119) in terms of $|\Phi_0\rangle$, we first use eq. (104),

(104)-1 $$\frac{|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} = \frac{S_\epsilon(0,\pm\infty)|\Phi_0\rangle}{\langle\Phi_0|S_\epsilon(0,-\infty)|\Phi_0\rangle}$$

$$\therefore \frac{\langle\Psi_0|\Psi_0\rangle}{|\langle\Phi_0|\Psi_0\rangle|^2} = \frac{\langle\Phi_0|S_\epsilon^{+}(0,\infty)S_\epsilon(0,-\infty)|\Phi_0\rangle}{|\langle\Phi_0|\Psi_0\rangle|^2}$$

$$= \frac{\langle\Phi_0|S_\epsilon(+\infty,0)S_\epsilon(0,-\infty)|\Phi_0\rangle}{|\langle\Phi_0|\Psi_0\rangle|^2} \quad \cdots (120)$$

($S_\epsilon(+\infty,0)S_\epsilon(0,-\infty) \rightarrow S_\epsilon(\infty,-\infty)$)

Similarly,

$$\frac{\langle\Psi_0|\hat{O}_H(t)|\Psi_0\rangle}{|\langle\Phi_0|\Psi_0\rangle|^2} = \frac{\langle\Phi_0|S_\epsilon(\infty,0)\hat{O}_H(t)S_\epsilon(0,-\infty)|\Phi_0\rangle}{|\langle\Phi_0|\Psi_0\rangle|^2}$$

$$\because \hat{O}_H(t) = e^{\frac{i}{\hbar}Ht}\hat{O}e^{-\frac{i}{\hbar}Ht} = e^{\frac{i}{\hbar}Ht}e^{-\frac{i}{\hbar}H_0t}e^{\frac{i}{\hbar}H_0t}\hat{O}e^{-\frac{i}{\hbar}H_0t} \times e^{\frac{i}{\hbar}H_0t}e^{-\frac{i}{\hbar}Ht}$$

$$= U^{\dagger}(t,0)\, O_I(t)\, U(t,0)$$

$$= S_\epsilon(0,t)\, O_I(t)\, S_\epsilon(t,0) \quad \cdots (121)\text{-}1$$

$$\therefore \frac{\langle \Psi_0 | \hat{O}_H(t) | \Psi_0 \rangle}{|\langle \Phi_0 | \Psi_0 \rangle|^2} = \frac{\langle \Phi_0 | S_\epsilon(\infty, t)\, \hat{O}_I(t)\, S_\epsilon(t, -\infty) | \Phi_0 \rangle}{|\langle \Phi_0 | \Psi_0 \rangle|^2} \quad \cdots (121)$$

Hence the ratio of eqs. (120) & (121) yields

$$\langle \hat{O}(t) \rangle = \frac{\langle \Phi_0 | S_\epsilon(\infty, t)\, \hat{O}_I(t)\, S_\epsilon(t, -\infty) | \Phi_0 \rangle}{\langle \Phi_0 | S_\epsilon(\infty, -\infty) | \Phi_0 \rangle} \quad \cdots (122)$$

Eq. (122) is a key result for establishing equilibrium Green's function (at T=0) as we are interested in averages w.r.t. the ground state.

The reason why it works in that way as shown in eq. (122) is the adiabatic turning on so that $S(\infty, -\infty) | \Phi_0 \rangle$ brings back $\langle \Phi_0 |$! ($\because$ the interaction is adabatic turning off at $t = \infty$!)

In the above derivation, we have made use of eq. (104)-1. In fact, $\langle \Phi_0 |$ needs not to be exactly $\langle \Phi_0 |$, and could be different by some phase e^{iL}, i.e., $S_\epsilon(\infty, -\infty) | \Phi_0 \rangle = e^{iL} | \Phi_0 \rangle$ — (123)

Using (123), one can derive (122) more concisely as:

$$\langle \hat{O}(t) \rangle = \underbrace{\langle \Phi_0 | S_\epsilon(-\infty, t)}_{\langle \Psi_I(t)|} \hat{O}_I(t) \underbrace{S_\epsilon(t, -\infty) | \Phi_0 \rangle}_{|\Psi_I(t)\rangle}$$

$$(S_\epsilon^{+}(t,-\infty) = S_\epsilon(-\infty, t))$$

$$= e^{-iL} \langle \Phi_0 | S_\epsilon(\infty, -\infty) \cdot S_\epsilon(-\infty, t) \hat{O}_I(t) S_\epsilon(t, -\infty) | \Phi_0 \rangle$$

↑ Hermitian Conjugate of (123)

$$= \frac{\langle \Phi_0 | S_\epsilon(\infty, t) \hat{O}_I(t) S_\epsilon(t, -\infty) | \Phi_0 \rangle}{\langle \Phi_0 | S_\epsilon(\infty, -\infty) | \Phi_0 \rangle}$$

$$e^{iL} = \langle \Phi_0 | S_\epsilon(\infty, -\infty) | \Phi_0 \rangle$$

One reproduces eq. (122).

Equilibrium Green's function at $T=0$

Since $S_\epsilon(t,-\infty) = T e^{-\frac{i}{\hbar}\int_{-\infty}^{t} \hat{V}_I(t_1)dt_1}$

& $S_\epsilon(\infty, t) = T e^{-\frac{i}{\hbar}\int_{t}^{\infty} \hat{V}_I(t_1)dt_1}$, eq. (122)

can be rewritten as

$$\langle O(t) \rangle = \frac{\langle \Phi_0 | \overbrace{T e^{-\frac{i}{\hbar}\int_{-\infty}^{\infty} V_I(t_1)dt_1}}^{S(\infty,-\infty)} \hat{O}_I(t) | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle} \quad \text{--- (124)}$$

The appearance of time ordering is due to the time ordering in the S-matrix itself.

The single-particle Green's function is the propagation of an electron from $\vec{r}', t'$ to $\vec{r}, t$.

It is therefore natural to define it by

$$i G_{\alpha\beta}(rt; r't') \equiv \frac{\langle \Phi_0 | T\, C_\alpha(rt)\, C^+_\beta(r't')\, S(\infty, -\infty) | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle} \quad \text{---(125)}$$

The appearance of i will be cancelled to make it as the evolution operator for the case of a single-particle Schrödinger equation

(Recall that $\int dt\, e^{\frac{i}{\hbar}(Et - Ht)} = \frac{\hbar/i}{E - H}$).

Here $C^+_\alpha(rt)$ & $C_\beta(r't')$ are the creation and annihilation operators in the interaction picture.

Using eq. (121)-1, one has

Heisenberg picture
$$\begin{cases} C^+_{\beta H}(r't') = S(0, t')\, C^+_\beta(r't')\, S(t', 0) \\ C_{\alpha H}(rt) = S(0, t)\, C_\alpha(rt)\, S(t, 0) \end{cases}$$

For $t > t'$, $T[C_\alpha(rt)\, C^+_\beta(r't')\, S(\infty, -\infty)]$

$$= S(\infty, t)\, C_\alpha(rt)\, S(t, t')\, C^+_\beta(r't')\, S(t', -\infty)$$

$\because S(t_1, t_2) S(t_2, t_3) = S(t_1, t_3)$

$$\therefore = S(\infty, 0) S(0, t)\, C_\alpha(rt)\, S(t, 0) S(0, t')\, C^+_\beta(r't')\, S(t', 0) S(0, -\infty)$$
$$= S(\infty, 0)\, C_{\alpha H}(rt)\, C^+_{\beta H}(r't)\, S(0, -\infty)$$

∴ For $t > t'$

$$\frac{\langle \Phi_0 | T\, C_\alpha(rt)\, C_\beta^+(r't')\, S(\infty,-\infty) | \Phi_0 \rangle}{|\langle \Phi_0 | \Psi_0 \rangle|^2}$$

$$= \frac{\langle \Phi_0 | S(\infty,0)\, C_{\alpha H}(rt)\, C_{\beta H}^+(r't')\, S(0,-\infty) | \Phi_0 \rangle}{|\langle \Phi_0 | \Psi_0 \rangle|^2}$$

$$= \frac{\langle \Psi_0 | C_{\alpha H}(rt)\, C_{\beta H}^+(r't') | \Psi_0 \rangle}{|\langle \Phi_0 | \Psi_0 \rangle|^2} \quad \cdots (126)$$

Ratio of (126) and (120) yields

$t > t'$

$$i G_{\alpha\beta}(rt, r't') = \frac{\langle \Psi_0 | C_{\alpha H}(rt)\, C_{\beta H}^+(r't') | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad \cdots (127)$$

Similarly, for $t < t'$

$$i G_{\alpha\beta}(rt; r't') = - \frac{\langle \Phi_0 | S(\infty,t')\, C_\beta^+(r't')\, C_\alpha(rt)\, S(t,-\infty) | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty,-\infty) | \Phi_0 \rangle}$$

↑ "−" due to exchange C_α C_β

$$= - \frac{\langle \Phi_0 | S(\infty,0)\, C_{\beta H}^+(r't')\, C_{\alpha H}(rt)\, S(0,-\infty) | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty,-\infty) | \Phi_0 \rangle}$$

$$= - \frac{\langle \Psi_0 | C_{\beta H}^+(r't')\, C_{\alpha H}(rt) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \quad \cdots (128)$$

Combing eqs. (127) & (128), we obtain the usual definition (in terms of Ψ_0 & Heisenberg picture)

$$i G_{\alpha\beta}(rt; r't') = \langle \Psi_0 | T[C_{\alpha H}(rt)\, C_{\beta H}^+(r't')] | \Psi_0 \rangle \quad \cdots (129)$$

(set $\langle \Psi_0 | \Psi_0 \rangle = 1$)

Examples of Green's function at T=0

To illustrate the corret definition given by eq. (129), we shall calculate the Green's function in the following three cases:

(i) <u>Empty Band</u> : One should recover the Green's function of one-particle Schrödinger eq.

In this case $|\Psi_0\rangle = |0\rangle$ = vacuum

$\therefore\ c|0\rangle = 0$ $\quad c$ = Schrödinger picture (c in)

$a|0\rangle = 0$ $\quad a$ = annihilation operator for phonon.

In this case, $H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}$, in the Heisenberg picture $c_H(t) = e^{\frac{i}{\hbar}Ht}\, c\, e^{-\frac{i}{\hbar}Ht}$

$$\therefore\ i\hbar \frac{dc_H}{dt} = [c_H(t), H]$$

$$i\hbar \frac{dc_{k\sigma}(t)}{dt} = [c_{k\sigma}(t), H]$$

we shall neglect the index "H"

At equal time, $\{c_{k\alpha}(t), c^\dagger_{k'\beta}(t)\} = \delta_{k,k'}\delta_{\alpha\beta}$

$$\therefore\ [c_{k\sigma}(t), \sum_{k'\sigma'} \varepsilon_{k'} c^\dagger_{k'\sigma'}(t) c_{k'\sigma'}(t)]$$

$$= \sum_{k'\sigma'} \varepsilon_{k'} \{c_{k\sigma}(t), c^\dagger_{k'\sigma'}(t)\} c_{k'\sigma'}(t) = \varepsilon_k c_{k\sigma}(t)$$

$$[A, BC] = ABC - BCA = ABC + BAC - BAC - BCA$$
$$= \{A, B\}C - B\{C, A\}$$

$$\therefore\ i\hbar \frac{dC_{k\sigma}(t)}{dt} = \epsilon_k C_{k\sigma}(t)$$

$$C_{k\sigma}(t) = e^{-\frac{i}{\hbar}\epsilon_k t} C_{k\sigma}(0)$$

At $t=0$. $C_{k\sigma}(0) = C_{k\sigma}$ (Schrödinger picture)

$$\therefore\ C_{k\sigma}(t) = e^{-\frac{i}{\hbar}\epsilon_k t} C_{k\sigma}$$

$\because\ C_{k\sigma}|0\rangle = 0$ $\quad\therefore\ T[C_{\alpha H}(rt)C^{+}_{\beta H}(r't')]|0\rangle$
$= \theta(t-t')\, C_{\alpha H}(rt)C^{+}_{\beta H}(r't')|0\rangle$

$\therefore\ iG_{\alpha\beta}(rt;r't')$

$$= \delta_{\alpha\beta}\left[\int \frac{d^dk}{(2\pi)^d} \langle 0|\, e^{-\frac{i}{\hbar}\epsilon_k t} C_{k\alpha}\, e^{+\frac{i}{\hbar}\epsilon_k t'} C^{+}_{k\beta}|0\rangle\right]\theta(t-t')$$

(with $\frac{d^dk}{(2\pi)^d} \to e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}$)

$$\equiv i\delta_{\alpha\beta}\int \frac{d^dk}{(2\pi)^d} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, G(k,t-t')$$

$$\therefore\ iG(k,t-t') = \theta(t-t')\, e^{-\frac{i}{\hbar}\epsilon_k(t-t')} \underbrace{\langle 0|C_{k\alpha}C^{+}_{k\alpha}|0\rangle}_{1}$$

$$\therefore\ G(k,t-t') = -i\theta(t-t')\, e^{-\frac{i}{\hbar}\epsilon_k(t-t')} \quad \cdots (130)$$

$$G(k,\omega) = \int d(t-t')\, e^{i\omega(t-t')}\, G(k,t-t')$$

$$= \int_0^\infty dt\, e^{i\omega t}\,(-i)\, e^{-\frac{i}{\hbar}\epsilon_k t}$$

To insure the convergence, one introduces $e^{-\epsilon t}$ fact $(\epsilon \to 0^+)$.

$\therefore \int_0^\infty dt \; e^{i(\omega - \frac{1}{\hbar}\epsilon_k + i\epsilon)t}$

$$= \frac{i}{\omega - \frac{\epsilon_k}{\hbar} + i\epsilon}$$

(131)

$G(k,\omega) = \frac{\hbar}{\hbar\omega - \epsilon_k + i0^+}$ which reproduces the Green's function for one-particle Green's function of the Schrödinger equation.

Here we see the cancellation of i. To remove $\hbar$, one can also define $i\hbar\, G_{\alpha\beta} = \langle T[C_{H\alpha} C^\dagger_{H\beta}]\rangle$.

(ii) Degenerate electron gas

$$\langle \Psi_0 | C^\dagger_{k\sigma} C_{k\sigma} | \Psi_0 \rangle = \theta(k_F - k) = \theta(-\xi_k)$$

$$\langle \Psi_0 | C_{k\sigma} C^\dagger_{k\sigma} | \Psi_0 \rangle = 1 - \theta(k_F - k) = \theta(k - k_F) = \theta(\xi_k)$$

(see below)

In this case, $H = \sum_{k\sigma} \xi_k C^\dagger_{k\sigma} C_{k\sigma}$

$$\xi_k = \epsilon_k - \epsilon_F$$

$C_{k\sigma}(t) = e^{-\frac{i}{\hbar}\xi_k t} C_{k\sigma}$
$C^\dagger_{k\sigma}(t) = e^{\frac{i}{\hbar}\xi_k t} C^\dagger_{k\sigma}$ are still correct.

But now $G^0(k, t-t') = -i\theta(t-t') e^{-\frac{i}{\hbar}\xi_k(t-t')} \langle \Psi_0 | C_{k\sigma} C^\dagger_{k\sigma} | \Psi_0 \rangle$

$$+ i\theta(t'-t) e^{-\frac{i}{\hbar}\xi_k(t-t')} \langle \Psi_0 | C^\dagger_{k\sigma} C_{k\sigma} | \Psi_0 \rangle$$

$$= -i\theta(t-t') e^{-\frac{i}{\hbar}\xi_k(t-t')} \theta(\xi_k) + i\theta(t'-t) e^{-\frac{i}{\hbar}\xi_k(t-t')} \theta(-\xi_k)$$

(132)

$$\therefore G^0(k,E) = -i\left[\theta(\xi_k)\int_0^\infty dt\, e^{i\frac{t}{\hbar}[E-\xi_k+i0^+]} - \theta(-\xi_k)\int_{-\infty}^0 dt\, e^{i\frac{t}{\hbar}(E-\xi_k-i0^+)}\right]$$

(E ↑ $\hbar\omega$)

where 0^+ are added to insure the convergence.

$$\therefore G^0(k,E) = \frac{\theta(\xi_k)}{E-\xi_k+i0^+} + \frac{\theta(-\xi_k)}{E-\xi_k-i0^+}$$

$(\hbar \equiv 1)$

or simply

$$G^0(k,E) = \frac{1}{E-\xi_k+i\delta_k} \qquad \delta_k = \delta \,\mathrm{sgn}\, \xi_k \quad \cdots (133)$$

(δ ↑ 0^+)

$(\xi_k > 0,\ i\delta_k = i0^+,\ \xi_k < 0,\ i\delta_k = -i0^+)$

(iii) Phonons

The Green's function for phonons is defined similarly:

$$i D(q,\lambda, t-t') \equiv \langle \Psi_0 | T[A_{q\lambda}(t) A_{q\lambda}(t)] | \Psi_0 \rangle$$

where $A_{q\lambda} \equiv a_{q\lambda} + a_{q\lambda}^\dagger$ is proportional to the displacement field and is in the Heisenberg picture. $a_{q\lambda}$, $a_{q\lambda}^\dagger$ are creation and annihilation operators for phonons with momentum $\hbar q$ and polarization $\hat{\epsilon}_{\lambda q}$.

At $T=0$, $|\Psi_0\rangle = |0\rangle$, $a_{q\lambda}|0\rangle = 0$ (↙ Schrödinger picture)

Consider unperturbed phonons. $H = \sum_{q\lambda} \hbar\omega_q a^+_{q\lambda} a_{q\lambda}$.

Following the derivation for $C_{k\sigma}(t)$, one has

$$i\hbar \frac{d a_{q\lambda}}{dt} = [a_{q\lambda}, H]$$

$\because$ $[A, BC] = ABC - BCA = ABC - BAC + BAC - BCA$

$= [A,B]C + B[A,C]$

$$\therefore \sum_{q'\lambda'} [a_{q\lambda}, a^+_{q'\lambda'} a_{q'\lambda'}] \hbar\omega_{q'\lambda'}$$

$$= \sum_{q'\lambda'} \hbar\omega_{q'} \underbrace{[a_{q\lambda}, a^+_{q'\lambda'}]}_{\delta_{qq'}\delta_{\lambda\lambda'}} a_{q'\lambda'} = \hbar\omega_q a_{q\lambda}$$

$$\therefore i\hbar \frac{d a_{q\lambda}}{dt} = \hbar\omega_q a_{q\lambda}, \quad a_{q\lambda}(t) = e^{-i\omega_q t} a_{q\lambda}$$

$$\therefore iD^0(q, t-t') = \langle 0 | T[a_{q\lambda} e^{-i\omega_q t} + a^+_{-q\lambda} e^{i\omega_q t}]$$
$$[a_{-q\lambda} e^{-i\omega_q t'} + a^+_{q\lambda} e^{i\omega_q t'}] | 0 \rangle$$

$$= \theta(t-t') [\langle 0 | a_{q\lambda} a^+_{q\lambda} e^{-i\omega_q (t-t')} | 0 \rangle$$
$$+ \langle 0 | a^+_{-q\lambda} a_{-q\lambda} e^{i\omega_q (t-t')} | 0 \rangle]$$

$$+ \theta(t'-t) [\langle 0 | a^+_{q\lambda} a_{q\lambda} e^{i\omega_q (t'-t)} | 0 \rangle$$
$$+ \langle 0 | a_{-q\lambda} a^+_{-q\lambda} e^{i\omega_q (t-t')} | 0 \rangle$$

$\because$ $\langle 0 | a_{q\lambda} a^+_{q\lambda} | 0 \rangle = 1$

$\langle 0 | a^+_{q\lambda} a_{q\lambda} | 0 \rangle = 0$

$\therefore \; iD^0(q, t-t')$

$$= \theta(t-t')\, e^{-i\omega_q(t-t')} + \theta(t'-t)\, e^{i\omega_q(t-t')}$$

(assuming $\omega_{-q} = \omega_q$)

$$D^0(q,\omega) = \int d(t-t') e^{i\omega(t-t')} D^0(q, t-t')$$

$$= -i\int_0^{\infty} dt\, e^{it(\omega-\omega_q+i0^+)} - i\int_{-\infty}^{0} dt\, e^{it(\omega-\omega_q-i0^+)}$$ } add 0^+ for convergence

$$= \frac{1}{\omega-\omega_q+i0^+} - \frac{1}{\omega-\omega_q-i0^+}$$

$$= \frac{2\omega_q}{\omega^2-\omega_q^2+i0^+} \quad \cdots \quad (134)$$

<u>Green's function</u> and <u>relation to observables</u>

Once the Green's function can be expressed as operators average w.r.t. the Ground state $|\Psi_0\rangle$ (c.f. eq. (129)), many equilibrium quantities / observables can be calculated by using the Green's function.

For example, for any single-particle operator, one has $\hat{O}(\vec{r}) = \sum_{\alpha\beta} C_\alpha^+(\vec{r})\, O_{\alpha\beta}(\vec{r})\, C_\beta(\vec{r})$

$$\langle \hat{O} \rangle = \frac{\langle \Psi_0 | \hat{O}(\vec{r}) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$$= \lim_{\vec{r}' \to \vec{r}} \sum_{\alpha\beta} O_{\alpha\beta}(\vec{r}) \frac{\langle \Psi_0 | C^\dagger_\alpha(\vec{r}') C_\beta(\vec{r}) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$$= -i \lim_{t' \to t^+} \lim_{\vec{r}' \to \vec{r}} \sum_{\alpha\beta} O_{\alpha\beta}(\vec{r})\, G_{\alpha\beta}(\vec{r}t; \vec{r}'t')$$

$$= -i \lim_{t' \to t^+} \lim_{\vec{r}' \to \vec{r}} \mathrm{Tr}\left[O(\vec{r})\, G(\vec{r}t; \vec{r}'t')\right] \quad \text{--- (135)}$$

examples:

$$\langle \hat{n}(\vec{r}) \rangle = -i\, \mathrm{Tr}\, G(\vec{r}t; \vec{r}t^+)$$

$$\langle \vec{S}(\vec{r}) \rangle = -i \frac{\hbar}{2} \mathrm{Tr}\left[\vec{\sigma}\, G(\vec{r}t; \vec{r}t^+)\right]$$

$$\langle \hat{T} \rangle = -i \int d^3\vec{r} \lim_{\vec{r}' \to \vec{r}} \frac{-\hbar^2 \nabla^2}{2m} \mathrm{Tr}\, G(\vec{r}t; \vec{r}'t^+)$$

($\hat{T}$: Kinetic energy)

What about the interaction

$$\hat{V} = \frac{1}{2} \sum_{\substack{\alpha\alpha' \\ \beta\beta'}} \int d^3\vec{r} \int d\vec{r}'\, C^\dagger_\alpha(\vec{r}) C^\dagger_\beta(\vec{r}')\, V(\vec{r}, \vec{r}')_{\alpha\alpha', \beta\beta'}\, C_{\beta'}(\vec{r}') C_{\alpha'}(\vec{r})$$

($V(\vec{r}, \vec{r}')_{\alpha\alpha',\beta\beta'} = V(\vec{r}', \vec{r})_{\beta\beta',\alpha\alpha'}$)

(t is suppressed)

Do we need two-particle Green's functions?

