25 Nov 2015

NEGF is a very useful tool for many part of condensed matter physics. Students of this group should know this theory / formalism very well in order to do good work. This notes is intended to give a solid fundation ~~as basics~~ of NEGF.

We begin with quantum-mechanics/Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H \psi$$

This is an equation for one single electron, e.g. In such case, it is computationally useful to discretize the wave function (in some basis)

$$\psi = \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ \\ C_N \end{pmatrix}$$

and write the Schrödinger equation in the tight-binding form

$$i\hbar \frac{d}{dt} \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_N \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1N} \\ & & \ddots & \\ H_{N1} & & & H_{NN} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_N \end{pmatrix}$$

or briefly just $\quad i\hbar \frac{d}{dt} C = H C$

where C is a column vector of complex numbers. H is the single particle Hamiltonian in a matrix form.

For many electron systems it is more convenient to work in occupation number representation and consider 2nd quantization Hamiltonian

$$\hat{H} = \hat{C}^{+} H \hat{C}$$

here H is the same matrix as before $\hat{C}$ is annihilation operator.

We drop the hat ^ on c

$$\hat{H} = c^\dagger H c \quad \text{and} \quad c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \text{ is column of}$$

annihilation operators and $c^\dagger = (c_1^\dagger \, c_2^\dagger \cdots \, c_N^\dagger)$ is row of creation operators.

The Heisenberg equation is

$$i\hbar \frac{dc}{dt} = Hc$$

This has exactly the same form as the Schrödinger equation on page 3.

☐ Exercise: Verify that $i\hbar \frac{dc}{dt} = [c, \hat{H}]$ produces the Schrödinger eq. Hint. Need use $c_i c_j^\dagger + c_j^\dagger c_i = 1$, $c_i^2 = 0$ etc. $[A, B] \equiv AB - BA$

Now, we consider <u>equilibrium</u> non-equilibrium Green's functions. Equilibrium means

$$\langle \cdots \rangle_{eq} \equiv \mathrm{Tr}\left(\frac{e^{-\beta(H - \mu N)}}{Z} \cdots \right) = \mathrm{Tr}(\rho_{eq} \cdots)$$

that is grand-canonical distribution where

$$Z = \mathrm{Tr}\left(e^{-\beta(H - \mu N)} \cdots\right)$$

$\mathrm{Tr}(\cdots)$ is over the Fock space, that is the eigen states of operator $\hat{n}_i = c_i^\dagger c_i$ $\quad i = 1, 2, \cdots N$

$|n_1 n_2 \cdots n_N\rangle$ Since each site (or state) can be, either occupied $n_i = 1$ or empty, we have exactly 2^N possible states. We trace over all those 2^N states in taking the averages $\langle \cdots \rangle_{eq}$.

In nonequilibrium open quantum systems, we don't have a nice formula for ρ, at best we can compute reduced density matrix. With the except of Hershfield density matrix $e^{-\beta(H-\Psi)}$ but this is purely formal.

We define several versions of Green's functions. In equilibrium, we only need to know one, as they are all related. But it is worthwhile to remember all the definitions. There is no excuse that you don't know the definitin

Greater:
$$G^{>}_{jk}(t,t') = -\frac{i}{\hbar}\langle \underbrace{c_j(t)}_{\text{t: Heisenberg evolution}} \underbrace{c^{+}_k(t')}_{\text{create 1st}} \rangle$$

since $i \equiv \sqrt{-1}$. I try avoid use i for the site/state.

Lesser:
$$G^{<}_{jk}(t,t') = +\frac{i}{\hbar}\langle c^{+}_k(t')\, c_j(t) \rangle$$

Since we swap a fermi operator we need + sign here. For Boson operator we do not have sign chage

$G^{>}$ is a matrix, so we can also write

$$G^{>}(t,t') = -\frac{i}{\hbar}\langle c(t)\, c^{+}(t') \rangle$$
$$= -\frac{i}{\hbar}\left\langle \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} (c_1^{+} c_2^{+} \cdots c_N^{+}) \right\rangle$$

$G^{<}$ can also be written in this compact ~~farm~~ form but it is a bit tricky. Please check that it is

$$G^{<}(t,t') = \frac{i}{\hbar}\left(\langle c^{+T}(t')\, c(t)^{T} \rangle\right)^{T}$$

But this is ugly, we'll not use it.

The retarded is most useful in a sense, since it is related to linear respose theory.

$$G^r(t,t') = \theta(t-t')\left(G^>(t,t') - G^<(t,t')\right)$$

or

$$G^r_{jk}(t,t') = -\frac{i}{\hbar}\theta(t-t')\langle \{ C_j(t), C_k^\dagger(t') \} \rangle$$

$\{A, B\} = AB + BA$ is anti-commutor.