The answer is no! This is the benefit of using the Heisenberg picture. From eq.(106), one has

$$i\hbar \frac{\partial}{\partial t} C_\alpha(\vec{r}, t) = [C_\alpha(\vec{r}, t), H] \quad \text{--- (136)}$$

(we shall surpress the index of H)

Now, $[C_\alpha(\vec{r},t), T]$ ∵ $T = \frac{-\hbar^2}{2m}\int d^3\vec{r} \sum_\alpha C_\alpha^+(\vec{r},t)\nabla^2 C_\alpha(\vec{r},t)$

$- \mu \sum_\alpha C_\alpha^+ C_\alpha$

$$= \underbrace{\left(\frac{-\hbar^2}{2m}\nabla^2 - \mu\right)}_{\hat{T}(\vec{r})} C_\alpha(\vec{r},t) \quad \text{--- (137)}$$

$[A, BC] = \{A, B\}C - B\{C, A\}$

$[C_\alpha(\vec{r},t), \hat{V}]$ $\left(B = C_\alpha^+(\vec{r},t),\ C = C_\beta^+(\vec{r}',t) \text{ in } V\right)$

$$= \frac{1}{2}\sum_{\alpha'\beta\beta'}\int d^3\vec{r}'\, C_\beta^+(\vec{r}',t)\, V(\vec{r},\vec{r}')_{\alpha\alpha';\beta\beta'} C_{\beta'}(\vec{r}',t)\, C_{\alpha'}(\vec{r},t)$$

$$- \frac{1}{2}\sum_{\alpha\beta\beta'}\int d^3\vec{r}'\, C_\beta^+(\vec{r}',t)\, V(\vec{r}',\vec{r})_{\beta\alpha;\alpha\beta'}\, C_{\beta'}(\vec{r}',t)\, C_{\alpha'}(\vec{r},t)$$

$\vec{r}', \beta \to \alpha, \vec{r}$

$\alpha, \vec{r} \to \beta, \vec{r}'$

rename $\beta' \to \alpha'$, $\alpha' \to \beta'$

$\to -U(\vec{r}',\vec{r})_{\beta\beta';\alpha\alpha'}\, C_{\beta'}(\vec{r},t)\, C_{\alpha'}(\vec{r},t)$

∵ $U(r,r')_{\alpha\alpha',\beta\beta'} = U(r',r)_{\beta\beta',\alpha\alpha'}$

$$\therefore = \sum_{\alpha'\beta\beta'}\int d^3\vec{r}'\, C_\beta^+(\vec{r}',t)\, U(\vec{r},\vec{r}')_{\alpha\alpha',\beta\beta'}\, C_{\beta'}(\vec{r}',t)\, C_{\alpha'}(\vec{r},t) \quad \text{--- (138)}$$

Combining eqs. (136), (137) & (138), we got

$$\left[i\hbar\frac{\partial}{\partial t} - \hat{T}(\vec{r})\right]\frac{\langle\Psi_0|C_{H\alpha}^+(\vec{r}',t')C_{H\alpha}(\vec{r},t)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

$$= \sum_{\alpha'\beta\beta'}\int d^3\vec{r}''\frac{\langle\Psi_0|C_{H\alpha}^+(\vec{r}',t')\, C_{H\beta}^+(\vec{r}'',t)\, V(\vec{r},\vec{r}'')_{\alpha\alpha',\beta\beta'}\, C_{H\beta'}(\vec{r}'',t) C_{H\alpha'}(\vec{r},t)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

Taking $t' \to t'$, $\vec{r}' \to \vec{r}$ & $\sum_\alpha$, the left hand side

$$= -i \lim_{t'\to t^+}\lim_{\vec{r}'\to\vec{r}}\left(i\hbar\frac{\partial}{\partial t} - \hat{T}(\vec{r})\right) G_{\alpha\alpha}(\vec{r}t, \vec{r}'t')$$

The right hand side $\hat{=}$ $2\langle \hat{V} \rangle$ (after integration over $\vec{r}'=\vec{r}$)

$$\therefore \langle \hat{V} \rangle = \frac{-i}{2} \int d^3\vec{r} \lim_{t'\to t} \lim_{\vec{r}'\to r} \left(i\hbar \frac{\partial}{\partial t} - \hat{T}(\vec{r})\right) G_{\alpha\alpha}(\vec{r}t, \vec{r}'t')$$

$$\therefore E = \langle \hat{T} + \hat{V} \rangle = \frac{-i}{2} \int d^3\vec{r} \lim_{t'\to t^+} \lim_{\vec{r}'\to r} \left(i\hbar \frac{\partial}{\partial t} + \hat{T}\right) \mathrm{Tr}\, G(\vec{r}t, \vec{r}'t')$$

$$= \frac{-i}{2} \int d^3\vec{r} \lim_{t'\to t} \lim_{\vec{r}'\to r} \left(i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2 \nabla^2}{2m}\right) \mathrm{Tr}\, G(\vec{r}t, \vec{r}'t') \quad \text{--- (139)}$$

In Fourier space, One has

$$G_{\alpha\beta}(\vec{r}t, \vec{r}'t') = \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} e^{i\vec{k}\cdot(\vec{r}-\vec{r}') - i\omega(t-t')} G_{\alpha\beta}(\vec{k}, \omega)$$

One obtains

$$N = \int d^3r\, n(\vec{r}) = -i \frac{V}{(2\pi)^4} \lim_{\eta\to 0^+} \int d^3\vec{k} \int d\omega\, e^{i\omega\eta}\, \mathrm{Tr}\, G(\vec{k}, \omega)$$

($e^{i\omega\eta} \sim e^{-i\omega(t-t')}$)

$$E = -\frac{i}{2} \frac{V}{(2\pi)^4} \lim_{\eta\to 0^+} \int d^3k \int d\omega\, e^{i\omega\eta} \left(\frac{\hbar^2 k^2}{2m} + \hbar\omega\right) \mathrm{Tr}\, G(\vec{k}, \omega) \quad \text{--- (140)}$$

Here, the usage of $\eta \to 0^+$ is to define the appropriate contour in the ω-integration.

Note that Eqs. (140) are also valid for bosons if $(-i)$ is changed into $+i$.

The Lehmann representation & analytic properties of G.

From the definition of $G_{\alpha\beta}$ in eq. (129), one has

$$iG_{\alpha\beta}(\vec{r}t, \vec{r}'t')$$

$$= \theta(t-t') \langle \Psi_0 | C_{H\alpha}(\vec{r}t) C^{+}_{H\beta}(\vec{r}'t') | \Psi_0 \rangle$$

$$- \theta(t'-t) \langle \Psi_0 | C^{+}_{H\beta}(\vec{r}'t') C_{H\alpha}(\vec{r}t) | \Psi_0 \rangle \quad \cdots (141)$$

We now insert $\sum_n |\Psi_n\rangle\langle\Psi_n| = \mathbb{1}$ between C & C^{+}.

where $\{|\Psi_n\rangle\}$ are a complete set of $\hat{H}$, with energies being E_n.

$|\Psi_n\rangle$ generally does not contain the same # of particles $|\Psi_0\rangle$. If # of particles for $|\Psi_0\rangle$ is N, the relevant $|\Psi_n\rangle$ contains $N \pm 1$ particles.

$$\because \hat{O}_H(t) = e^{i\hat{H}t/\hbar} \, \hat{O} \, e^{-i\hat{H}t/\hbar}$$

Eq. (141) becomes

$$iG_{\alpha\beta}(\vec{r}t, \vec{r}'t') = \sum_n \Big[\theta(t-t') \, e^{-\frac{i}{\hbar}(E_n - E)(t-t')} \langle \Psi_0 | C_\alpha(\vec{r}) | \Psi_n \rangle \langle \Psi_n | C^{+}_\beta | \Psi_0 \rangle$$

$$- \theta(t-t') \, e^{\frac{i}{\hbar}(E_n - E)(t-t')} \langle \Psi_0 | C^{+}_\beta(\vec{r}') | \Psi_n \rangle \langle \Psi_n | C_\alpha(\vec{r}) | \Psi_0 \rangle \Big]$$

$$\cdots (142)$$

For translationally invariant systems, the momentum is a good number. $\because$ $\hat{P} = \sum_\alpha \int d^3r \, C^{+}_\alpha(\vec{r}) \left(\frac{\hbar \vec{\nabla}}{i}\right) C_\alpha(\vec{r})$

$$= \sum_{\alpha k} \hbar k \, C^{+}_{k\alpha} C_{k\alpha}$$

$\therefore [\hat{C}_\alpha(\vec{r}), \hat{\vec{p}}] = \frac{\hbar\vec{\nabla}}{i}\hat{C}_\alpha(\vec{r})$

This is to be compared with the Heisenberg picture $i\hbar\frac{dC_H}{dt} = [C_H, H]$

$$C_H = e^{\frac{i}{\hbar}Ht} C e^{-\frac{i}{\hbar}Ht}$$

$$\therefore \hat{C}_\alpha(\vec{r}) = e^{-\frac{i\vec{p}\cdot\vec{r}}{\hbar}} \hat{C}_\alpha(0) e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$$

$\because \vec{p}$ is a constant of motion, $|\Psi_n\rangle$ can be taken as eigenstate of momentum, with eigenvalue $\vec{P}_n$.

$\therefore iG_{\alpha\beta}(\vec{r}t, \vec{r}'t')$

$$= \sum_n \Big[\theta(t-t')e^{-\frac{i}{\hbar}(E_n-E)(t-t')} e^{\frac{i}{\hbar}\vec{P}_n\cdot(\vec{r}-\vec{r}')} \langle\Psi_0|\hat{C}_\alpha(0)|\Psi_n\rangle\langle\Psi_n|\hat{C}_\beta^\dagger(0)|\Psi_0\rangle$$

$$-\theta(t'-t)e^{\frac{i}{\hbar}(E_n-E)(t-t')} e^{-i\frac{\vec{P}_n}{\hbar}\cdot(\vec{r}-\vec{r}')}\langle\Psi_0|\hat{C}_\beta^\dagger(0)|\Psi_n\rangle\langle\Psi_n|\hat{C}_\alpha(0)|\Psi_0\rangle\Big]$$

where the eigenvalue of momentum for $|\Psi_0\rangle = 0$.

We can now perform the Fourier transform

$$G_{\alpha\beta}(\vec{k}, \omega) = \int d^3(\vec{r}-\vec{r}')\int d(t-t')\, e^{-i\vec{k}\cdot(\vec{r}-\vec{r}')} e^{i\omega(t-t')} G_{\alpha\beta}(\vec{r}t, \vec{r}'t')$$

The spatial integration yields $V\sum_n \delta_{\vec{k}, \vec{P}_n/\hbar}$, so we shall set $\vec{P}_n = \hbar\vec{k}$, and $|\Psi_n\rangle = |n\vec{k}\rangle$.

$$\therefore G_{\alpha\beta}(\vec{k}, \omega) = V\sum_n \left[\frac{\langle\Psi_0|\hat{C}_\alpha(0)|n\vec{k}\rangle\langle n\vec{k}|\hat{C}_\beta^\dagger(0)|\Psi_0\rangle}{\omega - \hbar^{-1}(E_n - E) + i0^+}\right.$$

$$+ \frac{\langle \Psi_0 | \hat{C}_\beta^+(0) | n -\vec{k}\rangle \langle n-\vec{k} | C_\alpha(0) | \Psi_0\rangle}{\omega + \hbar^{-1}(E_n - E) - i0^+} \Bigg]$$

Note that in the 1st summation, $E = E(N)$,

$E_n = E_n(N+1)$. Let $E(N+1)$ be the ground state energy for $N+1$ particles.

We have

$$\omega - \hbar^{-1}(E_n(N+1) - E(N)) = \omega - \hbar^{-1}[E_n(N+1) - E(N+1)]$$
$$- \hbar[E(N+1) - E(N)]$$

$E(N+1) - E(N) = \mu$ (chemical potential)

$E_n(N+1) - E(N+1) = \varepsilon_n(N+1)$ = excitation energy of the $N+1$ particle system.

Similarly, in the 2nd summation, one has

$$\omega + \hbar^{-1}(E_n - E) = \omega - \hbar^{-1}[E(N) - E(N-1)]$$

(E_n: $E_n(N-1)$, E: $E(N)$)

$$+ \hbar^{-1}[E_n(N-1) - E(N-1)]$$

$$= \omega - \hbar^{-1}\mu + \hbar^{-1}\varepsilon_n(N-1)$$

Here we made use of $\mu(N+1) = \mu(N) + O(N^{-1})$

$$\therefore G_{\alpha\beta}(\vec{k},\omega) = \hbar V \sum_n \Bigg[\frac{\langle \Psi_0 | \hat{C}_\alpha(0) | n\vec{k}\rangle \langle n\vec{k} | \hat{C}_\beta^+(0) | \Psi_0\rangle}{\hbar\omega - \mu - \varepsilon_{n\vec{k}}(N+1) + i0^+}$$

$$+ \frac{\langle \Psi_0 | \hat{C}_\beta^+(0) | n -\vec{k}\rangle \langle n-\vec{k} | \hat{C}_\alpha(0) | \Psi_0\rangle}{\hbar\omega - \mu + \varepsilon_{n-\vec{k}}(N-1) - i0^+} \Bigg]$$

Now, for isotropic systems, the matrix of the Green's function $\mathbb{G}(\vec{k},\omega)$ can only depend on $\vec{k}$ and can be expanded in terms of the Pauli matrices

$$\therefore \mathbb{G}(\vec{k},\omega) = a\mathbb{1} + b\vec{\sigma}\cdot\vec{k}$$

where a & b are functions of ω & k^2.

$\vec{\sigma}$ = Pauli matrices

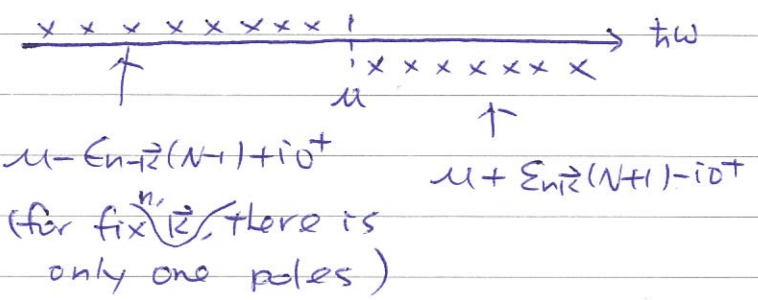
However, the term $\vec{\sigma}\cdot\vec{k}$ is not invariant under spatial reflection $(\vec{k}_1 \to -\vec{k}_1)$. Hence if the Hamiltonian & ground state are invariant under rotation and spatial reflections, one has $G_{\alpha\beta}(\vec{k},\omega) = \delta_{\alpha\beta}\, G(\vec{k},\omega) = \delta_{\alpha\beta}\, G(|\vec{k}|,\omega)$

$\therefore$ We can set $\alpha=\beta$ and $\sum_\alpha \cdot \frac{1}{2S+1}$

$$\therefore G(\vec{k},\omega) = \frac{\hbar V}{2S+1}\sum_{n,\alpha}\left[\frac{|\langle n\vec{k}|\hat{c}_\alpha^\dagger(0)|\Psi_0\rangle|^2}{\hbar\omega-\mu-\varepsilon_{n\vec{k}}(N+1)+i0^+} + \frac{|\langle n-\vec{k}|c_\alpha(0)|\Psi_0\rangle|^2}{\hbar\omega-\mu-\varepsilon_{n\vec{k}}(N-1)-i0^+}\right] \quad \text{--- (43)}$$

This is the Lehmann representation which exhibits the analytic properties of $G(\vec{k},\omega)$:

G has simple poles at exact excitation energies of the interacting system corresponding to a momentum $\hbar\vec{k}$!



For $\hbar\omega < \mu$, poles lie above the real axis.

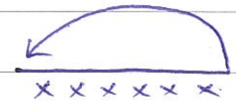
For $\hbar\omega > \mu$, poles lie in below the real axis.

Clearly, one can redefine the Green's function so that all poles are on one side of the real axis. There are retarded and advanced Green's functions:

retarded Green's function

$$G^R_{\alpha\beta}(k,\omega) = \hbar V \sum_n \left[\frac{\langle\Psi_0|\hat{C}_\alpha(0)|n\vec{k}\rangle\langle n\vec{k}|\hat{C}^+_\beta(0)|\Psi_0\rangle}{\hbar\omega - \mu - \varepsilon_{n\vec{k}}(N+1) + i0^+} + \frac{\langle\Psi_0|\hat{C}^+_\beta(0)|n-\vec{k}\rangle\langle n-\vec{k}|\hat{C}_\alpha(0)|\Psi_0\rangle}{\hbar\omega - \mu + \varepsilon_{n-\vec{k}}(N-1) + i0^+} \right] \quad (144)$$

So that $\int d\omega\, e^{-i\omega(t-t')} G^R_{\alpha\beta}(k,\omega)$, in the contour integral,



$t < t'$ $= 0$

$\therefore$ One changes $-\theta(t'-t)$ in eq. (141) to $\theta(t-t')$.

$$\therefore\ iG^R_{\alpha\beta}(\vec{r}t, \vec{r}'t') = \theta(t-t')\langle\Psi_0|\{C_{H\alpha}(\vec{r}t), C^+_{H\beta}(\vec{r}'t')\}|\Psi_0\rangle \quad (145)$$

Similarly, by changing $i0^+ \to -i0^+$ in eq. (144), one get $G^A(\vec{k}, \omega)$. Hence

$$iG^A(\vec{r}t, \vec{r}'t') = -\theta(t'-t)\langle \Psi_0 | \{ C_{H\alpha}(\vec{r}t), C^+_{H\beta}(\vec{r}', t') \} | \Psi_0 \rangle$$

$\llcorner$ - - (146)

Clearly, one has (for real ω)

$$[G^R_{\alpha\beta}(k, \omega)]^* = G^A_{\beta\alpha}(k, \omega) \quad \text{- - (147)}$$

$$(\langle n\vec{k} | C^+_\beta(0) | \Psi_0 \rangle^* = \langle \Psi_0 | C_\beta(0) | n\vec{k} \rangle)$$

$\hbar\omega > \mu$ $\quad G^R_{\alpha\beta}(k, \omega) = G_{\alpha\beta}(k, \omega)$

$\hbar\omega < \mu$ $\quad G^A_{\alpha\beta}(k, \omega) = G_{\alpha\beta}(k, \omega)$

Thermodynamic limit

In the thermodynamic limit, one may replace

$\sum_n$ by $\int d\varepsilon \underbrace{\frac{dn}{d\varepsilon}}_{\text{density of states}}$ because $\Delta E_n \to 0$ as $V \to \infty$.

$$\frac{V}{(2S+1)} \sum_{\alpha, n} \frac{|\langle n\vec{k} | \hat{C}^+_\alpha(0) | \Psi_0 \rangle|^2}{\hbar\omega - \mu - \varepsilon_{n\vec{k}}(N+1) + i0^+} \qquad (\text{eq. (143)})$$

$$\to \frac{V}{(2S+1)} \int d\varepsilon \frac{dn}{d\varepsilon} \frac{(- - -)}{\hbar\omega - \mu - \varepsilon + i0^+}$$

$$\equiv \int_0^\infty d\omega' \frac{A(\vec{k}, \omega')}{\omega - \hbar^{-1}\mu - \omega' + i0^+}$$

Similarly,

$$\frac{V}{2S+1}\sum_{n,\alpha}\frac{|\langle n-\vec{k}|\hat{c}_\alpha(0)|\Psi_0\rangle|^2}{\hbar\omega-\mu-\varepsilon_{n\vec{k}}(N-1)-i0^+}$$

$$\rightarrow \int_0^\infty d\omega' \frac{B(\vec{k},\omega')}{\omega-\hbar^{-1}\mu+\omega'-i0^+}$$

$$\therefore\ G(\vec{k},\omega)=\int_0^\infty d\omega'\left[\frac{A(\vec{k},\omega')}{\omega-\hbar^{-1}\mu-\omega'+i0^+}+\frac{B(\vec{k},\omega')}{\omega-\hbar^{-1}\mu+\omega'-i0^+}\right]$$

(In the thermodynamic limit.) ← (148)

Similarly,

$$G^{R,A}(\vec{k},\omega)=\int_0^\infty d\omega'\left[\frac{A(\vec{k},\omega')}{\omega-\hbar^{-1}\mu-\omega'\pm i0^+}+\frac{B(\vec{k},\omega')}{\omega-\hbar^{-1}\mu+\omega'\pm i0^+}\right]$$

→ they satisfy the Kramer-Kronig relations

(Hence they are analytic in upper/lower Complex plane.) ← (149)

Therefore, in the thermodynamic limit, there is now a <u>branch cut along the real ω axis</u>. because the discrete poles have merged into a branch line.

Eqs. (148) & (149) show that all Green's functions can be constructed if A and B are known.

Now,
$$A=\frac{V}{(2S+1)\hbar}\sum_\alpha\frac{dn}{d\varepsilon}|\langle n\vec{k}|c_\alpha^\dagger(0)|\Psi_0\rangle|^2$$

$$B=\frac{V}{(2S+1)\hbar}\frac{dn}{d\varepsilon}\sum_\alpha|\langle n-\vec{k}|c_\alpha(0)|\Psi_0\rangle|^2$$

No.
Date.

Furthermore, if we consider the average of anti-commutator $\{\hat{C}_\alpha(r,t), \hat{C}_\beta(\vec{r}',t)\} = \delta(\vec{r}-\vec{r}')$, we obtain

$$\langle \Psi_0 | \{\hat{C}_\alpha(r), \hat{C}_\beta^{+}(\vec{r}')\} | \Psi_0 \rangle = \delta(\vec{r}-\vec{r}')$$

Similar analysis of the above equation leads to

$$\delta(\vec{r}-\vec{r}') = \frac{1}{(2S+1)} \sum_{n,\alpha} \Big[e^{\frac{i\vec{P}_n\cdot(\vec{r}-\vec{r}')}{\hbar}} |\langle \Psi_n | \hat{C}_\alpha^{+}(0) | \Psi_0 \rangle|^2 + e^{-\frac{i}{\hbar}\vec{P}_n\cdot(\vec{r}-\vec{r}')} |\langle \Psi_n | \hat{C}_\alpha(0) | \Psi_0 \rangle|^2 \Big]$$

So that after Fourier transformation, one obtains

$$1 = \frac{V}{(2S+1)} \sum_n \Big[|\langle n \vec{k} | \hat{C}_\alpha^{+}(0) | \Psi_0 \rangle|^2 + |\langle n -\vec{k} | \hat{C}_\alpha(0) | \Psi_0 \rangle|^2 \Big]$$

which becomes (in the thermodynamic limit)

$$1 = \int_0^\infty d\omega \, [A(\vec{k},\omega) + B(\vec{k},\omega)] \quad \text{--- (150)}$$

Eq. (150) implies that when $|\omega| \to \infty$

Eqs. (147) & (148) $\Rightarrow$ $G(k,\omega) = G^R(k,\omega) = G^A(k,\omega)$

$$\sim \frac{1}{\omega} \int_0^\infty d\omega' \, [A(\vec{k},\omega') + B(\vec{k},\omega')] \sim \frac{1}{\omega}.$$

General dynamics & time-loop S matrix

The adiabatic switch on ($-\infty$, to 0) and off (0 to ∞) enables the S matrix $S_\varepsilon(\infty, -\infty)$ to take $|\Phi_0\rangle$ at $t=-\infty$ to $|\Phi_0\rangle$ at $t=\infty$.

As a result, one can perform all calculations w.r.t. Φ_0 as shown, for example, eq. (122).

The real S-matrix, $S(\infty, -\infty)$, however, does not have this property, i.e., $S(\infty,-\infty)|\Phi_0\rangle \neq e^{i\delta}|\Phi_0\rangle$!

How to deal $S(\infty,-\infty)$ without adiabatic turning on?

Schwinger (1961) (also Keldysh) suggested another way to handle $t\to\infty$. The method (usually referred as Keldysh formalism) turns out to be a general method that can even treat non-equilibrium properties.

The idea is to go from $-\infty$ to ∞ and then from ∞ back $-\infty$. By doing so, the initial & final state are the known state $|\Phi_0\rangle$!
(the state $\Psi(t=\infty)$ is avoided)
The integration path is a time loop now as indicated in below.

The formalism can be derived by going back to the interacting picture. Here we shall assume

$$H = H_0 + V(t)$$

with explicitly-time-dependant $V(t)$, so that one can deal with non-equilibrium situations.

To see how Schwinger's proposal works, we start by noting that for one operator,

$\langle O \rangle_t = \langle \Psi(t) | \hat{O} | \Psi(t) \rangle$ is the most general expectation value, including non-equilibrium properties.

In the Heisenberg picture, one reexpresses

$$\langle \hat{O} \rangle = \langle \Psi(0) | \underbrace{U^{+}(t)\, \hat{O}\, U(t)}_{\hat{O}_H(t)} \underbrace{|\Psi(0)\rangle}_{|\Psi_H\rangle} ,$$

where it is no longer possible to write $U(t) = e^{-\frac{i}{\hbar} H t}$ as V is now time-dependant.

Now, in the interaction picture, one has

$$|\Psi_I(t)\rangle = \underbrace{U_0^{+}(t)\, U(t)}_{U_I(t)} |\Psi(0)\rangle , \quad U_0(t) = e^{-\frac{i}{\hbar} H_0 t}$$

$\therefore |\Psi(0)\rangle = U_I^{+}(t)\,|\Psi_I(t)\rangle \quad (U_I U_I^{+} = \mathbb{I})$

$\therefore \langle O \rangle_t = \langle \Psi_I(t) | U_I(t)\, U^{+}(t)\, \hat{O}\, U(t)\, U_I^{+}(t)\, | \Psi_I(t) \rangle$

$$= \langle \Psi_I(t) | \underbrace{U_0^{+}(t)\, \hat{O}\, U_0(t)}_{\hat{O}_I(t)} | \Psi_I(t) \rangle \quad \cdots (151)$$

In addition, $|\Psi_I\rangle$ at different times are related by the S-matrix as follows:

$$|\Psi_I(t)\rangle = U_I(t)\, |\Psi(0)\rangle$$

$$= \underbrace{U_I(t)\, U_I^{+}(t')}_{S(t,t')}\, |\Psi_I(t')\rangle \quad \cdots (152)$$

$\because \; i\hbar \frac{\partial U(t)}{\partial t} = H\, U(t), \quad i\hbar \frac{\partial U_0}{\partial t} = H_0 U_0$

$$\therefore i\hbar \frac{\partial U_I}{\partial t} = i\hbar \frac{\partial U_0^{+}}{\partial t} U + i\hbar U_0^{+} \frac{\partial U}{\partial t}$$

$$= H_0 U_0^{+} U + U_0^{+} (H U)$$

$$= U_0^{+} \underbrace{(H - H_0)}_{V} U_0 U_0^{+} U$$

$$= V_I(t)\, U_I(t)$$

$\therefore$ As done before, one gets $U_I(t) = T\, e^{\frac{-i}{\hbar}\int_0^t V_I(t')\,dt'}$

Similarly, $i\hbar \frac{\partial S(t,t')}{\partial t} = i\hbar \frac{\partial U_I(t)}{\partial t} U_I^{+}(t')$

$$= V_I(t)\, S(t,t'), \quad S(t',t') = \mathbb{I}$$

$$\therefore S(t,t') = T\, e^{\frac{-i}{\hbar}\int_{t'}^{t} V_I(t_1)\,dt_1} \quad \cdots (153)$$

Taking $t' \to -\infty$ and denote $|\Psi_I(-\infty)\rangle = |\Phi_0\rangle$ which is presumed to the ground state of H_0, eqs. (151) & (152) give

$$\langle O \rangle_t = \langle \Phi_0 | S^+(t,-\infty)\, \hat{O}_I(t)\, S(t,-\infty) | \Phi_0 \rangle$$

$$= \langle \Phi_0 | S(-\infty,t)\, \hat{O}_I(t)\, S(t,-\infty) | \Phi_0 \rangle \quad \text{--- (154)}$$

This is what is shown on the figure of page 121 ($\tau \equiv t$). One does return to Φ_0. However, returning to $|\Phi_0\rangle$ is not the issue, the problem is that the combination of $S(-\infty,t)$, $\hat{O}_I(t)$ & $S(t,-\infty)$ can not be unified under "time-ordering" which is ~~the natural representation~~ of S-matrix as shown in eq. (153)

$$S(t,-\infty) = T\, e^{-\frac{i}{\hbar}\int_{-\infty}^{t} V_I(t')\,dt'}$$

In the case of equilibrium, this is overcome by inserting $S(-\infty,\infty)\, S(\infty,-\infty) = \mathbb{I}$ in eq. (154)

$$\therefore \langle O \rangle_t = \langle \Phi_0 | S(-\infty,\infty)\, \underbrace{S(\infty,t)\, O_I(t)\, S(t,-\infty)}_{=\; T\, e^{-\frac{i}{\hbar}\int_{-\infty}^{\infty} U_I(t')\,dt'}\, O_I(t)} | \Phi_0 \rangle$$

where $S(\infty,t)\, O_I(t)\, S(t,-\infty)$ can be unified under time-ordering.

$\therefore \langle O \rangle_t = \langle \Phi_0 | S(-\infty, \infty) T[S(\infty,-\infty) O_I(t)] | \Phi_0 \rangle$ --- (155)

As implied by adiabatically switching on/off,

$S(\infty,-\infty)|\Phi_0\rangle = e^{iL}|\Phi_0\rangle$, eq. (155) becomes

$\langle O \rangle_t = e^{-iL} \langle \Phi_0 | T e^{\frac{-i}{\hbar}\int_{-\infty}^{\infty} V_I(t')dt'} \hat{O}_I(t) | \Phi_0 \rangle$

and leads to eq. (124) for equilibrium case.

For general $V(t)$,

$S(\infty,-\infty)|\Phi_0\rangle = e^{iL}|\Phi_0\rangle$ --- (156)

is no longer true, then how to unify $S(-\infty,t)$, $\hat{O}_I(t)$ & $S(t,-\infty)$ in eq. (154)?

Eq. (155) is essentially the Schwinger's proposal. One first goes from $-\infty$ to ∞ (Time ordering) and goes from $t=\infty$ to $-\infty$ via anti-time ordering: $\bar{T} \equiv$ anti-time ordering

$S(-\infty,\infty) = S^{+}(\infty,-\infty) = \bar{T} e^{\frac{i}{\hbar}\int_{-\infty}^{\infty} V_I(t')dt'}$ --- (157)

Overall, one combines time-ordering and anti-time ordering as the time-loop path ordering T_C: (contour-ordering)

$$\langle O\rangle_t = \langle \Phi_0 | T_c\left[e^{-\frac{i}{\hbar}\int_c V_I(t')dt'} O_I(t)\right] | \Phi_0 \rangle \quad \text{--- (158)}$$

where $S(\infty,-\infty) = \mathbb{I}$ ∴ we don't need to divide it out in the denominator.

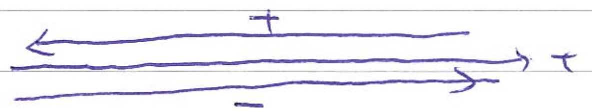
This is the case for a single operator. It's soon realized that if one has more than one operator, one needs to distinguish whether the operator is in the <u>time-ordering branch</u> or <u>anti-time-ordering branch</u>.

Hence the Green's function should be generally defined by

$$iG_{\alpha\beta}(rs; r's') \equiv \langle \Phi_0 | T_c\left[e^{-\frac{i}{\hbar}\int_c V_I(t)dt} C_\alpha(rs) C^{+}_\beta(r's')\right] | \Phi_0\rangle \quad \text{--- (159)}$$

where C_α, C^+_β are in the interaction picture and s & s' are time labels along the contour.

For a given time t, t can be either in time-ordering ($-$) branch or anti-time ordering branch ($+$). ∴ <u>$s = t^{\pm}$</u>

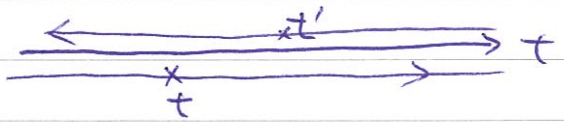


Clearly, one has 4 possible combination and 4 kinds of Green's functions. Together with the retarded and advanced Green's functions, one obtain six Green's functions.

<u>Six Green's functions</u>

(i) $s = t^-$, $s' = t'^+$ $\qquad G \equiv G^>$ (greater component)
$\qquad\qquad\qquad\qquad\qquad\qquad (G^{-+})$

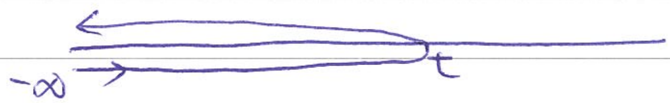
$$G^>_{\alpha\beta}(\vec{r}t, \vec{r}'t') = -i \langle \Phi_0 | S(-\infty, t) C_\alpha(r,t) S(t, \infty)$$
$$S(\infty, t') C^+_\beta(r', t') S(t', -\infty) | \Phi_0 \rangle \quad \leftarrow \ldots (160)$$



Just as in the case of equilibrium formalism, it is possible to express eq. (160) in the Heisenberg picture.

If one takes $t = -\infty$ as the reference point to define the Heisenberg / interaction picture (i.e., not restrict $e^{\frac{i}{\hbar}H}$ as the definition shown in eq. (151)), eq. (154) implies

$$\hat{O}_H(t) = S(-\infty, t)\, \hat{O}_I(t)\, S(t, -\infty) \quad \leftarrow \ldots (161)$$



$\because\ S(t,\infty)\,S(\infty,t') = S(t,t')$

$= S(t,-\infty)\,S(-\infty,t')$, $\therefore$ eq. (160) becomes

$$G^{>}_{\alpha\beta}(\vec{r}t;\vec{r}'t') = -i\,\langle\Phi_0|\,S(-\infty,t)\,C_\alpha(\vec{r}t)\,S(t,-\infty)\,S(-\infty,t')\,C^{+}_{\beta}(\vec{r}'t')\,S(t',-\infty)\,|\Phi_0\rangle$$

$$= -i\,\langle C_{\alpha H}(\vec{r}t)\,C^{+}_{\beta H}(\vec{r}'t')\rangle \quad \text{--- (161)}$$

where one does not have restrict $t=-\infty$

$|\Psi_I(t=-\infty)\rangle = |\Phi_0\rangle$ (ground state of non-interacting Hamiltonian H_0), and at $t=-\infty$, $|\Psi_I\rangle = |\Psi_H\rangle$ can be any state, including the intearcting Ground state.

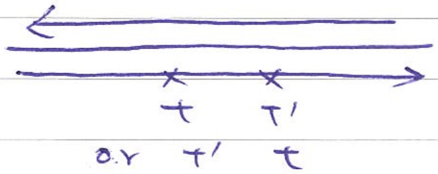
(ii) $s = t^{+}$, $s = t'^{-}$, $G \equiv G^{<}$ (lesser component) (G^{+-})

$$G^{<}_{\alpha\beta}(\vec{r}t;\vec{r}'t') = i\,\langle\Phi_0|\,S(-\infty,t')\,C^{+}_{\beta}(\vec{r}',t')\,S(t',\infty)\,S(\infty,t)\,C_\alpha(\vec{r},t)\,S(t,-\infty)\,|\Phi_0\rangle$$

$$= i\,\langle C^{+}_{\beta H}(\vec{r}'t')\,C_{\alpha H}(\vec{r},t)\rangle$$

(iii) $s = t^{-}$, $s = t'^{-}$

$G =$ time-ordered Green's function $\equiv G^{--}$



$$i\,G_{\alpha\beta}(\vec{r}t;\vec{r}'t') = \langle\Phi_0|\,T\left[S(-\infty,\infty)\,C_\alpha(rt)\,C^{+}_{\beta}(r't')\right]S(\infty,-\infty)\,|\Phi_0\rangle$$

For $t < t'$

$$iG_{\alpha\beta} = \langle \Phi_0 | \underline{S(-\infty, t)\, C_\alpha(\vec{r}, t)\, S(t, t')\, C^{+}_{\beta}(\vec{r}', t')\, S(t', \infty)}\, S(\infty, -\infty) | \Phi_0 \rangle$$

$$= \langle \Phi_0 | S(-\infty, t)\, C_\alpha(\vec{r}, t)\, S(t, t')\, C^{+}_{\beta}(\vec{r}', t')\, S(t', -\infty) | \Phi_0 \rangle$$

$$\uparrow \quad S(t, -\infty)\, S(-\infty, t')$$

$$= \langle \Phi_0 | C_{\alpha H}(\vec{r}, t)\, C^{+}_{\beta H}(\vec{r}', t') | \Phi_0 \rangle = \langle C_{\alpha H}(\vec{r}t)\, C^{+}_{\beta H}(\vec{r}'t') \rangle$$

Similarly, for $t' < t$

$$iG_{\alpha\beta} = -\langle \Phi_0 | S(\infty, t')\, C^{+}_{\beta}(\vec{r}'t')\, S(t', t)\, C_\alpha(\vec{r}, t)\, S(t, -\infty)\, S(\infty, -\infty) | \Phi_0 \rangle$$

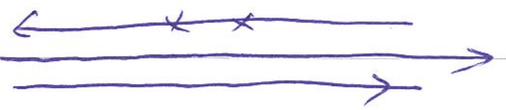
$$= -\langle C^{+}_{\beta H}(\vec{r}', t')\, C_{\alpha H}(\vec{r}, t) \rangle$$

$$\therefore\ iG_{\alpha\beta}(\vec{r}t, \vec{r}'t') = \langle T [C_{\alpha H}(\vec{r}t)\, C^{+}_{\beta H}(\vec{r}'t')] \rangle$$

which is exactly the same form as the one we defined for the equilibrium case.

(iv) $s = t^{+}$, $s' = t'^{+}$

$G =$ anti-time-ordered Green's function



$= G^{++}$

One obtains

$$iG^{++}_{\alpha\beta}(\vec{r}t; \vec{r}'t') = \langle \tilde{T} [C_{\alpha H}(\vec{r}t)\, C^{+}_{\beta H}(\vec{r}'t')] \rangle$$

(V)/(Vi) . In addition to (i) ~ (iv), one also has the retarded Green's function (eq. (145))

$$i G^R_{\alpha\beta}(\vec{r}t, \vec{r}'t') = \theta(t-t') \langle \{ C_{H\alpha}(\vec{r}t), C^+_{H\beta}(\vec{r}'t') \} \rangle$$

$$= \theta(t-t') \langle C_{H\alpha}(\vec{r}t) C^+_{H\beta}(\vec{r}'t') \rangle$$

$$- \theta(t'-t) \langle C^+_{H\beta}(\vec{r}'t') C_{H\alpha}(\vec{r}t) \rangle$$

$$+ \theta(t'-t) \langle C^+_{H\beta}(\vec{r}'t') C_{H\alpha}(\vec{r}t) \rangle + \theta(t-t')$$

$$\langle C^+_{H\beta}(\vec{r}'t') C_{H\alpha}(\vec{r}t) \rangle$$

$$= \langle T[C_{H\alpha}(\vec{r}t) C^+_{H\beta}(\vec{r}'t')] \rangle + \langle C^+_{H\beta}(\vec{r}'t') C_{H\alpha}(\vec{r}t) \rangle$$

↑ $\theta(t-t') + \theta(t'-t) = 1$

$\therefore$ $G^R = G^{--} - G^<$ is not an independent one.

Other expressions are equally well:

$$G^R = \theta(t-t') [G^<(t,t') - G^>(t,t')]$$

$$= G^> - G^{++}$$

$$G^{--} + G^{++} = G^< + G^> = G^{-+} + G^{+-}$$

Similarly, from eq. (146), one also obtains

$$i G^A_{\alpha\beta}(\vec{r}t, \vec{r}'t') = -\theta(t'-t) \langle \{ C_{H\alpha}(\vec{r}t), C^+_{H\beta}(\vec{r}'t') \} \rangle$$

$$G^A = \theta(t'-t) [G^<(t,t') - G^>(t,t')]$$

$$= G^{--} - G^> = G^< - G^{++}$$

The Keldysh Formalism

As we have seen, in the most general situation, one has 3 independent Green's functions.

$$(G^{++} + G^{--} = G^{-+} + G^{+-})$$

Keldysh arranged them into a 2x2 matrix Green's function

$$\hat{G}(1,2) \equiv \begin{pmatrix} G^{--}(1,2) & G^{-+}(1,2) \\ G^{+-}(1,2) & G^{++}(1,2) \end{pmatrix}$$

where $1 \equiv (\alpha, \vec{r}, t)$, $2 \equiv (\beta, \vec{r}', t')$

From $\hat{G}$, one developes the perturbation theory for non-equilibrium systems. This is known as the keldysh Formalism.

Note that since there are only 3 independent Green's functions, it is possible to rotate $\hat{G}$ by

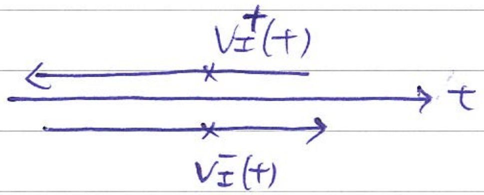
$$\bar{G} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \hat{G} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} G^R & G^{+-} + G^{-+} \\ 0 & G^A \end{pmatrix}$$ to exhibit 3 independent components,

where $G^{+-} + G^{-+} \equiv G^K$ is the so-called Keyldysh Green's function.

In addition to the complication due to more components in the Green's functions, the interaction also proliferates in the non-equilibrium problem.

This can be seen by noting that the involved S-matrix is $T_c \int e^{\frac{-i}{\hbar}\int_c V_I(t')dt'}$



Hence $V_I(t)$ is doubled into V_I^- & V_I^+

In this case, V_I^+ results from anti-time ordering,

$$\bar{T} e^{\frac{i}{\hbar}\int_{-\infty}^{\infty} V_I(t')dt'}$$

Therefore, $V_I^+(t) = -V_I(t)$, $V_I^- = V_I(t)$

V_I^- & V_I^+ can be arranged as $V_I(t)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. It is understood that + components have to come after − components.

<u>Quantum Kinetic equation</u>

The Keldysh formalism has close connection to the Quantum Kinetic equation, which is the generalization of the Boltzman equation, based on the Wigner function

$$f^{\omega}(\vec{r},\vec{p},t) \equiv \int d^3\xi\, e^{-\frac{i\vec{p}\cdot\vec{\xi}}{\hbar}} \langle C^+(r-\xi/2,t)\, C(r+\xi/2,t)\rangle$$

Clearly, f^{ω} is the integration of G^{+-} ($G^<$) with $t'\to t$.

It is known that even though f^{ω} is the quantum generalization of classical distribution function $f(\vec{r},\vec{p},t)$ used in the Boltzman equation, f^{W} is not always positive.

Nonetheless, if one averages f^{W} over the scale of h^d (h = Planck constant, d = dimension), one finds

$$\int_h \frac{d^d\vec{p}\, d^d\vec{r}}{h^d} f^{W}(\vec{r},\vec{p},t) = f(\vec{r},\vec{p},t) + O(h^d).$$

(the integration region h is centered at $\vec{r},\vec{p}$)

Hence f^{W} is the proper quantum generalization of $f(\vec{r},\vec{p},t)$.

Based on the Keldysh formalism, one can derive the equation that $f^{W}(\vec{r},\vec{p},t)$ obeys. This is known as the quantum kinetic equation, which is the generalization of the Boltzman equation and is the proper equation to investigate the non-equilibrium properties of quantum systems. We shall not be able to discuss details of the derivation for the quantum kinetic equation but only refer it to any textbook with the derivation. (see, for example, Quantum Theory of Many-Body Systems by Zagoskin)

Perturbation theory and linked cluster expansion

From eq. (125)

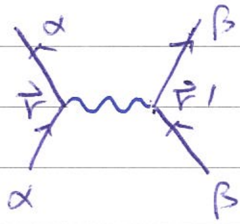
$$iG(\vec{r},\vec{r}\,') = \frac{\langle \Phi_0 | T\, C(\vec{r})\, C^+(\vec{r}\,')\, S(\infty,-\infty) | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty,-\infty) | \Phi_0 \rangle} \quad \cdots (162)$$

where we abbreviate $\vec{r}+t\,\alpha$ as a single index $\vec{r}$ for convenience.

and $S(\infty,-\infty) = T e^{-\frac{i}{\hbar}\int_{-\infty}^{\infty} V_I(t)\,dt}$, one can develope the perturbation theory for G by expanding $S(\infty,-\infty) = T \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \left(\int_{-\infty}^{\infty} V_I(t)\,dt\right)^n$.

Here $V_I(t) = \frac{1}{2}\sum_{\substack{\alpha\alpha' \\ \beta\beta'}} \int d^3 r \int d^3 r'\, C_\alpha^+(\vec{r},t)\, C_\beta^+(\vec{r}\,',t)\, V(\vec{r},\vec{r}\,')\, C_\beta(\vec{r}\,',t)\, C_\alpha(\vec{r},t)$

represented by



$$= \frac{1}{2}\sum_{\substack{\alpha\alpha' \\ \beta\beta'}} \int d^4 r \int d^4 r'\, C_\alpha^+(\vec{r}\,t)\, C_\beta^+(\vec{r}\,',t')\, V(\vec{r},\vec{r}\,')\,\delta(t-t')\, C_\beta(\vec{r}\,',t')\, C_\alpha(\vec{r},t) \quad (d^4 r = d^3 r\, dt)$$

and $|\Phi_0\rangle$ = non-interacting Fermi gas, filled up to k_F

As we have seen, w.r.t. $|\Phi_0\rangle$, the Green's functions are given by

$$G^0_{\alpha\beta}(k,\omega) = \delta_{\alpha\beta}\left[\frac{\theta(k-k_F)}{\omega-\varepsilon_k+i0^+} + \frac{\theta(k_F-k)}{\omega-\varepsilon_k-i0^+}\right]$$

& $$D^0(q,\omega) = \frac{2\omega_q}{\omega^2-\omega_q^2+i0^+}$$

Clearly, expanding the numerator of eq. (162) takes the following form

$$iG(\vec{r},\vec{r}') = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \cdots \int_{-\infty}^{\infty} dt_n$$

$$\times \frac{\langle \Phi_0 | T[V_I(t_1) V_I(t_2) \cdots V_I(t_n)\, C(\vec{r}) C^+(\vec{r}')] | \Phi_0 \rangle}{\langle \Phi_0 | S(\infty, -\infty) | \Phi_0 \rangle}$$

∴ The numerator takes the form
$\equiv i\tilde{G}$

$$i\tilde{G}(\vec{r},\vec{r}') = iG_0(\vec{r},\vec{r}') + \left(\frac{-i}{\hbar}\right) \sum_{\substack{\alpha\alpha' \\ \beta\beta'}} \frac{1}{2} \int d\vec{r}_1 \int d\vec{r}_1{}'$$

$$\langle \Phi_0 | T[C^+(\vec{r}_1) C^+(\vec{r}_1{}') V(\vec{r}_1,\vec{r}_1{}') C(\vec{r}_1{}') C(\vec{r}_1) C(\vec{r}) C^+(\vec{r}') | \Phi_0 \rangle$$

$$+ \cdots \qquad (162)-1$$

Therefore the fundamental expression one needs to evaluate is

$$I_n = \langle \Phi_0 | T[\hat{C}_1(t_1) \hat{C}_1^+(t_1') \cdots \hat{C}_n(t_n) \hat{C}_{n'}^+(t_n') | \Phi_0 \rangle \qquad (163)$$

The theorem that enables one to evaluate (163) systematically is the Wick's theorem.

Which states (weaker form)

$$I_n = \sum_{\substack{\text{all possible} \\ \text{pairs of } i \& j^{-1}}} (-1)^P \langle \Phi_0 | T\, C_i(t_i) \hat{C}_{j'}^+(t_j') | \Phi_0 \rangle \cdots \langle \Phi_0 | C_k(t_k) C_{k'}^+(t_k') | \Phi_0 \rangle \qquad (163)-1$$

The Wick's theorem is an identity in the operator form and the above is the identity with respect to the average of Φ_0, so it is a weaker form.

We shall not prove the Wick's theorem rigorously but only show its weaker form is correct.

For this purpose, it is convenient to go to the Fourier k space. In the k space, $C_I = e^{\frac{i}{\hbar}H_0 t} C e^{-\frac{i}{\hbar}H_0 t}$ become $C e^{-\frac{i}{\hbar}\xi_k t}$ and $C_I^+ = C^+ e^{\frac{i}{\hbar}\xi_k t}$ ---- (164)

We have

$$\hat{V}_I(t) = \frac{1}{2}\sum_{k',k,q} V(q)\, C^+_{k+q}(t) C^+_{k'-q}(t) C_{k'}(t) C_k(t)$$

and the Green's function becomes

$$iG(k, t-t') = \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!}\int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n$$

$$\times \frac{\langle T[C_k(t) V_I(t_1) V_I(t_2) \cdots V(t_n)\, C_k^+(t')]\rangle_0}{\langle S(-\infty,\infty)\rangle_0}$$

The fundamental average I_n then becomes

$$I_n = \left(\frac{1}{V}\right)^n \sum_{\substack{k_1,k_1'\\ \vdots \\ k_n,k_n'}} e^{i(\vec{k}_1\cdot\vec{r}_1 + \vec{k}_2\cdot\vec{r}_2 + \cdots + \vec{k}_n\cdot\vec{r}_n)}\, e^{-i(\vec{k}_1'\cdot\vec{r}_1' + \vec{k}_2'\cdot\vec{r}_2' + \cdots + \vec{k}_n'\cdot\vec{r}_n')}$$

$$\langle\Phi_0|T[C_{k_1}(t_1)\, C^+_{k_1'}(t_1')\, C_{k_2}(t_2)\, C^+_{k_2'}(t_2') \cdots C_{k_n}(t_n)\, C^+_{k_n'}(t_n')]|\Phi_0\rangle \quad \text{--- (165)}$$

where the spin indices are suppressed and included in k.

Now because of eq. (164), we are essentially evaluating

$$I_n' = \langle \Phi_0 | c_{k_1} c_{k_2} \cdots c_{k_n} c^+_{k_1'} c^+_{k_2'} \cdots c^+_{k_n'} | \Phi_0 \rangle .$$

Because #s of electrons of $|\Phi_0\rangle$ & $\langle \Phi_0|$ are fixed to be N, I_n' is nonvanishing only when # of c^+ = # of c. Furthermore, k' in c^+ must appear again in c so that # of electrons in various k modes are the same!

$$\therefore I_n' = \sum_{\substack{\{P_1 \ldots P_n\} \\ = \{k_1 \ldots k_n\}}} (-1)^P \langle \Phi_0 | c_{P_1} c^+_{P_1} | \Phi_0 \rangle \langle \Phi_0 | c_{P_2} c^+_{P_2} | \Phi_0 \rangle \cdots \langle \Phi_0 | c_{P_n} c^+_{P_n} | \Phi_0 \rangle$$

where $(-1)^P$ keeps track of minus sign resulting from commuting $c^+_{P_k}$ to the right hand side of c_{P_k}!

Since the time ordering operator in eq. (165) only introduces global (-1) sign according to ordering of t_k in $e^{\pm \frac{i}{\hbar} \varepsilon_k t_k}$, we conclude

$$\langle \Phi_0 | T[c_{k_1}(t_1) c^+_{k_1'}(t_1') c_{k_2}(t_2) c^+_{k_2'}(t_2') \cdots c_{k_n}(t_n) c^+_{k_n'}(t_n')] | \Phi_0 \rangle$$

$$= \sum_{\substack{\text{all possible} \\ \text{pair among } c \,\&\, c^+}} (-1)^P \langle \Phi_0 | c_{k_i}(t_i) c^+_{k_j'}(t_j') | \Phi_0 \rangle \cdots \langle \Phi_0 | c_{k_\alpha}(t_\alpha) c^+_{k_\beta'}(t_\beta') | \Phi_0 \rangle$$

If we further perform integrations over k_i & $k_{j'}$,

We conclude that even in real space, I_n

$$= \sum_{\substack{\text{all possible}\\ \text{pairs of } i \,\&\, j'}} (-1)^P \langle \Phi_0 | T\, C_i(t_i)\, C_{j'}^+(t_{j'}) | \Phi_0 \rangle \cdots$$

as shown in eq. (163)-1 !

As examples, we have that for the 2nd term of (162)-1

$$\langle T[C^+(\vec r_1) C^+(\vec r_1') C(\vec r_1') C(\vec r_1) C(\vec r) C^+(\vec r')] \rangle_0 \quad (\times V(\vec r_1, \vec r_1'))$$

$(\vec r \equiv (\vec r, t))$

(i) $= \langle T[C^+(\vec r_1) C^+(\vec r_1') C(\vec r_1') C(\vec r_1) C(\vec r) C^+(\vec r')] \rangle_0$

$= (-1) \langle T\, C^+(\vec r_1) C(\vec r_1') \rangle_0 \langle T\, C^+(\vec r_1') C(\vec r_1) \rangle_0 \langle T (C(\vec r) C^+(\vec r')) \rangle_0$

$= (-1)^3 i^3\, G_0(\vec r_1', \vec r_1)\, G_0(\vec r_1, \vec r_1')\, G_0(\vec r, \vec r')$

$\langle T C C^+ \rangle$
$= iG$

(ii) $= \langle T[C^+(\vec r_1) C^+(\vec r_1') C(\vec r_1') C(\vec r_1) C(\vec r) C^+(\vec r')] \rangle_0$

$= (-1)^2 \langle T\, C^+(\vec r_1) C(\vec r_1) \rangle_0 \langle T\, C^+(\vec r_1') C(\vec r_1') \rangle_0 \langle T (C(\vec r) C^+(\vec r')) \rangle_0$

$= (-1)^4 i^3\, G_0(\vec r_1, \vec r_1)\, G_0(\vec r_1', \vec r_1')\, G_0(\vec r, \vec r')$

(iii) $= \langle T[C^+(\vec r_1) C^+(\vec r_1') C(\vec r_1') C(\vec r_1) C(\vec r) C^+(\vec r')] \rangle_0$

$= (-1)^5 i^3\, G_0(\vec r, \vec r_1)\, G_0(\vec r_1', \vec r_1')\, G_0(\vec r_1, \vec r')$

(iv)

$$= \langle T[c^{+}(\vec r_1)\, c^{+}(\vec r_1{}')\, c(\vec r_1{}')\, c(\vec r_1)\, c(\vec r)\, c^{+}(\vec r\,')]\rangle_0$$

$$= (-1)^4 i^3\, G_0(\vec r_1{}', \vec r_1)\, G_0(\vec r, \vec r_1{}')\, G(\vec r_1, \vec r\,')$$

(v)

$$= \langle T[c^{+}(\vec r_1)\, c^{+}(\vec r_1{}')\, c(\vec r_1{}')\, c(\vec r_1)\, c(\vec r)\, c^{+}(\vec r\,')]\rangle_0$$

$$= (-1)^4 i^3\, G_0(\vec r, \vec r_1)\, G_0(\vec r_1, \vec r_1{}')\, G_0(\vec r_1{}', \vec r\,')$$

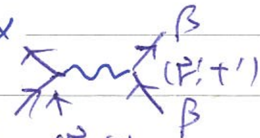
(vi) $= \langle T[c^{+}(\vec r_1)\, c^{+}(\vec r_1{}')\, c(\vec r_1{}')\, c(\vec r_1)\, c(\vec r)\, c^{+}(\vec r\,')]\rangle_0$

$$= (-1)^3 i^3\, G_0(\vec r_1, \vec r_1)\, G_0(\vec r, \vec r_1{}')\, G_0(\vec r_1{}', \vec r\,')$$

Diagram representation — Feynman diagram

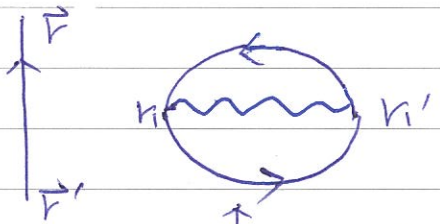
The above terms can be represented by diagrams with

*  representing $G_0(x, y)$, running from y to x

* 

vertex is labelled by $(\vec r, t)$

∴ (i)

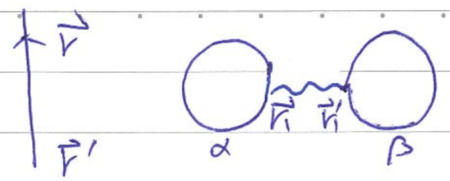


closed loop (equal time)

$$= \left(\frac{-i}{\hbar}\right)(-1)\, i^3 \boxed{\frac{1}{2}\sum_\alpha} \int d^4 r_1 \int d^4 r_1{}'\; V(\vec r_1, \vec r_1{}')\, \delta(t_1 - t_1{}')\, G_0(\vec r_1, \vec r_1{}')\, G_0(\vec r_1{}', \vec r_1)$$

(I, $G_0(\vec r t; \vec r\,' t')$; arrows: $\vec r_1, t_1$ and $\vec r_1{}', t_1{}'$)

(ii)

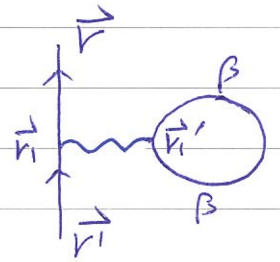


$$\left(\frac{-i}{\hbar}\right)(-1)^4 i^3 \overbrace{\frac{1}{2}\sum_\alpha\sum_\beta}^{2}$$

$$\times \int d^4\vec{r}_1 \int d^4\vec{r}_1{}' \; V(\vec{r}_1,\vec{r}_1{}')\,\delta(t_1-t_1{}')$$

$$\times G_0(\vec{r}_1,\vec{r}_1)\, G_0(\vec{r}_1{}',\vec{r}_1{}')$$

(iii')



$$\left(\frac{-i}{\hbar}\right)(-1)^5 i^3 \overbrace{\frac{1}{2}\sum_\beta}^{1} \int d^4\vec{r}_1 \int d^4\vec{r}_1{}'$$

$$V(\vec{r}_1,\vec{r}_1{}')\,\delta(t_1-t_1{}')\, G_0(\vec{r}_1,\vec{r}{}')\, G_0(\vec{r},\vec{r}_1)$$

$$\times G_0(\vec{r}_1{}',\vec{r}_1{}')$$

after removing i $\Rightarrow$ $(-1)\frac{i}{\hbar}$ (1th order)

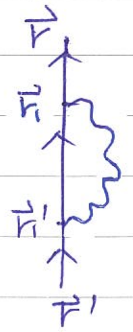
(iv)

$$\left(\frac{-i}{\hbar}\right)(-1)^4 i^3 \; \frac{1}{2}\int d^4\vec{r}_1 \int d^4\vec{r}_1{}'$$

$$V(\vec{r}_1,\vec{r}_1{}')\,\delta(t_1-t_1{}')\; G_0(\vec{r}_1,\vec{r}{}')\, G_0(\vec{r}_1{}',\vec{r}_1)\, G_0(\vec{r},\vec{r}_1{}')$$

after removing i $\Rightarrow$ $(+1)\frac{i}{\hbar}$

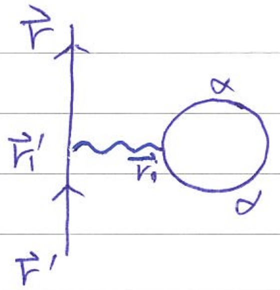
(v)



$$\left(\frac{-i}{\hbar}\right)(-1)^4 i^3 \; \frac{1}{2}\int d^4\vec{r}_1 \int d^4\vec{r}_1{}'$$

$$V(\vec{r}_1,\vec{r}_1{}')\,\delta(t_1-t_1{}')\; G_0(\vec{r}_1{}',\vec{r}{}')\; G_0(\vec{r}_1,\vec{r}_1{}')\; G_0(\vec{r},\vec{r}_1)$$

(vi)



$$\left(\frac{-i}{\hbar}\right)(-1)^3 i^3 \; \frac{1}{2}\sum_\alpha \int d^4\vec{r}_1 \int d^4\vec{r}_1{}'$$

$$V(\vec{r}_1,\vec{r}_1{}')\,\delta(t_1-t_1{}')\; G_0(\vec{r}_1{}',\vec{r}{}')\, G_0(\vec{r},\vec{r}_1{}')$$

$$G_0(\vec{r}_1,\vec{r}_1)$$

Several important features are exhibited in the above diagrams:

* Diagrams (iv) & (v) are the same as they differ only by permutation of $\vec{r}_1$ & $\vec{r}_1{}'$

Similarly, diagrams (iv) & (v) are the same,

These result from <u>equivalent ways of connecting internal indices to external</u> (fixed by $\vec{r}$ & $\vec{r}\,'$) <u>indices (sometimes, called external legs)</u>.

Numbers due to equivalent permutation of internal (to be integrated) indices are <u>Combinatoric factors</u>. When combined with $\frac{1}{n!}$ & $(\frac{1}{2})^n$.

* Diagrams can be classified as disconnected (such as (i) & (ii)) and connected diagrams.

Parts of disconnected diagrams also appear in the denominator eq. (162). These are <u>closed loops with equal time</u>.

$\langle\Phi_0|S(\infty,-\infty)|\Phi_0\rangle$

$$= 1 + \sum_{\substack{\alpha\alpha' \\ \beta\beta'}} \frac{1}{2}\int d\vec{r}_1 \int d\vec{r}_1{}' \langle\Phi_0| T\left[C^+(\vec{r}_1)C^+(\vec{r}_1{}')\,V(\vec{r}_1,\vec{r}_1{}')\,C(\vec{r}_1{}')C(\vec{r}_1)\right]|\Phi_0\rangle$$

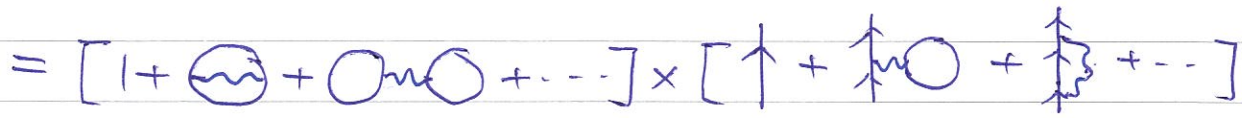
$+ \cdots$

$= 1 +$  $+ \cdots$

From the above observation, one naturally deduces

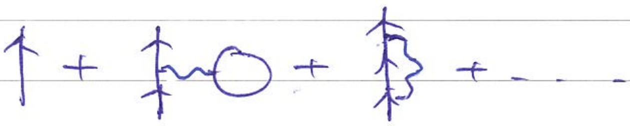
that

the numerator of eq. (162) for evaluation G



while the denominator =

Hence G =



Contains only connected diagrams!

Indeed, this can be proved and known as

the cancellation theorem.

Cancellation theorem

The numerator of eq. (162), i.e., $i\tilde{G}$, can be generally expressed as

(The numerator: N th term in the)

$$i\hat{G}_{\alpha\beta}(\vec{r},\vec{r}\,') = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\left(\frac{-i}{\hbar}\right)^{n+m(=N)} \delta_{N,n+m}\frac{1}{N!}\frac{N!}{m!\,n!}$$

($\frac{N!}{m!\,n!}$: combinatoric # for permuting V_I between connected & closed loops)

$$\times \int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2\cdots\int_{-\infty}^{\infty}dt_m \langle\Phi_0|T[V_I(t_1)\cdots V_I(t_m)C_\alpha(\vec{r})C^\dagger_\beta(\vec{r}\,')]|\Phi_0\rangle$$

(Connected diagrams)

$$\times \int_{-\infty}^{\infty}dt_{m+1}\cdots\int_{-\infty}^{\infty}dt_N \langle\Phi_0|T[V_I(t_{m+1})\cdots V_I(t_N)]|\Phi_0\rangle$$

(closed loops)

$\because$ $i\tilde{G}_{\alpha\beta} = \sum_N i\hat{G}_{\alpha\beta}^{(N)}$, and after summation over N, $\delta_{N,n+m}$ is removed. We get

$$i\tilde{G}_{\alpha\beta}(\vec{r},\vec{r}') = \sum_{m=0}^{\infty}\left(\frac{-i}{\hbar}\right)^m \frac{1}{m!}\int_{-\infty}^{\infty}dt_1 \cdots \int_{-\infty}^{\infty}dt_m$$

$$\times \langle\Phi_0|T[V_I(t_1)\cdots V_I(t_m)\, C_\alpha(\vec{r})\, C_\beta^+(\vec{r}')]|\Phi_0\rangle_{\text{connected}}$$

$$\underbrace{\times\sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!}\int_{-\infty}^{\infty}\underset{\substack{\uparrow\\ t_{m+1}}}{dt_1'}\cdots\int_{-\infty}^{\infty}\underset{\substack{\uparrow\\ t_N}}{dt_n'}\,\langle\Phi_0|T[V_I(t_1')\cdots V(t_n')]|\Phi_0\rangle}_{\substack{\| \\ \langle\Phi_0|S(\infty,-\infty)|\Phi_0\rangle}}$$

$$\therefore\ iG_{\alpha\beta}(\vec{r},\vec{r}') = \sum_{m=0}^{\infty}\left(\frac{-i}{\hbar}\right)^m \frac{1}{m!}\int_{-\infty}^{\infty}dt_1 \cdots \int_{-\infty}^{\infty}dt_m$$

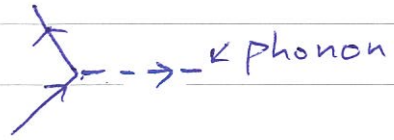
$$\times \langle\Phi_0|T[V_I(t_1)\cdots V_I(t_m)\, C_\alpha(\vec{r})\, C_\beta^+(\vec{r}')]|\Phi_0\rangle_{\text{connected}}.$$

Q.E.D.

With the cancellation theorem, we have Feynman rules for the linked cluster expansion of G in real space as follows:

(a) Draw all topologically distinct connected diagrams with n interaction lines (〰) and $\overset{(4n+2)/2}{\overset{\|}{2n+1}}$ directed Green's functions. Fermion lines run from $\vec{r}'$ to $\vec{r}$ for $G^0(\vec{r},\vec{r}')$ or close on themselves (Fermion loops)

In the presence of phonons, one includes

Vertices 

(b) Label each vertex with $(\vec{r}, t) \equiv \vec{r}$

(c) Each line is associated with $G_0(\vec{r}', \vec{r})$ running from $\vec{r}, t$ to $\vec{r}', t'$

(d) Each ~~~ line represents $U(r, r')$

(e) Integrate all internal variables

(f) Assign (-1) to any Fermion loop,
∴ overall $(-1)^F$, F = # of Fermion loop
(example: (iii) & (iv))

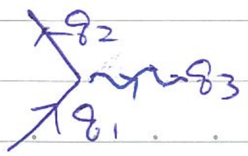
(g) Assign $(\frac{i}{\hbar})^n$ to each n^{th} order term
(example: (iii) & (iv))

(h) Green's functions with equal time should be interpretated as $G_0(rt, r', t^+)$.

Since $G_0(rt, r't') = G_0(r-r', t-t')$ and $U(r, r') = v(r-r')$, the whole system is translational invariant. It's more convenient to work in the Fourier $(\vec{k}, \omega)$ space.

$$G(\vec{r}, t, \vec{r}'t') = \int \frac{d^3\vec{k}}{(2\pi)^3} \int \frac{d\omega}{2\pi} e^{i\vec{k}\cdot(\vec{r}-\vec{r}') - i\omega(t-t')} G(\vec{k}, \omega)$$

$$V(q) = \int d(\vec{r}-\vec{r}')\, V(r-r')\, e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')}$$



$$\int d^3\vec{r} \int dt\, e^{i\vec{q}_1\cdot\vec{r}} e^{-i\vec{q}_2\cdot\vec{r}} e^{-i\vec{q}_3\cdot\vec{r}} \times e^{i\omega_1 t - i\omega_2 t - i\omega_3 t} = (2\pi)^3 \delta(\vec{q}_1 - \vec{q}_2 - \vec{q}_3)\, (2\pi)\delta(\omega_1 - \omega_2 - \omega_3)$$

i.e., momentum & energy have to be conserved at each vertex.

With these observations, we have the following Feynman rules in the momentum – frequency space.

Feynman rules in momentum – frequency space

(a) Draw all possible topologically – distinct connected diagrams with phonons, electrons & interactions

(b) Assign a direction to each interaction, electron and phonon lines.

(c) Assign a directed momentum & frequency to each line

(d) Conserve momentum and frequency at each vertex

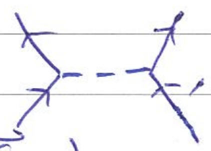
(e) For each electron line, introduce

$$G^0_{\alpha\beta}(\vec{k},\omega) = \frac{1}{\omega - \hbar^{-1}\xi_k + i\delta_k} \qquad \delta_k = 0^+ \,\mathrm{sign}\, \xi_k$$

(f) For each phonon line, introduce

$$D^0(\vec{q},\omega) = \frac{2\omega_q}{\omega^2 - \omega_q^2 + i\delta}$$

(g) For ~~each electron – phonon vertex~~ each phonon line introduce



$$|M_q|^2 = \frac{\hbar}{2MV\omega_{q\lambda}} V_q(\vec{q}\cdot\vec{\epsilon}_{q\lambda})$$

(h) For Each interaction line, introduce $V(q)$

(i) Integration over all internal momentum & frequencies

(j) Affix a factor

$$\frac{i^m}{(2\pi\hbar)^{4m}} (2S+1)^F (-1)^F$$

↑ for each loop $\sum_{spin} = (2S+1)$

F = # of closed loops

m = # of internal phonons + interaction line

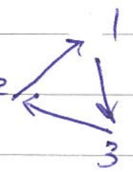
and combinatoric factors

(k) Simple closed loops are assigned the factor $e^{i\omega 0^+} G_0(\vec{k},\omega)$.

Note that the $(2\pi)^{-4}$ factor has assumed $V \to \infty$.

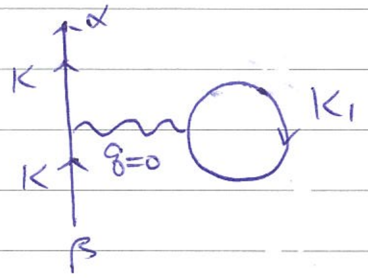
The (-1) sign for each Fermion loop can be understood as follows by a simple example:

$\langle C_1 C_2^+ C_2 C_3^+ C_3 C_1^+ \rangle$ is a loop



Which is permuted of $C_2^+ C_2 C_3^+ C_3 C_1^+ C_1$ by odd # of permutations. ∴ There is a minus sign for each closed loop.

Examples :

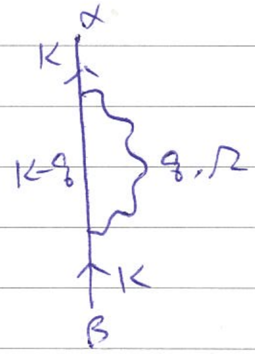


$$G^{(a)}_{\alpha\beta}(\vec{k},\omega)$$

$2S+1=1$

$$= (-1)\,\frac{i}{\hbar}\,\frac{1}{(2\pi)^4}\int d^3\vec{k}_1\int d\omega_1\, G^0(\vec{k}_1,\omega_1)\,e^{i\omega_1 0^+}$$

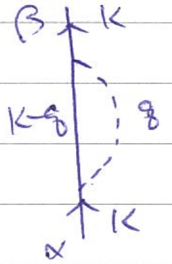
$$\times\, G^0(\vec{k},\omega)\, G^0(\vec{k},\omega)\, \delta_{\alpha\beta}$$



$$G^{(b)}_{\alpha\beta}(\vec{k},\omega)$$

$$= \frac{i}{\hbar}\,\frac{1}{(2\pi)^4}\int d^3\vec{q}\int d\Omega\, V(q)\, G^0(k-q,\omega-\Omega)$$

$$\times\, G^0(\vec{k},\omega)\, G^0(k,\omega)\, \delta_{\alpha\beta}.$$



$$G^{(c)}_{\alpha\beta}(\vec{k},\omega)$$

$$= \frac{i}{\hbar}\,\frac{1}{(2\pi)^4}\int d^3\vec{q}\int d\Omega\, |M_q|^2 D^0(q,\Omega)$$

$$G_0(k-q,\omega-\Omega)\times\left[G^0(\vec{k},\omega)\right]^2 \delta_{\alpha\beta}.$$

Dyson's equation & self-energy

From the topology of the diagrams for the Green's function, one can further classify connected diagrams as one-particle reducible (OPR) and one-particle irreducible (OPI) diagrams.

A diagram is OPI if one can not seperate it into two disjoint diagrams by cutting a line. A diagram is one-particle reducible if it is not OPI.

Clearly, from the definition, one has

$G =$ 

$+ \cdots$

We shall denote (OPI) by Σ, which will be termed as self energy.

If we denote $\Rightarrow$ as G, one has

 --- (166)

In the momentum-frequency space, eq. (166) becomes (Becaus V has no spin dependence, $\Sigma_{\alpha\beta} \propto \delta_{\alpha\beta}$ too!)

$$G_{\alpha\beta}(\vec{k},\omega) = G^0_{\alpha\beta}(\vec{k},\omega) + G^0_{\alpha\gamma}(k,\omega)\,\Sigma_{\gamma\delta}(\vec{k},\omega)\,G_{\delta\beta}(\vec{k},\omega)$$

$$\therefore\ (1-G^0\Sigma)\,G = G^0$$

$$G_{\alpha\beta}(k,\omega) = \Bigg[\overbrace{\frac{G^0(k,\omega)}{1-G^0(k,\omega)\,\Sigma(k,\omega)}}^{G}\Bigg]\delta_{\alpha\beta}$$

$$\therefore\ G(\vec{k},\omega) = \frac{1}{G^{0\,-1}-\Sigma} = \frac{1}{\omega-\hbar^{-1}\epsilon_k+i\delta_k-\Sigma(\vec{k},\omega)}$$

--- (167)

Eq. (167) is the Dyson's equation.

In the real space or in the case when one doesn't have translational invariance, the Dyson's equation takes the following

$$G_{\alpha\beta}(\vec{r},\vec{r}') = G^{0}_{\alpha\beta}(\vec{r},\vec{r}') + \int d^4 r_1 \int d^4 \vec{r}_1{}' \, G^{0}_{\alpha\gamma}(\vec{r},\vec{r}_1)\Sigma(\vec{r}_1,\vec{r}_1{}')_{\gamma\delta}$$
$$\times G_{\delta\beta}(\vec{r}_1{}',\vec{r}') \quad \text{--- (168)}$$

Analytic properties and pole approximation

From the Lehmann representation, it is clear that $\mathrm{Im}\,\Sigma(\vec{k},\omega) \geq 0$ for $\hbar\omega < \mu$

$\mathrm{Im}\,\Sigma(\vec{k},\omega) \leq 0$ for $\hbar\omega > \mu$.

$\therefore$ $\mathrm{Im}\,\Sigma(\vec{k},\omega)$ changes sign at $\hbar\omega = \mu$.

It is clear that the above behavior of Σ is for the time-ordered Green's function, where $\omega \to \omega + i\delta_k$ is used.

The retarded (advanced) Green's function can be obtained via replacing $i\delta_k$ by $i0^+$ or $i0^-$ in all diagrams. In that case, one also obtains

$$G^{R/A}(\vec{k},\omega) = \frac{1}{\omega - \hbar^{-1}\xi_k \pm i0^+ - \Sigma^{R/A}(\vec{k},\omega)}$$

Pole approximation

A particular simple approximation to the Green's function is to work on G^R or G^A.

For the non-interacting degenerate electrons, one has $G^0 = \frac{\theta(\xi_k)}{\omega - \hbar^{-1}\xi_k + i0^+} + \frac{\theta(-\xi_k)}{\omega - \hbar^{-1}\xi_k - i0^+}$.

This is not particularly convenient as 0^+ changes sign below/above the Fermi surface.

For G^A/G^R, we have

$$G_0^{R/A} = \frac{\theta(\xi_k) + \theta(-\xi_k)}{\omega - \hbar^{-1}\xi_k \pm i0^+} = \frac{1}{\omega - \hbar^{-1}\xi_k \pm i0^+} \quad \text{--- (170)}$$

which exhibit a simple pole at $\hbar^{-1}\xi_k$.

This indicates $A(\vec{k},\omega') = \delta(\omega' - \hbar^{-1}\xi_k)$ in eq. (148). --- (170)-1

In general, if the interaction does not change the properties too dramatically, it is expected that $G^{R/A}$ also have a simple pole but at modified $\hbar^{-1}\varepsilon_k^R$.

In this case, one writes $\Sigma = \Sigma_R + i\Sigma_I$ and assumes $|\Sigma_I|, |\Sigma_R| \ll 1$ so that the pole (zero) of $\omega - \xi_k - \Sigma(\vec{k},\omega)$ is determined by

Such free-electron-like are called quasiparticles.

An interacting fermionic system with such quasiparticles (near Fermi surface) is called a Fermi-liquid.

Such single-particle-like excitations are no longer exact eigenstate of the system since the interaction permits scattering in and out of the Bloch state and results in finite Z_k.

If one performs the Fourier transformation of (170) back to t space, one finds

$$G^R(k,t) \sim \theta(t)\, Z_k\, e^{-i\xi_k t}\, e^{-t/\tau_k}$$

Which eventually decays to zero, indicating the quasi-particle is not an exact eigenstate. However, as we shall see later, $\tau_k \propto (E-E_F)^{-2}$, the state becomes asymptotically exact at the Fermi surface.

The above is the analysis based on the retarded /advanced Green's functions. Since time-ordered Green's function is obtained by changing 0^+ into $0^+ \operatorname{sign} \xi_k = \delta_k$, one gets

$$G(\vec{k},\omega) = \frac{Z_k\,\theta(\xi_k^R)}{\omega-\xi_k^R+i/\tau_k} + \frac{Z_k\,\theta(-\xi_k^R)}{\omega-\xi_k^R-i/\tau_k}$$

$$\omega - \xi_k - \Sigma_R(\vec{k}, \omega) = 0 \quad \text{---} \quad (169) \quad (\hbar \equiv 1)$$

whose solution is ξ_k^R

$$\therefore \quad \xi_k^R = \xi_k + \quad (\vec{k}, \xi_k^R)$$

Expanding w.r.t. ξ_k^R, we get

$$\Sigma(\vec{k}, \omega) \cong \Sigma_R(\vec{k}, \xi_k^R) + (\omega - \xi_k^R) \left.\frac{d\Sigma_R}{d\omega}\right|_{\omega = \xi_k^R}$$

$$+ i\,\Sigma_I(\vec{k}, \xi_k^R)$$

$$\therefore \quad \omega - \xi_k - \Sigma(\vec{k}, \omega)$$

$$\simeq (\omega - \xi_k^R) - (\omega - \xi_k^R) \left.\frac{d\Sigma_R}{d\omega}\right|_{\xi_k^R} - i\,\Sigma_I(\vec{k}, \xi_k^R)$$

$$\therefore \quad G^R(\vec{k}, \omega) = \frac{Z_k}{\omega - \xi_k^R + i/\tau_k} \quad \text{---} \quad (170)$$

where

$$Z_k = \frac{1}{1 - \left.\frac{d\Sigma_R}{d\omega}\right|_{\omega = \xi_k^R}}$$

$$\frac{1}{\tau_k} = -\frac{\Sigma_I(k, \xi_k^R)}{1 - \left.\frac{d\Sigma_R}{d\omega}\right|_{\omega = \xi_k^R}} = -\frac{\Sigma(k, \xi_k^R)}{1 - \left.\frac{d\Sigma_R}{d\omega}\right|_{\omega = \xi_k^R}}$$

In comparison to the non-interacting case (eq. (170)), one sees that in addition to the shift of pole: $\xi_k \to \xi_k^R$, the residue is changed from 1 to Z_k and the lifetime becomes finite. $0^+ \to \tau_k$.

In general, on physical grounds, one expects that at higher energies, because electrons move faster and have less time to interact with others, the effect of interaction is expected to be smaller. ∴ One expects $\Sigma(k,\omega)$ is a decreasing function of ω.

$$\left.\frac{d\Sigma_R}{d\omega}\right|_{\omega=\xi_k^R} < 0 \quad \therefore Z_k < 1$$

If $Z_k > 0$, Z_k is called a normalization factor.

From the identity for the Green's function,

$$G(r,r') = \sum_n \frac{\phi_n^*(r)\,\phi_n(r')}{E-E_n} = \frac{1}{V}\sum_k \frac{e^{ik\cdot(\vec{r}'-\vec{r})}}{E-\xi_k},$$

one sees that Z_k is related to the normalization of eigenstates. It's also known as the wave-function renormalization constant.

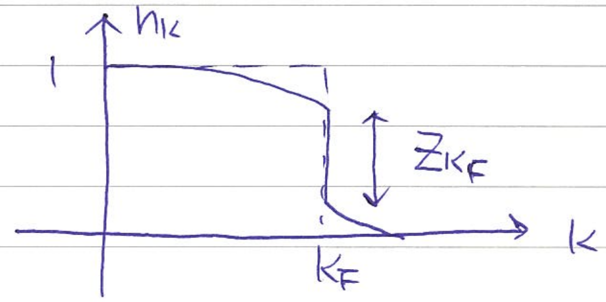
For degenerate Fermi gas, one is interested in $k=k_F$. The pole approximation describes the situation that if $Z_{k_F}>0$, the excitations are similiar to non-interacting electron gas and are single-particle like with suppressed amount.

Hence, the spectral weight (eq. (170)-1)

$$A(k,\omega) = Z_k \, \delta(\omega - \hbar^{-1}\xi_k^R)$$

is reduced and which is the quantity that experiments usually try to measure.

In addition, the step of the Fermi surface becomes



The magnitude of discontinuity on the Fermi surface is precisely the quasi-particle residue, which is considered to be the hallmark of a Fermi-liquid.

The Fermi-liquid is only one possible phase of interacting electrons. We will come back to its detailed properties and justification later.

Hartree-Fock Approximation of Green's functions

The real-space Dyson equation (eq. (168)) implies an effective Schrödinger equation for a single particle excitation in the presence of other particles. We shall assume $G_{\alpha\beta} = G\,\delta_{\alpha\beta}$

For $G^0(\vec{r}t;\vec{r}'t')$, one has

$$G^0(\vec{k},\omega) = \frac{1}{\omega - \hbar^{-1}\xi_k + i\delta_k}.$$

Hence
$$G^0(\vec{r}t;\vec{r}'t') = \sum_{k,\omega} \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}') - i\omega(t-t')}}{\omega - \hbar^{-1}\xi_k + i\delta_k}$$

&
$$\Big[i\hbar\frac{\partial}{\partial t} - \underbrace{\Big(-\frac{\hbar^2\nabla^2}{2m} - \mu\Big)}_{\hat{T}(\vec{r})}\Big] G^0(\vec{r}t;\vec{r}'t') = \hbar\,\delta(\vec{r}-\vec{r}')\,\delta(t-t') \qquad \text{---(171)}$$

Combining eq. (168) & eq. (171), we obtain

$$\Big[i\hbar\frac{\partial}{\partial t} - \hat{T}\Big] G(\vec{r}t;\vec{r}'t') = \hbar\,\delta(r-r')\,\delta(t-t') + \int d\vec{r}_1' \,\Sigma(\vec{r}t;\vec{r}_1' t_1)\, G(\vec{r}_1', t_1; \vec{r}'t').$$

i.e
$$\Big(i\hbar\frac{\partial}{\partial t} - \hat{T} - \hat{V}\Big) G = \hbar\,\delta(r-r')\,\delta(t-t') \quad \text{with}$$

non-local potential (Time-dependent)
$$\hat{V}G \equiv \hbar \int d^4\vec{r}_1' \,\Sigma(\vec{r}t;\vec{r}_1 t_1)\, G(r_1 t_1, \vec{r}'t') \qquad \text{---(172)}$$

In the case when $\Sigma = \Sigma(t-t_1)$; $G = G(t_1 - t')$ (time-translationally invariant), Eq. (172), after Fourier transformation in time, becomes

$$(\hbar\omega - \hat{T} - \hat{V}(\omega))\, G = \hbar\, \delta(r - r')$$

with $\hat{V} G = \hbar \int d^3 \vec{r}_1\, \Sigma(\vec{r}, \vec{r}_1; \omega)\, G(\vec{r}_1, \vec{r}', \omega)$.

It implies that G can be constructed from the energy eigenfunction to $\hat{T} + \hat{V}(\omega)$ for a given ω

$$[\hat{T} + \hat{V}(\omega)]\, \phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r}) \quad \text{--- (173)}$$

as

$$G(\vec{r}t, \vec{r}'t') = \sum_j e^{-i\omega(t-t')} \phi_j(\vec{r}) \phi_j^*(\vec{r}') \left[\frac{\theta(\epsilon_j - \epsilon_F)}{\omega - \hbar^{-1}\epsilon_j + i0^+} + \frac{\theta(\epsilon_F - \epsilon_j)}{\omega - \hbar^{-1}\epsilon_j - i0^+} \right] \quad \text{--- (174)}$$

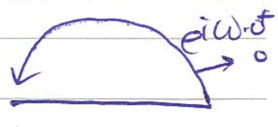
Here in general, ϵ_j & ϕ_j depends on ω. The eigenvalue, ϵ_j, as we shall see, has the meaning of excitation energy as it enters into the total energy of the system. To see it, from eq. (139), we have that the total energy

$$E = \frac{-i}{2} \underbrace{(2S+1)}_{\text{sum of spin}} \int \frac{d\omega}{2\pi} e^{i\omega 0^+} \int d^3\vec{r} \lim_{\vec{r}' \to r} [\hbar\omega + \hat{T}]\, G(\vec{r}, \vec{r}'; \omega)$$

With

$$G(\vec{r}, \vec{r}', \omega) = \sum_j \phi_j(\vec{r}) \phi_j^*(\vec{r}') \left[\frac{\theta(\epsilon_j - \epsilon_F)}{\omega - \hbar^{-1}\epsilon_j + i0^+} + \frac{\theta(\epsilon_F - \epsilon_j)}{\omega - \hbar^{-1}\epsilon_j - i0^+} \right] \quad \text{--- (175)}$$

The integration $\int \frac{d\omega}{2\pi} e^{i\omega 0^+}$ enforces the contour to be closed in the upper complex plane



We shall assume the ω-dependence of ϕ_j & ϵ_j does not contribute and set $\omega = \epsilon_j$ in ϕ_j & ϵ_j.

Hence only $\theta(\epsilon_F-\epsilon_j)$ contributes.

Now $\because\ \hat{T}G(\vec{r},\vec{r}',\omega)=\sum_j\left[\epsilon_j\phi_j(\vec{r})\phi_j^*(\vec{r}')-(\hat{V}\phi_j(\vec{r}))\phi_j^*(\vec{r}')\right]$

$$\times\left[\frac{\theta(\epsilon_j-\epsilon_F)}{\omega-\hbar^{-1}\epsilon_j+i0^+}+\frac{\theta(\epsilon_F-\epsilon_j)}{\omega-\hbar^{-1}\epsilon_j-i0^+}\right]$$

In this case,

the pole contribution of the $\hbar\omega$ term $=\frac{-i}{2}\times\frac{1}{2\pi}\times 2\pi i\times\hbar(\hbar^{-1}\epsilon_j)=\frac{\epsilon_j}{2}$,

while the pole contribution to the first term of $\hat{T}G$

is $\frac{-i}{2}\times\frac{1}{2\pi}\times 2\pi i\times\epsilon_j=\epsilon_j/2$

$\because\ \int d\vec{r}\,\phi_j(\vec{r})\phi_j^*(\vec{r})=1$, we find

$$E=\sum_j\epsilon_j\,\theta(\epsilon_F-\epsilon_j)-\frac{1}{2}\int d^3\vec{r}_1\int d^3\vec{r}_2\sum_j\left[\phi_j^*(\vec{r}_1)\,\hbar\Sigma(\vec{r}_1,\vec{r}_2)_{\omega=\epsilon_j}\,\phi_j(\vec{r}_2)\,\theta(\epsilon_F-\epsilon_j)\right]\quad\cdots(176)$$

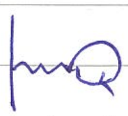
The meaning of ϵ_j is clearly exhibited in (176)

with $\hbar\Sigma(\vec{r}_1,\vec{r}_2)$ being non-local potential among

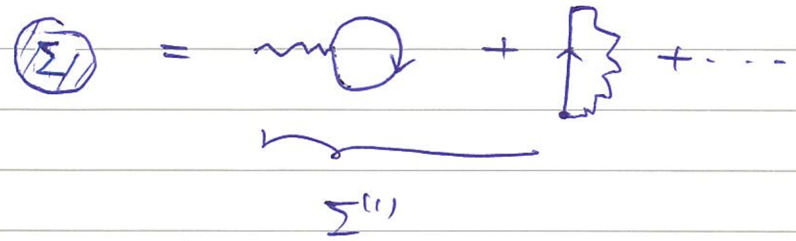
states below the Fermi energy ϵ_F.

Hartree–Fock terms

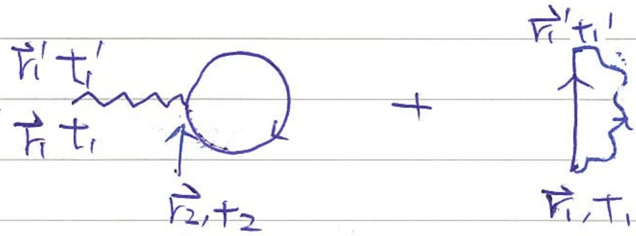
As we have seen, in the lowest orders (1st order),

only  and  contributes to G.

This implies that the self energy in this order is



$\therefore \Sigma^{(1)}(\vec{r}_1 t_1, \vec{r}_1' t_1') =$



$$= \frac{i}{\hbar}(2s+1)\,\delta(t_1-t_1')\,\delta(\vec{r}_1-\vec{r}_1')\int d^3\vec{r}_2\; G_0(\vec{r}_2,t_2;\vec{r}_2,t_2^+)\; V(\vec{r}_1-\vec{r}_2)$$

$$+\frac{i}{\hbar}(2s+1)\,\delta(t_1-t_1')\,V(\vec{r}_1-\vec{r}_1')\,G_0(\vec{r}_1 t_1;\vec{r}_1' t_1^+)$$

Clearly, when substituting $\Sigma^{(1)}$ into eq. (172), the $\delta(t_1-t_1')$ is integrated out, one gets a non-local potential:

$$\hbar\Sigma^{(1)}(r_1,r_1') = -i\,\delta(\vec{r}_1-\vec{r}_1')\int d^3\vec{r}_2\; V(\vec{r}_1-\vec{r}_2)\int\frac{d\omega}{2\pi}e^{i\omega 0^+}G_0(\vec{r}_2,\vec{r}_2,\omega)$$

$$+\,i\,V(\vec{r}_1-\vec{r}_1')\int\frac{d\omega}{2\pi}e^{i\omega 0^+}G_0(\vec{r}_1,\vec{r}_1',\omega) \qquad \text{(177)}$$

$\therefore$ $\Sigma^{(1)}$ has no ω-dependance! one case use eq. (176)

In the self-consistant calculation, one replaces G_0 by G in (177).

$$(-i)\int\frac{d\omega}{2\pi}e^{i\omega\cdot 0^+}G(\vec{r}_2,\vec{r}_2,\omega) = \sum_{\ell}\phi_{\ell}(\vec{r}_2)\,\phi_{\ell}^*(\vec{r}_2)\;\theta(\epsilon_F-\epsilon_{\ell})$$

Hence, eq. (176) becomes

$$E^{(1)} = \sum_j \epsilon_j \theta(\epsilon_F - \epsilon_j) - \frac{1}{2}\sum_{j,l} \theta(\epsilon_F - \epsilon_j)\theta(\epsilon_F - \epsilon_l)$$

$$\int d^3\vec{r}_1 \int d^3\vec{r}_2 \; V(\vec{r}_1,\vec{r}_2)\left[|\phi_j(\vec{r}_1)|^2 |\phi_l(\vec{r}_2)|^2 - \phi_j^*(\vec{r}_1)\phi_l(\vec{r}_1)\phi_l^*(\vec{r}_2)\phi_j(\vec{r}_2)\right]$$

which is clearly the usual Hartree-Fock result.

In the free electron limit, one adopts G_0 in eq. (177).

$$\text{H}i)\int \frac{d\omega}{2\pi} e^{i\omega 0^+} G_0(\vec{r}_2,\vec{r}_2,\omega) = \sum_k \theta(k_F - k) = n$$

$$i\int \frac{d\omega}{2\pi} e^{i\omega 0^+} G_0(\vec{r}_1,\vec{r}_1',\omega) = -\sum_{k'} \frac{1}{V} e^{ik(\vec{r}_1-\vec{r}_1')}\theta(k_F - k')$$

$$\therefore \hbar\Sigma^{(1)}(\vec{k}) = n\,V(\vec{k}=0) - \int \frac{d^3k'}{(2\pi)^3} V(k-k')\theta(k_F - k')$$

$$\uparrow$$

$$\int d(\vec{r}_1-\vec{r}_1')\, e^{i\vec{k}(\vec{r}_1-\vec{r}_1')}\Sigma^{(1)}(\vec{r}_1-\vec{r}_1') \qquad \therefore \xi_k = \xi_k^0 + \hbar\Sigma^{(1)}(\vec{k})$$

(eq. (173))

$$\text{Eq (176)} \Rightarrow E = V\int \frac{d^3k}{(2\pi)^3}\left[\xi_k - \frac{\hbar}{2}\Sigma^{(1)}(\vec{k})\right]\theta(k_F - k)$$

$$= V\int \frac{d^3k}{(2\pi)^3}\left[\xi_k^0 + \frac{\hbar}{2}\Sigma^{(1)}(\vec{k})\right]\theta(k_F - k).$$

One sees that the self energy $\Sigma(k)$ corrects the total energy. In the presence of ion potentials, one needs to introduce $v(\vec{r})$ and solves eq. (177) with $G_0 \rightarrow G$ self consistently!

self-consistency

When one solves eq. (173), one holds ω fixed. From there, ϵ_j & ϕ_j are obtained and thus by neglecting the contribution of ω in ϵ_j & ϕ_j, one gets E in eq. (176).

The reason why one can neglect the ω dependence in ϵ_j, ϕ_j & $\Sigma(\vec{r},\vec{r}';\omega)$ when one evaluates $\int \frac{d\omega}{2\pi} e^{i\omega 0^+}$ in E is because eventually one has to set $\omega = \epsilon_j \hbar^{-1}$.

In real calculation, one needs to do it self-consistently by setting $\omega = \hbar^{-1}\epsilon_j^0$ in $\hat{V}(\omega)$ at the beginning, one then obtains ϵ_j^1. In the 2nd step, one sets $\omega = \hbar^{-1}\epsilon_j^1$ in $\hat{V}(\omega)$ and obtains ϵ_j^2 . . . until finally, one gets self-consistently ϵ_j. Hence in eq. (176), ϵ_j is the self-consistent energy for solution!

Finite-temperature Green's function

At finite temperatures, it is natural to define

$$iG_{\alpha\beta}(\vec{r}t;\vec{r}'t') = \frac{\sum_n e^{-\beta(E_n-\mu N)} \langle\Psi_n| T[c_{\alpha H}(\vec{r}t)\, c^{\dagger}_{\beta H}(\vec{r}'t')] |\Psi_n\rangle}{\sum_n e^{-\beta(E_n-\mu N)}}$$

which extends eq. (120) at $T=0$. Here $\beta=\frac{1}{k_B T}$

Formally, this can be written as

$$iG_{\alpha\beta}(\vec{r}t;\vec{r}'t') = \frac{\mathrm{Tr}\, e^{-\beta(H-\mu N)}\, T[c_{\alpha H}(\vec{r}t)\, c^{\dagger}_{\beta H}(\vec{r}'t')]}{\mathrm{Tr}\, e^{-\beta(H-\mu N)}} \quad \text{--- (178)}$$

which is known as the real-time time-ordered Green's function.

Since $e^{-\beta\Omega} = \mathrm{Tr}\, e^{-\beta(H-\mu N)}$, one can
($\uparrow$ Grand-potential)

simple rewrite (178) as

$$iG_{\alpha\beta}(\vec{r}t;\vec{r}'t') = \mathrm{Tr}\left\{e^{-\beta(H-\Omega)}\, T[c_{\alpha H}(\vec{r}t)\, c^{\dagger}_{\beta H}(\vec{r}'t')]\right\} \quad \text{--- (179)}$$

where we absorb's $-\mu N$ into H.

Similarly, the finite temperature real-time retarded/advanced Green's function is (in k space)

$$G_R(k;t-t') = -i\theta(t-t')\, \langle\{c_{kH}(t), c^{\dagger}_{kH}(t')\}\rangle$$
$$= -i\theta(t-t')\, \mathrm{Tr}\left\{e^{-\beta(H-\Omega)} \{c_{kH}(t), c^{\dagger}_{kH}(t')\}\right\} \quad \text{--- (180)}$$

$$G_A(k, t-t') = i\theta(t'-t) \langle \{ C_{kH}(t), C^{+}_{kH}(t') \} \rangle \quad \text{--- (181)}$$

Matsubara Green's functions

A simple investigation on the form of eqs (179) – (181) shows that the factor $e^{-\beta H}$ gives the trouble of writing the whole expression as a single time-ordered exponential × unperturbed part :

$$\mathrm{Tr}\left[e^{-\beta H} C_{\alpha H}(rt) C^{+}_{\beta H}(r't') \right]$$

$$= \mathrm{Tr}\left[e^{-\beta H} S(0,t) \, C_\alpha(rt) \, S(t\,t') \, C^{+}_\beta(r't') \, S(t',0) \right]$$

in the interaction picture

$\longleftrightarrow$ eq. (125)-1 $\quad e^{-\beta H} \longleftrightarrow \langle\Phi_0| S(\infty,0) S(0,-\infty) |\Phi_0\rangle$ ← unperturbed Ground state

where $S = T e^{-\frac{i}{\hbar}\int V_I(t)\,dt}$. Because $e^{-\beta H}$ $\neq S(\infty,0)S(0,-\infty)$, one can't combine it with other terms into a single time-ordered exponential.

How does one treat the $e^{-\beta H}$ factor ?

A solution invented by Matsubara is to use the imaginary time : $it \to \tau$ and picture. performs the analytic continuation back later by setting $\tau = it$.

By doing so, one has the imaginary-time Heisenberg picture

$$\hat{O}_H(\tau) = e^{\tau H}\hat{O}e^{-\tau H},\quad \hat{O}_H^{+}(\tau) = e^{\tau H}\hat{O}^{+}e^{-\tau H}$$

$$\left(\leftrightarrow\ \hat{O}_H(t) = e^{\frac{i}{\hbar}Ht}\hat{O}e^{-\frac{i}{\hbar}Ht}\right)$$

and the imaginary-time interaction picture

$$\hat{O}_I(\tau) = e^{\tau H_0}\hat{O}e^{-\tau H_0}$$
, ... (182)

$$U_I(\tau) = e^{\tau H_0}e^{-\tau H},\quad S(\tau,\tau') = e^{\tau H_0}e^{-(\tau-\tau')H}e^{-\tau' H_0}$$

$$\left(\leftrightarrow S(t,t') = U_I(t)U_I^{+}(t') = e^{\frac{i}{\hbar}H_0t}e^{-\frac{i}{\hbar}H(t-t')}e^{-\frac{i}{\hbar}H_0t'}\right)$$

$$\therefore S(\tau,\tau_1)S(\tau_1,\tau') = S(\tau,\tau')$$

$$,\ \frac{d}{d\tau}S(\tau,\tau') = e^{\tau H_0}(H_0-H)e^{-(\tau-\tau')H}e^{-\tau' H_0}$$

$$= -V_I(\tau)S(\tau,\tau')$$

$$\therefore S(\tau,\tau') = T_\tau\, e^{-\int_{\tau'}^{\tau}d\tau_1 \hat{V}_I(\tau_1)} \quad \cdots (183)$$

Furthermore, by using eq. (182), setting $\tau'=0$, $\tau=\beta$

$$e^{-\beta H} = e^{-\beta H_0}S(\beta,0) \quad -- (184)$$

$$\therefore \mathrm{Tr}\left[e^{-\beta H}C_{\alpha H}(r\tau)C_{\beta H}^{+}(r'\tau')\right]$$

$$= \mathrm{Tr}\left[e^{-\beta H_0}S(\beta,0)S(0,\tau)C_{\alpha I}(r\tau)S(\tau,\tau')C_{\beta I}^{+}(r'\tau')S(\tau',0)\right]$$

$$= \mathrm{Tr}\left[e^{-\beta H_0}S(\beta,\tau)C_{\alpha I}(r\tau)S(\tau,\tau')C_{\beta I}^{+}(r'\tau')S(\tau',0)\right]$$

Which, now, can be written as

$$\mathrm{Tr}\left[e^{-\beta H_0} T_\tau \left(S(\beta,0)\, C_{\alpha I}(r\tau)\, C^{+}_{\beta I}(r'\tau')\right)\right]$$

— (185)

where T_τ is τ-ordering : $\tau > \tau'$

$$T_\tau[C_{\alpha I}(r\tau_1)\, C^{+}_{\beta I}(r'\tau')] = C_{\alpha I}(r\tau_1)\, C^{+}_{\beta I}(r'\tau')$$

~~Clearly, if we start from t'>t~~

$-\mathrm{Tr}\left[e^{-\beta H} C^{+}_{\beta H}(r't')\, C_{\alpha H}(rt)\right]$, we

end up with $-\mathrm{Tr}\left[e^{-\beta H_0} T_\tau\left(S(\beta,0) C^{+}_{\beta I}(r'\tau')\, C_{\alpha I}(r\tau)\right)\right]$.

Hence, instead of working on eq. (178) directly, one defines <u>the Matsubara Green's functions</u> as

$$G_{AB}(\tau,\tau') \equiv -\langle T_\tau [A(\tau)\, B(\tau')]\rangle$$

$$= -\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta H_0} T_\tau\left(\hat{S}(\beta,0)\, \hat{A}(\tau)\, \hat{B}(\tau')\right)\right]$$

— (186)

where $Z = \mathrm{Tr}\, e^{-\beta H} = \mathrm{Tr}\left[e^{-\beta H_0} S(\beta,0)\right]$, and

$$T_\tau[A(\tau) B(\tau')] = \theta(\tau-\tau')\, A(\tau) B(\tau') \pm \theta(\tau'-\tau)\, B(\tau') A(\tau)$$

+ for bosons

− for fermions.

Here <u>H has absorbed $-\mu N$</u>.

Such defined Mastubara · Green's functions have ~~the following properties~~

(i) $G_{AB}(\tau, \tau') = G_{AB}(\tau-\tau')$

$\tau > \tau'$

$$G_{AB}(\tau, \tau') = \frac{\mp 1}{Z} \mathrm{Tr}\left[e^{-\beta H} e^{\tau H} A e^{-\tau H} e^{\tau' H} B e^{-\tau' H}\right]$$

$$= \frac{\mp 1}{Z} \mathrm{Tr}\left[e^{-\tau' H} e^{-\beta H} e^{\tau H} A e^{-(\tau-\tau')H} B\right]$$

$$= \frac{\mp 1}{Z} \mathrm{Tr}\left[e^{-\beta H} e^{(\tau-\tau')H} A e^{-(\tau-\tau')H} B\right]$$

$= G_{AB}(\tau-\tau', 0)$, here one requires $\tau-\tau' \leq \beta$ for convergence at $E_n \to \infty$

Similarly

for $\tau < \tau'$ $\quad G_{AB}(\tau, \tau') = \frac{\pm 1}{Z} \mathrm{Tr}\, e^{-\beta H} e^{\tau' H} B e^{-\tau' H} e^{\tau H} A e^{-\tau H}$

$$= \frac{\pm 1}{Z} \mathrm{Tr}\, e^{-\beta H} e^{(\tau'-\tau)H} B e^{-(\tau'-\tau)H} A$$

is a function of $\tau-\tau'$.

The convergence for large energies requires $\tau-\tau' \geq -\beta$

$\therefore$ $-\beta \leq \tau-\tau' \leq \beta$

(ii) $G_{AB}(\tau) = \pm G_{AB}(\tau+\beta)$ for $\tau < 0$. $(-\beta \leq \tau \leq \beta)$

$$G_{AB}(\tau+\beta) = \frac{\mp 1}{Z} \mathrm{Tr}\left[e^{-\beta H} e^{(\tau+\beta)H} A e^{-(\tau+\beta)H} B\right]$$

$$= \frac{\mp 1}{Z} \mathrm{Tr}\left[e^{\tau H} A e^{-\tau H} e^{-\beta H} B\right]$$

$$= \frac{\mp 1}{Z} \mathrm{Tr}\left[e^{-\beta H} B \underbrace{e^{\tau H} A e^{-\tau H}}_{A(\tau)}\right]$$

$$= \frac{-1}{Z} \cdot \mathrm{Tr}\left[e^{-\beta H} \chi(\pm) T_\tau (A(\tau) B) \right] \quad (\tau < 0)$$

$$= \pm G_{AB}(\tau)$$

i.e. $G_{AB}(\tau)$ is periodic or antiperiodic in τ

and only

From the above properties, one can perform the Fourier transformation on τ for $-\beta < \tau < \beta$

Fourier transformation & Matsubara frequency

Clearly, the function we encounter for the imaginary time formalism is $f(\tau)$ with $-\beta \leq \tau \leq \beta$ but $f(\tau + \beta) = \pm f(\tau)$ for $\tau < 0$. This implies

$$f(\tau) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos \frac{n\pi\tau}{\beta} + b_n \sin \frac{n\pi\tau}{\beta} \right]$$

with β being the period of either periodic or antiperiodic cases.

Here one can find

$$a_n = \frac{1}{\beta} \int_{-\beta}^{\beta} d\tau\, f(\tau) \cos \frac{n\pi\tau}{\beta}$$

$$b_n = \frac{1}{\beta} \int_{-\beta}^{\beta} d\tau\, f(\tau) \sin \frac{n\pi\tau}{\beta}$$

Another way to write $f(\tau)$ is to combine cos & sin into $e^{i n\pi\tau/\beta}$.

∴ One defines

$$f(i\omega_n) \equiv \frac{\beta}{2}(a_n + i b_n) = \frac{1}{2}\int_{-\beta}^{\beta} dz\, f(z)\, e^{i\frac{n\pi z}{\beta}}$$

($\frac{n\pi}{\beta}$ ~ ω_n)

$$\therefore \quad f(z) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-in\pi z/\beta} f(i\omega_n) \quad \text{--- (187)}$$

Eq. (187) can be further reduced according to whether it's bosonic or fermionic system.

<u>Boson</u> : $f(z) = f(z+\beta) \quad -\beta \le z < 0$

$$f(i\omega_n) = \frac{1}{2}\left(\int_0^\beta + \int_{-\beta}^0 dz\right) f(z)\, e^{i\frac{n\pi}{\beta}z}$$

(the $\int_{-\beta}^0$ term $= \int_0^\beta$ with $f(z) \to f(z+\beta)$, $z+\beta \equiv z$)

$$= \frac{1}{2}(1 + e^{-in\pi}) \int_0^\beta dz\, f(z)\, e^{i\frac{n\pi}{\beta}z}$$

∴ Only <u>n = even</u>, $f(i\omega_n) \neq 0$ ∴ $\underline{\omega_n = \frac{2n\pi}{\beta}}$

& $f(i\omega_n) = \int_0^\beta dz\, f(z)\, e^{i\omega_n z}$

$$f(z) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\omega_n z} f(i\omega_n).$$

<u>Fermion</u> : $f(z) = -f(z+\beta) \quad -\beta \le z < 0$

$$f(i\omega_n) = \frac{1}{2}(1 - e^{-in\pi}) \int_0^\beta f(z)\, e^{i\frac{n\pi}{\beta}z}$$

∴ Only <u>n = odd</u>, $f(i\omega_n) \neq 0$ ∴ $\underline{\omega_n = \frac{(2n+1)\pi}{\beta}}$

In this case,

$$f(i\omega_n) = \int_0^\beta d\tau\, f(\tau)\, e^{i\omega_n \tau}$$

$$f(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau} f(i\omega_n)$$

are still the same.

Finite temperature Lehmann representation and its analytic continuation

We first construct the Lehmann representation for the retarded real-time Green's function.

$$G_A^R(t-t') = -i\theta(t-t')\, e^{\beta\Omega} \sum_n \langle n|\, e^{-\beta H} [A(t)A^+(t') + \xi A^+(t')A(t)]|n\rangle$$

$e^{\beta\Omega}$ ↑ $\frac{1}{Z}$

insert $\mathbb{1} = |m\rangle\langle m|$

$\xi = -1$ for bosons
$= 1$ for fermions

$$= -i\theta(t-t')\, e^{\beta\Omega} \sum_{m,n} e^{-\beta E_n} \Big[\langle n|A(t)|m\rangle \langle m|A^+(t')|n\rangle + \xi \langle n|A^+(t')|m\rangle \langle m|A(t)|n\rangle\Big]$$

$\because A(t) = e^{i\frac{Ht}{\hbar}} A\, e^{-i\frac{Ht}{\hbar}}$

$$\langle n|A(t)|m\rangle = e^{i\frac{1}{\hbar}(E_n - E_m)t} \langle n|A|m\rangle$$

$$\therefore G_A^R(t-t') = -i\theta(t-t')\, e^{\beta\Omega} \sum_{m,n} e^{-\beta E_n} \Big\{ e^{\frac{i}{\hbar}(E_n-E_m)(t-t')} |\langle n|A|m\rangle|^2 + \xi e^{-\frac{i}{\hbar}(E_n-E_m)(t-t')} |\langle m|A|n\rangle|^2 \Big\}$$

Exchange n & m in the 2nd term, one gets

$$G_A^R(t-t') = -i\theta(t-t')\, e^{\beta\Omega}$$

$$\sum_{n,m} |\langle n|A|m\rangle|^2 e^{\frac{i}{\hbar}(E_n-E_m)(t-t')}\left[e^{-\beta E_n} + \xi e^{-\beta E_m}\right]$$

$$\therefore G_A^R(\omega) = \int_0^\infty dt\, e^{i(\omega+i0^+)(t-t')} G_A^R(t-t')$$

$$= e^{\beta\Omega}\sum_{n,m} |\langle n|A|m\rangle|^2 (e^{-\beta E_n} + \xi e^{-\beta E_m}) \frac{1}{\omega + \hbar^{-1}(E_n-E_m)+i0^+}$$

$\leftarrow$ (188)

Now, for Matsubara Green's function,

one starts from

$$G_A(\tau) = -\langle T_\tau \hat{A}(\tau)\hat{A}^\dagger(0)\rangle$$

$$G_A(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau} G_A(\tau)$$

$\tau > 0$ $\quad G_A(\tau) = -e^{\beta\Omega}\sum_{n,m}\langle n|e^{-\beta H} A(\tau)|m\rangle\langle m|A^\dagger(0)|n\rangle$

$\uparrow \frac{1}{Z}$ $\qquad \uparrow 1 = |m\rangle\langle m|$

$$= e^{-\beta\Omega}\sum_{n,m}|\langle n|A|m\rangle|^2 e^{-\beta E_n} e^{\tau(E_n-E_m)}$$

$$\therefore G_A(i\omega_n) = -e^{-\beta\Omega}\sum_{n,m}|\langle n|A|m\rangle|^2 e^{-\beta E_n}\int_0^\beta d\tau\, e^{i\omega_n\tau} e^{\tau(E_n-E_m)}$$

$$= e^{\beta\Omega}\sum_{n,m}|\langle n|A|m\rangle|^2 \frac{\xi e^{-\beta E_m} - e^{-\beta E_n}}{i\omega_n + E_n - E_m}$$

$\uparrow$ $e^{i\omega_n\beta} = -\xi = +1$ for bosons, -1 for fermions

$$= e^{\beta\Omega}\sum_{n,m} |\langle n|A|m\rangle|^2 \, \frac{e^{-\beta E_m} + \xi e^{-\beta E_m}}{i\omega_n + E_n - E_m}$$

$\cdots$ (189)

From eqs. (188) & (189), one gets

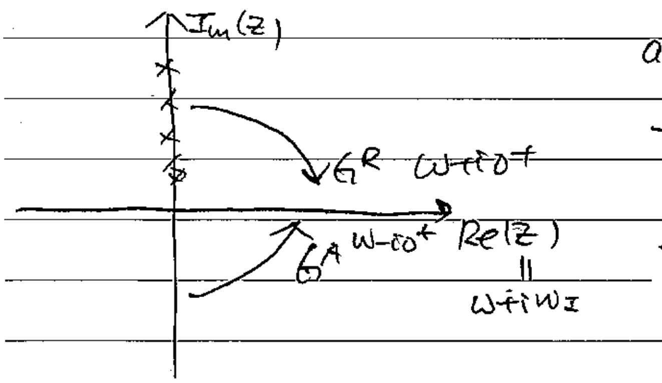
$$G_A^R(\omega) = \hbar\, G_A(i\omega_n \to \hbar\omega + i0^+) \quad \cdots (190)$$

In other words, it indicates that to get the real-time retarded Green's function, one simply replaces $i\omega_n$ by $\omega + i0^+$ in the Matsubara Green's function.

Similarly, to get the real-time advanced Green's function, one replaces $i\omega_n$ by $\omega - i0^+$

$$G_A^A(\omega) = \hbar\, G_A(i\omega_n \to \hbar\omega - i0^+) \quad \cdots (191)$$

Note that the replacement analytically continues from $i\omega \to$ to real axis (see the figure on below) and it has to be done after the integral is performed:



$$f(i\omega_n) = \int_0^\beta e^{i\omega_n \tau} f(\tau)\, d\tau$$

$\updownarrow$

$\omega \pm i0^+$

Noninteracting Matsubara Green's function

We shall check the analytic continuation for free fermions.

Consider $\hat{H}_0 = \sum_k \xi_k c_k^\dagger c_k$

$$c_k(\tau) = e^{\tau H_0} c_k e^{-\tau H_0}$$

$$\therefore \frac{\partial c_k}{\partial \tau} = [H_0, c_k] = -\xi_k c_k$$

$$\therefore c_k(\tau) = e^{-\xi_k \tau} c_k$$

Now $c_k^\dagger(\tau) = e^{\xi_k \tau} c_k^\dagger \neq [c_k(\tau)]^\dagger = e^{-\tau H_0} c_k^\dagger e^{\tau H_0}$ ($= e^{-\xi_k\tau} c_k^\dagger$)

Instead $c_k^\dagger(\tau) = e^{\tau H_0} c_k^\dagger e^{-\tau H_0}$, $\frac{\partial c_k^\dagger}{\partial \tau} = [H_0, c_k^\dagger] = +\xi_k c_k^\dagger$

$$\therefore c_k^\dagger(\tau) = e^{\xi_k \tau} c_k^\dagger$$

$$\therefore g_k^0(\tau - \tau') \equiv -\langle T_\tau c_k(\tau) c_k^\dagger(0) \rangle \quad (\tau' = 0)$$

$$= -\theta(\tau)\langle c_k(\tau) c_k^\dagger(0)\rangle - \zeta\theta(-\tau)\langle c_k^\dagger(0) c_k(\tau)\rangle$$

$$= -[\theta(\tau)\langle c_k c_k^\dagger\rangle + \zeta\theta(-\tau)\langle c_k^\dagger c_k\rangle] e^{-\xi_k\tau}$$

For fermions, $\zeta = -1$

$$\therefore \theta(\tau)\langle c_k c_k^\dagger\rangle + \zeta\theta(-\tau)\langle c_k^\dagger c_k\rangle$$

$$= \theta(\tau)\langle 1 - c_k^\dagger c_k\rangle - \theta(-\tau)\langle c_k^\dagger c_k\rangle$$

$$= \theta(\tau) - n_F(k)$$

$$\therefore g_k^0(\tau) = -\theta(\tau) e^{-\xi_k\tau} + n_F(k) e^{-\xi_k\tau}, \quad n_F(k) \equiv \langle c_k^\dagger c_k\rangle$$

$$g^0_K(i\omega_n) = \int_0^\beta e^{i\omega_n(\tau)} g^0_K(\tau)\, d\tau$$

$$= -(1-n_F(K)) \int_0^\beta e^{i\omega_n\tau} e^{-\xi_K\tau} d\tau$$

$$= -(1-n_F(K)) \frac{1}{i\omega_n - \xi_K} e^{i\omega_n\tau - \xi_K\tau} \Big|_0^\beta$$

$\because e^{i\omega_n \cdot \beta} = -1$ for fermion $\omega_n = \frac{(2n+1)\pi}{\beta}$

$$\therefore g^0_K(i\omega_n) = -(1-n_F(K)) \left[-e^{-\xi_K\beta} - 1\right] \frac{1}{i\omega_n - \xi_K}$$

Now, $1 - n_F(K) = 1 - \frac{1}{e^{\beta\xi_K}+1} = \frac{e^{\beta\xi_K}}{e^{\beta\xi_K}+1}$

$$= \frac{1}{1+e^{-\xi_K\beta}}$$

$$\therefore g^0_K(i\omega_n) = \frac{1}{i\omega_n - \xi_K} \qquad \omega_n = \frac{(2n+1)\pi}{\beta}$$

After the analytic continuation, one gets the real-time (retarded) Green's function:

$$G^0_R(k,\omega) = \frac{1}{\omega + i0^+ - \xi_K\hbar^{-1}}$$

which reproduces the $T=0$ result (eq. 131)

Phonons. Similarly, for phonons, we start by considering the Matsubara Green's function

$$\mathcal{D}^0_K(\tau) = -\langle T_\tau A(q,\tau) A(-q,0) \rangle$$

Here $A(q,\tau) = a_q(\tau) + a_{-q}^{+}(\tau)$ with the index q including polarization λ.

$$a_q(\tau) = e^{\tau H_0} a_q e^{-\tau H_0} \qquad H_0 = \sum_q \hbar\omega_q a_q^{+} a_q$$

$$= e^{-\tau\omega_q} a_q$$

$$a_q^{+}(\tau) = e^{\tau\omega_q} a_q^{+}$$

$$\therefore \mathcal{D}_K^0(\tau) = -\theta(\tau) \langle (a_q e^{-\tau\omega_q} + a_{-q}^{+} e^{\tau\omega_q})(a_{-q} + a_q^{+}) \rangle$$

$$-\theta(-\tau) \langle (a_q + a_q^{+})(a_q e^{-\tau\omega_q} + a_{-q}^{+} e^{\tau\omega_q}) \rangle$$

Let $\langle a_q^{+} a_q \rangle$, $\langle a_q a_q^{+} \rangle = n_B + 1$

$$= \frac{1}{e^{\beta\omega_q} - 1} = n_q$$

$$= n_B(\omega_q)$$

One gets

$$\mathcal{D}_K^0(\tau) = -\theta(\tau)\left[(n_B+1) e^{-\tau\omega_q} + n_B e^{\tau\omega_q}\right]$$

$$-\theta(-\tau)\left[n_B e^{-\tau\omega_q} + (n_B+1) e^{\tau\omega_q}\right]$$

$$= -n_B(e^{-\tau\omega_q} + e^{\tau\omega_q}) - \theta(\tau) e^{-\tau\omega_q} - \theta(-\tau) e^{\tau\omega_q}$$

$$\mathcal{D}_K^0(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n \tau} \mathcal{D}_K^0(\tau)$$

$$= - \int_0^\beta d\tau\, e^{i\omega_n\tau}\left[e^{-\tau\omega_q}(n_B+1) + e^{\tau\omega_q} n_B\right]$$

$$= - \left[\frac{1+n_B}{i\omega_n - \omega_q} e^{i\omega_n\tau - \omega_q\tau}\Big|_0^\beta + n_B \frac{e^{i\omega_n\tau + \tau\omega_q}}{i\omega_n + \omega_q}\Big|_0^\beta\right]$$

$\therefore \omega_n = \frac{2\pi n}{\beta}, \quad e^{i\omega_n \beta} = 1.$

$$\therefore \mathcal{D}^0_k(i\omega_n) = -\left[\frac{(1+n_B)(e^{-\beta\omega_q}-1)}{i\omega_n - \omega_q} + \frac{n_B(e^{\beta\omega_q}-1)}{i\omega_n + \omega_q}\right]$$

$$\because \quad 1+n_B = \frac{e^{\beta\omega_q}}{e^{\beta\omega_q}-1} = \frac{-1}{e^{-\beta\omega_q}-1}$$

$n_B = \frac{1}{e^{\beta\omega_q}-1}$ $\therefore$ 1st & 2nd numerators $= 1$ & -1

$$\mathcal{D}^0_k(i\omega_n) = \frac{1}{i\omega_n - \omega_q} - \frac{1}{i\omega_n + \omega_q}.$$

which clearly generalizes the $T=0$ result (eq. 134) to finite temperature:

$$\mathcal{D}^0_R(k,\omega) = \frac{1}{\omega - \omega_q + i0^+} - \frac{1}{\omega + \omega_q + i0^+}$$

<u>Wick theorem</u> & <u>Matsubara frequency sums</u>

When evaluating the Matsubara Green's function (for electron) (eq (186)), one can substitute $S(\beta,0)$ from eq. (183) into eq (186) and obtains the general expression one needs to evaluate:

$$\mathcal{G}_0^{(n)} \equiv (-1)^n \langle T_\tau [c_{k_1}(\tau_1) c_{k_2}(\tau_2) \cdots c_{k_n}(\tau_n) c^+_{k_n'}(\tau_n') \cdots c^+_{k_1'}(\tau_1')\rangle_0 \quad \text{--- (192)}$$

where $\langle \cdots \rangle_0 \equiv \frac{\mathrm{Tr}\, e^{-\beta H_0}(\cdots)}{\mathrm{Tr}\, e^{-\beta H_0}}$ and <u># of c^+ = # c.</u>

$\therefore \dfrac{\partial C_{k_i}(z_i)}{\partial z_i} = -\xi_{k_i} C_{k_i}(z_i)$

$\therefore$ we get

$$\underbrace{\left(-\partial z_i + \xi_{k_i}\right)}_{g_{0i}^{-1}} g_0^n = \sum_{j=1}^{n} \delta_{k_i, k_j'} \, \delta(z_i - z_j') \, (-1)^{\alpha} \quad \text{--- (193)}$$

$$\times \, g_0^{n-1} (\text{without } k_i, k_j')$$

Here $\alpha = (-1)$ for the case i & j are nearest neighbours.

In general, one can move j next to i.

There is (-1) sign from $-\frac{\partial}{\partial z_i}$

$(-1)^n$ from g_0^n's definition

$(-1)^{n-1}$ " g_0^{n-1}'s "

$(-1)^{n-j}$ moving $C_{k_j'}^+$ across other $C_{k_n'}^+$

$$\underbrace{C_{k_n'}^+ \cdots}_{n-j \text{ terms}} \underbrace{C_{k_j'}^+ \cdots C_{k_1'}^+}_{j}$$

$(-1)^{n-i}$ moving $C_{k_j'}^+$ across C_{k_n}

$$\cdots C_{k_i} \underbrace{\cdots C_{k_n}}_{n-i \text{ terms}} C_{k_j'}^+$$

$\therefore$ total sign $= (-1)^{1+n+n-1+n-i+n-j} = (-1)^{i+j}$

$$\therefore \left(-\partial z_i + \xi_{k_i}\right) g_0^n = \sum_{j=1}^{n} \delta_{k_i, k_j'} \, \delta(z_i - z_j') \, (-1)^{i+j} \, g_0^{n-1} (\text{without } k_i, k_j') \quad \text{--- (194)}$$

The reason why # of c^+ = # of c is because $\langle n|e^{-\beta H_0}|n'\rangle \neq 0$ only when # of particles in $|n\rangle$ & $|n'\rangle$ are the same for H_0 that we are working on.

Hence

$$\mathrm{Tr}\, e^{-\beta H_0} c^+ c^+ = \sum_{n,m} \langle n|e^{-\beta H_0}|m\rangle\langle m|c^+c^+|n\rangle$$

$$= \sum_n \langle n|e^{-\beta H_0}|n\rangle \underbrace{\langle n|c^+c^+|n\rangle}_{0}$$

$$= 0$$

To evaluate $g_0^{(n)}$ in eq. (192), we perform the operation $-\frac{\partial}{\partial z_i}$ and find the equation of motion. To find $\frac{\partial}{\partial z_i}$, one notices that any exchange between any nearest-neighbour pair of i, j introduces ~~a minus sign.~~

$$g_0^n = [\cdots \theta(z_i - z_j') \cdots] \langle \cdots c_{k_i}(z_i)\, c_{k_j}^{+}(z_j') \cdots \rangle$$

$$\pm [\cdots \theta(z_j' - z_i) \cdots] \langle \cdots c_{k_j}^{+}(z_j')\, c_{k_i}(z_i) \cdots \rangle$$

Hence $-\partial_{z_i} g_0^n$

due to $-\frac{\partial}{\partial z}\theta$

$$= \mp [\cdots] \langle \cdots \underbrace{[c_{k_i}(z_i), c_{k_j}^{+}(z_j')]_{\pm}}_{\delta_{k_i,k_j}\,\delta(z_i - z_j')} \cdots \rangle\, \delta(z_i - z_j')$$

$+$ = anticommutator
$-$ = commutator

$$+ (-1)^n \langle T_z [c_{k_1}(z_1) \cdots \frac{\partial c_{k_i}(z_i)}{\partial z_i} \cdots] \rangle$$

Now, since $(\partial_{\tau_i} + \xi_{k_i})\, g_0(k_i\tau_i, k_j'\tau_j')$

$$= \delta_{k_i,k_j'}\,\delta(\tau_i - \tau_j'),$$

replacing $\delta_{k_i,k_j'}\delta(\tau_i-\tau_j')$ on RHS of eq (194) and removing $(\partial_{\tau_i}+\xi_{k_i})$ leads to

$$g_0^n = \sum_{j=1}^{n} (\pm 1)^{i+j}\, g_0(k_i\tau_i;\, k_j'\tau_j')\, g_0^{n-1}(\underbrace{k_1\tau_1,\ldots,k_n\tau_n}_{\text{without } i};\, \underbrace{k_1'\tau_1'\ldots k_n'\tau_n'}_{\text{without } j})$$

+ for Boson, − for fermions

Clearly, the above result is the Laplace expansion of a determinant.

∴ For fermions, one gets

$$g_0^n(1,\ldots n, 1', \ldots n') = \begin{vmatrix} g_0(1,1') & g_0(1,2') & \cdots & g_0(1,n') \\ g_0(2,1') & g_0(2,2') & \cdots & g_0(2,n') \\ \vdots & \vdots & & \vdots \\ g_0(n,1') & g_0(n,2') & \cdots & g_0(n,n') \end{vmatrix} \quad \cdots (195)$$

For bosons, one gets

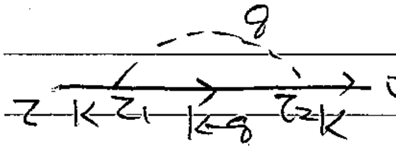
$$g_0^n(1,\ldots,n,1',\ldots n') = \sum_{\substack{\text{all}\\ \text{possible}\\ \text{pairs}}} g_0(k_i, k_{j'})\, g_0(k_\alpha, k_\beta')\cdots \quad \cdots (196)$$

Eqs. (195) & (196) are the Wick's theorems at finite temperature, which allows one to break the average into $g_0(\alpha,\beta)$ (two-particle Green's function).

Feynman rules & frequency sums

With the Wick's theorem, the finite temperature perturbation theory is similar to the perturbation theory at $T=0$ except that (i) τ plays the role of t. (ii) there is a $(-1)^n$ for each order. (not $\left(\frac{i}{\hbar}\right)^n$ for nth order)

Example:

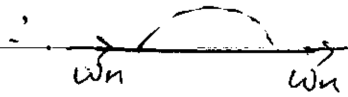


$$= -\sum_q |M_q|^2 \int_0^\beta d\tau_1 \int_0^\beta d\tau_2$$

$$\times\, \mathcal{G}_k^0(\tau-\tau_1)\, \mathcal{G}_{k-q}^0(\tau_1-\tau_2)\, \mathcal{G}_k^0(\tau_2\quad)\, \mathcal{D}_q^0(\tau_1-\tau_2)$$

Now, $\because$ $f(\tau) = \frac{1}{\beta}\sum_n e^{-i\omega_n \tau} f(i\omega_n)$

$$f(i\omega_n) = \int_0^\beta f(\tau)\, e^{i\omega_n \tau} d\tau$$

$\therefore$ 

$= \mathcal{G}^{(2)}(k, i\omega_n)$

$$= -\sum_q |M_q|^2 \left(\frac{1}{\beta}\right)^4 \sum_{\substack{n_1 n_2\\ n_3 m}} \mathcal{D}^0(q, i\Omega_m)\, \mathcal{G}^0(k, i\omega_{n_1})\, \mathcal{G}^0(k-q, i\omega_{n_2})$$

$$\times\, \mathcal{G}^0(k, i\omega_3)$$

$$\times \int_0^\beta d\tau \int_0^\beta d\tau_1 \int_0^\beta d\tau_2\; e^{i\omega_n \tau}\; e^{-i\omega_{n_1}(\tau-\tau_1) - i\omega_{n_2}(\tau_1-\tau_2) - i\omega_{n_3}\tau_2}$$

$$\times\, e^{-i\Omega_m(\tau_1-\tau_2)}$$

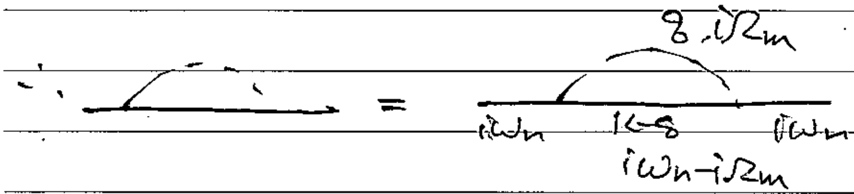
Where $\Omega_m = \frac{2\pi m}{\beta}$ & $\omega_n = \frac{(2n+1)\pi}{\beta}$

The τ-integration yields frequency conservation:

$$\frac{1}{\beta}\int_0^\beta d\tau\, e^{i\tau(\omega_n-\omega_{n_1})} = \delta_{\omega_n,\omega_{n_1}}$$

$$\frac{1}{\beta}\int_0^\beta d\tau_1\, e^{i\tau_1(\underbrace{\omega_{n_1}-\omega_{n_2}}_{\text{even}}-\underbrace{\Omega_m}_{\text{even}})} = \delta_{\omega_{n_1},\omega_{n_2}+\Omega_m}$$

$$\frac{1}{\beta}\int_0^\beta d\tau_2\, e^{i\tau_2(\omega_{n_2}-\omega_{n_3}+\Omega_m)} = \delta_{\omega_{n_3},\omega_{n_2}+\Omega_m}$$

$\therefore$ 

$\Sigma^{(2)}(k, i\omega_n)$

$$= g^{(2)}(k,i\omega_n) = \frac{-1}{\beta}\sum_q\sum_{i\Omega_m}|M_q|^2\mathcal{D}^0(q,i\Omega_m)\,g^0(k-q,i\omega_n-i\Omega_m)$$

$$\times\left[g^0(k,i\omega_n)\right]^2$$

Clearly, we have the same Feynman diagrams with the following Feynman rules:

1. Each electron line $g^0(k, i\omega_n)$
2. Each phonon line $|M_q|^2\mathcal{D}^0(q, i\Omega_n)$
3. Each Coulomb line (~~) $v_q = \frac{4\pi e^2}{q^2}$
4. Momentum & frequencies are conserved with $\omega_n = \frac{\pi(2n+1)}{\beta}$ & $\Omega_m = \frac{2\pi m}{\beta}$.

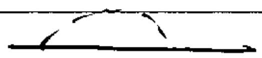
5. mth order (phonon's mth order = # of internal phonon lines)

$$\Rightarrow \frac{(-1)^{m+F}}{\beta^m}(2S+1)^F \qquad F = \#\text{ of Fermion loops.}$$

Frequency summation

Unlike integration over frequencies, in the finite temperature perturbation theory, one needs to evaluate summation over internal frequencies.

For example, in the previous example,

, one needs to evaluate

$$\sum_{i\Omega_m} \mathcal{D}^0(q, i\Omega_m)\, \mathcal{G}^0(k-q, i\omega_n - i\Omega_m)$$

There are two kinds of frequency summations (in the perturbation theory)

(i)

$$S = -\frac{1}{\beta}\sum_{m} f(i\Omega_m) \qquad \Omega_m = \frac{2\pi m}{\beta} \quad \text{(Bosonic series)}$$

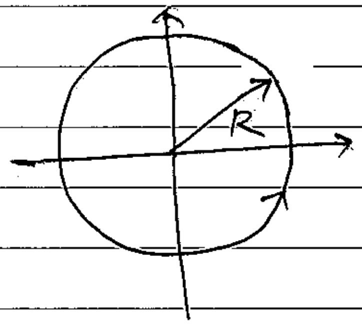
In this case, we choose $n_B(z)$ for consideration to generate $\Omega_m = \frac{2\pi m}{\beta}$ because $n_B(z)$ has poles at $z = i\frac{2\pi m}{\beta}$; $n_B(z) = \frac{1}{e^{\beta z} - 1}$

$$\underset{z=i\Omega_m}{\text{Residue}}\left[n_B(z)\right] = \lim_{z\to i\Omega_m} \frac{z-i\Omega_m}{e^{\beta z}-1}$$

$$= \lim_{z\to i\Omega_m} \frac{1}{\beta e^{\beta z}} = \frac{1}{\beta}$$

Assuming $f(z)\to 0$ in the circle $R\to\infty$,

$$I = \oint_{R\to\infty} \frac{dz}{2\pi i} f(z)\, n_B(z) = 0$$, and $f(z)$ has no



poles at $z=i\Omega_m$, one gets

$$I = \frac{1}{\beta}\sum_m f(i\Omega_m) + \text{other residue}$$

$\therefore S =$ other residue

example: $I = -\frac{1}{\beta}\sum_m \mathcal{D}^0(q, i\Omega_m)\, \mathcal{G}^0(p, i\omega_n + i\Omega_m)$, $\Omega_m = \frac{2\pi m}{\beta}$

$$= \frac{1}{\beta}\sum_{m=-\infty}^{\infty} \frac{2\omega_q}{\Omega_m^2+\omega_q^2}\, \frac{1}{i\omega_n + i\Omega_m - \xi_p}$$

$$= \frac{-1}{\beta}\sum_m f(i\Omega_m)$$

$$f(z) = \frac{2\omega_q}{z^2-\omega_q^2}\, \frac{1}{i\omega_n + z - \xi_p}$$

$\because f(z) \to \infty$ on the $|z| = R \to \infty$ circle.

Other residues:

$z = \omega_q \qquad R_1 = \dfrac{1}{i\omega_n + \omega_q - \xi_p} n_B(\omega_q)$

$z = -\omega_q \qquad R_2 = \dfrac{-1}{i\omega_n - \omega_q - \xi_p} n_B(-\omega_q)$, with $n_B(-\omega_q) = -(1 + n_B(\omega_q))$

$= \dfrac{1 + n_B(\omega_q)}{i\omega_n - \omega_q - \xi_p}$

$z = i\omega_n - \xi_p \qquad R_3 = \dfrac{2\omega_q \, n_B(\xi_p - i\omega_n)}{(i\omega_n - \xi_p)^2 - \omega_q^2}$

$\because n_B(\xi_p - i\omega_n) = \dfrac{1}{e^{\beta(\xi_p - i\omega_n)} - 1} = \dfrac{-1}{e^{\beta\xi_p} + 1} = -n_F(\xi_p)$

(second step uses $e^{-i\beta\omega_n} = -1$, since $\omega_n = \dfrac{\pi(2n+1)}{\beta}$)

$\therefore R_3 = -\dfrac{2\omega_q n_F(\xi_p)}{(i\omega_n - \xi_p)^2 - \omega_q^2} = \dfrac{n_F(\xi_p)}{i\omega_n + \omega_q - \xi_p} - \dfrac{n_F(\xi_p)}{i\omega_n - \omega_q - \xi_p}$

$\therefore I = R_1 + R_2 + R_3$

$= \dfrac{n_B(\omega_q) + n_F(\xi_p)}{i\omega_n + \omega_q - \xi_p} + \dfrac{n_B(\omega_q) + 1 - n_F(\xi_p)}{i\omega_n - \omega_q - \xi_p}$

(ii) Fermionic series

$$S = -\frac{1}{\beta}\sum_n f(i\omega_n) \qquad \omega_n = \frac{(2n+1)\pi}{\beta}$$

In this case, we use $n_F(z) = \frac{1}{e^{\beta z}+1}$

to generate $\omega_n = \frac{(2n+1)\pi}{\beta}$ because $n_F(z)$

has poles at $z = i\frac{(2n+1)\pi}{\beta}$

$$\underset{z=i\omega_n}{\text{Res}}[n_F(z)] = \lim_{z\to i\omega_n} \frac{z-i\omega_n}{e^{\beta z}+1}$$

$$= \lim_{z\to i\omega_n} \frac{1}{\beta e^{\beta z}} = \frac{-1}{\beta}$$

$$I = \oint_{R\to\infty} n_F(z) f(z)\, dz = \frac{-1}{\beta}\sum_n f(i\omega_n) + \text{other residues}$$

$\therefore$ $S = -$ other residues.

example.

$$I = \frac{1}{\beta}\sum_{m=-\infty}^{\infty} \frac{2\omega_q}{\Omega_m^2+\omega_q^2}\,\frac{1}{i\omega_n + i\Omega_m - \xi_p}$$ (same sequence in (i))

$$= \frac{1}{\beta}\sum_n \frac{2\omega_q}{(\omega_n-\omega_m)^2+\omega_q^2}\,\frac{1}{i\omega_n - \xi_p}, \qquad \omega_n = \frac{(2n+1)\pi}{\beta}$$

$$\omega_m = \frac{(2m+1)\pi}{\beta}$$

One needs to choose:

$$f(z) = \frac{2\omega_q}{(z-i\omega_m)^2-\omega_q^2}\ \frac{1}{z-\xi_p}$$

$$I = \frac{-1}{\beta}\sum_n f(i\omega_n)$$

Other residues

$z=\xi_p$. $\quad R_1 = \dfrac{n_F(\xi_p)\,2\omega_q}{(\xi_p-i\omega_m)^2-\omega_q^2}$

$$= n_F(\xi_p)\left[\frac{1}{i\omega_m-\xi_p-\omega_q} - \frac{1}{i\omega_m-\xi_p+\omega_q}\right]$$

$z=i\omega_m-\omega_q \qquad R_2 = -\dfrac{2\omega_q}{2\omega_q}\ \dfrac{n_F(i\omega_m-\omega_q)}{i\omega_m-\xi_p-\omega_q}$

$$= -\frac{n_B(\omega_q)+1}{i\omega_m-\xi_p-\omega_q}$$

$$n_F(i\omega_m-\omega_q) = \frac{1}{e^{\beta(i\omega_m-\omega_q)}+1}$$

$$= \frac{1}{-e^{-\beta\omega_q}+1} = \frac{e^{\beta\omega_q}}{e^{\beta\omega_q}-1}$$

$$= n_B(\omega_q)+1$$

$z=i\omega_m+\omega_q \qquad R_3 = \dfrac{n_F(i\omega_m+\omega_q)}{i\omega_m+\omega_q-\xi_p} = \dfrac{-n_B(\omega_q)}{i\omega_m+\omega_q-\xi_p}$

$$\therefore I = -R_1-R_2-R_3 = \frac{n_B(\omega_q)+n_F(\xi_p)}{i\omega_m-\xi_p+\omega_q} + \frac{n_B(\omega_q)+1-n_F(\xi_p)}{i\omega_m-\xi_p-\omega_q}$$

Other summation formula:

(a) $$\frac{1}{\beta}\sum_m g^0(k, i\omega_m)\, g^0(p, i\omega_m + i\omega_n) = \frac{n_F(\xi_k) - n_F(\xi_p)}{i\omega_n + \xi_k - \xi_p}$$

$$\omega_n = \frac{(2n+1)\pi}{\beta}, \quad \omega_m = \frac{(2m+1)\pi}{\beta}$$

(b) $$\frac{-1}{\beta}\sum_m g^0(k, i\omega_m)\, g^0(p, i\omega_n - i\omega_m) = \frac{1 - n_F(\xi_k) - n_F(\xi_p)}{i\omega_n - \xi_k - \xi_p}$$

(c) $$\frac{1}{\beta}\sum_n g^0(k, i\omega_n) = n_F(\xi_k) \qquad \omega_n = \frac{(2n+1)\pi}{\beta}$$

Finally, one also encounters summations over functions with branch cuts.

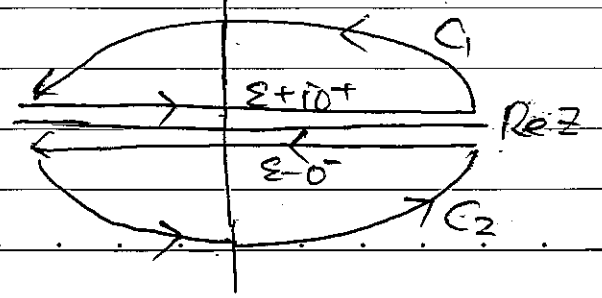
(iii) functions with branch cuts

In this case, one needs to avoid the cuts by going around it to up/down of the cuts.

For example,

$$g_k(\tau) = \frac{1}{\beta}\sum_n g_k(i\omega_n)\, e^{i\omega_n \tau} \qquad \tau > 0, \ \omega_n = \frac{(2n+1)\pi}{\beta}$$

$g_k(z)$ has a branch cut along $Re[z]$ as follows



In this case, one chooses $C_1 + C_2$ ($R \to \infty$)

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In this case, clearly one has

$$\int_{C_1+C_2} \frac{dz}{2\pi i} n_F(z) g_K(z) e^{z\tau}$$

$$= \frac{-1}{\beta} \sum_K g_K(i\omega_n) e^{i\omega_n \tau}$$ as $g_K(z)$ has no other poles except for the branch cut.

On the other hand, we have

$$\int_{C_1} \frac{dz}{2\pi i} n_F(z) g_K(z) e^{z\tau} = \underbrace{\int_{\frown,\, R\to\infty} \frac{dz}{2\pi i} n_F(z) g_K(z) e^{z\tau}}_{\to 0}$$

$$+ \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} n_F(\epsilon) g_K(\epsilon + i0^+) e^{\epsilon\tau}$$

$$\int_{C_2} \frac{dz}{2\pi i} n_F(z) g_K(z) e^{z\tau} = \underbrace{\int_{\smile,\, R\to\infty} \frac{dz}{2\pi i} n_F(z) g_K(z) e^{z\tau}}_{\to 0}$$

$$- \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi i} n_F(\epsilon) g_K(\epsilon - i0^+) e^{\epsilon\tau} \qquad \left(= [g_K(\epsilon + i0^+)]^* \right)$$

$$\therefore\ g_K(\tau) = -\int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi i} n_F(\varepsilon) \underbrace{\left[g_K(\varepsilon + i0^+) - g_K(\epsilon - i0^-) \right]}_{= 2i\, \mathrm{Im}\, G_R(K, \epsilon)} e^{\epsilon\tau}$$

$$\therefore\ g_K(\tau) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} n_F(\epsilon) A(K, \omega) e^{\epsilon\tau}$$

$\uparrow$ spectral weight $= -2\,\mathrm{Im}\, G_R$

example: $\langle c_K^\dagger c_K \rangle = g_K(\tau = 0^-)$ $\left(= -\langle T_\tau c_K(\tau = 0^-) c_K^\dagger(0) \rangle \right)$

$$= \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} n_F(\epsilon)\, A(k,\epsilon) \quad \text{--- (197)}$$

For free electrons, $G_R^0(k,\omega) = \dfrac{1}{\omega - \xi_k + i0^+}$

$$\therefore \mathrm{Im}\, G_R^0(k,\omega) = -\pi\,\delta(\omega - \xi_k)$$

$$\therefore A^0(k,\epsilon) = -2\,\mathrm{Im}\, G_R^0(k,\omega) = 2\pi\,\delta(\omega - \xi_k)$$

$\therefore$ Eq. (197) reproduces $\langle c_k^\dagger c_k \rangle = n_F(\xi_k)$

<u>T=0 limit</u>

The frequency summation, $\frac{1}{\beta}\sum_n f(i\omega_n)$,

in the $T \to 0$, naturally goes over to

the integration over ω:

$$\omega_n = \frac{2\pi n}{\beta} \text{ or } \frac{(2n+1)\pi}{\beta}$$

$$\therefore \Delta\omega_n = \frac{2\pi}{\beta}$$

$$\therefore \frac{1}{\beta}\sum_n f(i\omega_n) = \frac{1}{2\pi}\Delta\omega \sum_n f(i\omega_n)$$

$$\xrightarrow[T\to 0]{} \int \frac{d\omega}{2\pi} f(i\omega)$$

Spectral density function:

The retarded Green's function is the most natural extended Green's function. On one hand, it respects the causality, on the other hand, it can be easily calculated from the Matsubara Green's function by analytic continuation $i\omega_n \to \omega + i0^+$.

From the Lehmann representation, eq. (188), one can insert the identity $1 = \int d\omega' \delta(\omega' + \hbar^{-1}(E_n - E_m))$ and obtains

$$G_A^R(\omega) = \int \frac{d\omega'}{2\pi} \frac{R_A(\omega')}{\omega - \omega' + i0^+} \quad \cdots \quad (198)$$

where $R_A(\omega) = 2\pi e^{\beta\Omega} \sum_{n,m} |\langle n|A|m\rangle|^2 (e^{-\beta E_n} + \xi e^{-\beta E_m})$

$$\times \delta(\omega + \hbar^{-1}(E_n - E_m)) \quad \cdots \quad (199)$$

is called the spectral function of $\hat{A}$

$\because \frac{1}{\omega - \omega' + i0^+} = P\frac{1}{\omega - \omega'} - i\pi\delta(\omega - \omega')$

and $R_A(\omega) =$ real

$$\therefore R(\omega) = -2\,\mathrm{Im}\, G_A^R(\omega) \quad \cdots \quad (200)$$

In particular, for electrons, $A = C_k$,

one gets

$$\mathrm{Im}\, G^R(k,\omega) = -\pi\, e^{\beta\Omega}\sum_{n,m} |\langle n|C_k|m\rangle|^2 \left(e^{-\beta E_n}+e^{-\beta E_m}\right) \times \delta(\omega+E_n-E_m)$$

∴ The spectral function

$$A(k,\omega) = -2\,\mathrm{Im}\, G^R(k,\omega)$$

$$= 2\pi\, e^{\beta\Omega}\sum_{n,m}|\langle n|C_k|m\rangle|^2\left(e^{-\beta E_n}+e^{-\beta E_m}\right)\delta(\omega+E_n-E_m) \geq 0 \quad \cdots (201)$$

and $$G^R(k,\omega)=\int\frac{d\omega'}{2\pi}\,\frac{A(k,\omega')}{\omega-\omega'+i0^+} \quad\cdots (202)$$

From eq. (201), one gets

$$\int \frac{d\omega}{2\pi}A(k,\omega) = e^{\beta\Omega}\sum_{n,m}|\langle n|C_k|m\rangle|^2\left(e^{-\beta E_n}+e^{-\beta E_m}\right)$$

(exchange n ⇄ m)

$$= e^{\beta\Omega}\sum_{nm} e^{-\beta E_n}\left\{\langle n|C_k|m\rangle\langle m|C_k^\dagger|n\rangle + \langle m|C_k|n\rangle\langle n|C_k^\dagger|m\rangle\right\}$$

$$= e^{\beta\Omega}\sum_{n} e^{-\beta E_n}\left\{\underbrace{\langle n|C_kC_k^\dagger + C_k^\dagger C_k|n\rangle}_{1}\right\} = 1$$

$$\therefore \int \frac{d\omega}{2\pi}A(k,\omega) = 1 \quad \cdots (203)$$

Hence $A(k,\omega)$ has the meaning of weight at ω.
(see (201) & (202))

As we have seen, in the case of non-interacting electrons, $A^0(k,\omega) = 2\pi\,\delta(\omega - \xi_k)$ is nonvanishing only when $\omega = \xi_k$.

In general, $A(k,\omega) \neq 2\pi\,\delta(\omega - \xi_k)$ and contributes

$$\langle c_k^\dagger c_k \rangle = \int \frac{d\omega}{2\pi} n_F(\omega)\, A(k,\omega) \quad (\text{eq. } (197))$$

Similarly, for bosons, one finds

$$\langle A_q^\dagger A_q \rangle = \int \frac{d\omega}{2\pi} n_B(\omega)\, B(q,\omega)$$

where $A_q = a_q + a_{-q}^\dagger$ for phonons and

$B(q,\omega) = -2\,\mathrm{Im}\, D_R(q,\omega)$ (retarded Green's functions of phonons)

In the case of interacting electrons, one has

$$G_R(k,\omega) = \frac{1}{\omega + i0^+ - \xi_k - \Sigma_R(k,\omega)} \quad (\text{Dyson's eq.})$$

$$A(k,\omega) = \frac{-2\,\mathrm{Im}\,\Sigma_R(k,\omega)}{(\omega - \xi_k - \mathrm{Re}\,\Sigma_R)^2 + (\mathrm{Im}\,\Sigma_R)^2}.$$

In the frequency region, $\mathrm{Im}\,\Sigma_R = 0$, one has

$$A(k,\omega) = 2\pi\, \delta(\omega - \xi_k - \mathrm{Re}\,\Sigma_R(k,\omega)) \quad \cdots (204)$$

This is the pole approximation we discussed.

Since $\delta(g(x)) = \dfrac{\delta(x-x_0)}{|g'(x_0)|}$ where $g(x_0)=0$,

we get

$$A(k,\omega) = 2\pi Z_k\, \delta(\omega - \xi_k^R) \quad \cdots (205)$$

where $\xi_k^R = \xi_k + \mathrm{Re}\,\Sigma_R(k, \xi_k^R)$

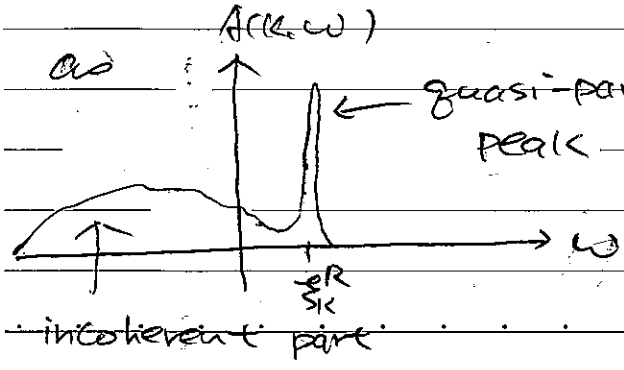
and $Z_k = \left| 1 - \dfrac{\partial}{\partial\omega} \mathrm{Re}\,\Sigma_R(k,\omega) \right|^{-1}_{\omega = \xi_k^R}$

is called a renormalization factor.

Note that eq. (205) can not be correct for all ω region as it contradicts to the result

$$\int \frac{d\omega}{2\pi} A(k,\omega) = 1$$

In real systems, $A(k,\omega)$ does not obey (205) in other ω region, e.g. $A(k,\omega)$ behaves as



$$A(k,\omega) = 2\pi Z_k \delta(\omega - \xi_k^R) + A_{in}(k,\omega)$$

The δ peak is usually referred as resolution limited peak. In reality, there exists a life time τ, $\therefore 2\pi Z_k \delta(\omega - \xi_k^R)$

$$\rightarrow \frac{2Z_k/\tau}{(\omega-\xi_k^R)^2+(1/\tau)^2}$$

<u>Effective mass</u> : ξ_k^R can be used to define the effective mass m^* of the electron.

$$\xi_k^R = \xi_0 + \frac{\hbar^2 k^2}{2m^*} + O(k^4)$$

$$\therefore \frac{m}{m^*} = \left.\frac{\partial \xi_k^R}{\partial \varepsilon_k}\right|_{\varepsilon_k \to 0} \qquad \varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

From $\xi_k^R = \xi_k + Re\,\Sigma_R(k, \overset{\omega}{\overset{\shortparallel}{\xi_k^R}})$, one gets

$$\frac{\partial \xi_k^R}{\partial \varepsilon_k} = 1 + \frac{\partial}{\partial \varepsilon_k} Re\,\Sigma_R(k,\omega) + \frac{\partial}{\partial \omega} Re\,\Sigma_R(k,\omega)\frac{\partial \xi_k^R}{\partial \varepsilon_k}$$

$$\therefore \frac{\partial \xi_k^R}{\partial \varepsilon_k} = \frac{1+\frac{\partial}{\partial \varepsilon_k} Re\,\Sigma_R(k,\xi_k^R)}{1-\frac{\partial}{\partial \xi_k^R} Re\,\Sigma_R(k,\xi_k^R)}$$

$$\frac{m}{m^*} = \lim_{\varepsilon_k \to 0} \frac{1+\frac{\partial}{\partial \varepsilon_k} Re\,\Sigma_R(k,\xi_k^R)}{1-\frac{\partial}{\partial \xi_k^R} Re\,\Sigma_R(k,\xi_k^R)}$$