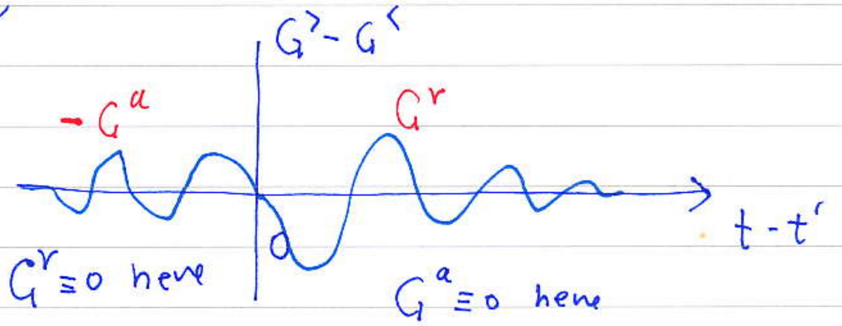
For boson, we use commutator.

$$G^a(t,t') = -\theta(t'-t)\left(G^>(t,t') - G^<(t,t')\right)$$

Let define $G^> - G^< = G^r - G^a = -iA$

Since $\theta(t-t') + \theta(t'-t) = 1$

G^r is the positive half, G^a is negative half with a sign flipped.



A is an important quantity. It's Fourier transform is $2\pi \times$ density of states. A is the spectrum function.

Equation of motion

We compute $i\hbar\frac{\partial}{\partial t}$ to the Green's function and find

$$\left(i\hbar\frac{\partial}{\partial t} - H\right) G^{>,<}(t,t') = 0$$

$$\left(i\hbar\frac{\partial}{\partial t} - H\right) G^r(t,t') = +\delta(t-t') I$$

They are the Green's function for the Schrödinger equation in the classical physics/math sense.

Let prove the 2nd Equation

$$G^r_{jk}(t,t') = -\frac{i}{\hbar}\theta(t-t')\langle c_j(t)c^\dagger_k(t') + c^\dagger_k(t')c_j(t)\rangle$$

differentiate with respect to t

$$i\hbar\frac{\partial}{\partial t}G^r_{jk}(t,t') = i\hbar\left(-\frac{i}{\hbar}\right)\left[\frac{\partial}{\partial t}\theta(t-t')\right]\langle c_j(t)c^\dagger_k(t')$$

$$+ c^\dagger_k(t')c_j(t)\rangle + \left(-\frac{i}{\hbar}\right)\langle i\hbar\frac{\partial}{\partial t}c_j(t)\, c^\dagger_k(t') + c^\dagger_k(t')\, i\hbar\frac{\partial c_j(t)}{\partial t}\rangle$$

$$= \delta(t-t')\langle c_j(t)c^\dagger_k(t') + c^\dagger_k(t')c_j(t)\rangle$$

$$+ \left(-\frac{i}{\hbar}\right)\langle \sum_\ell H_{j\ell}c_\ell(t)\,c^\dagger_k(t') + \sum_\ell c^\dagger_k(t')\,H_{j\ell}\,c_j(t)\rangle$$

We have used the fact that $\frac{d}{dt}\theta(t-t') = \delta(t-t')$

and $i\hbar\frac{dc}{dt} = Hc$

due to the δ-function in the 1st term we can set $t'=t$

but $\{c_j, c^\dagger_k\} = \delta_{jk}$ at equal time

so $$i\hbar\frac{\partial}{\partial t}G^r_{jk}(t,t') = \delta(t-t')\delta_{jk} + \sum_\ell H_{j\ell}G^r_{\ell k}(t,t')$$

In matrix form $$i\hbar\frac{\partial}{\partial t}G^r(t,t') = \delta(t-t')\,I + H\,G^r(t,t')$$

or $$i\hbar\frac{\partial}{\partial t}G^r(t,t') - H\,G^r(t,t') = \delta(t-t')\,\underline{I}.$$

We can solve the retarded Green's function easily if we go to energy space (ie. frequency domain)

we define $$\tilde{G}(E) \equiv \int_{-\infty}^{+\infty} dt\, e^{i\frac{E}{\hbar}t}\,G(t)$$

The inverse transform is $G(t) = \int_{-\infty}^{+\infty} \frac{dE}{2\pi\hbar} e^{i\frac{E}{\hbar}t} \tilde{G}(E)$

we can also identify $\omega = E/\hbar$

but I prefer to use E. Moreover

we have $\delta(t) = \int \frac{dE}{2\pi\hbar} e^{-i\frac{Et}{\hbar}} \cdot 1$

It is clearly $G^r(t,t') \equiv G^r(t-t')$ in practice

equilibrium Green's function is always time translationally

invariant. we have only one argument

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

becomes. in E-space

$$I = \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}$$

N-dimensional identity matrix

$$\left\{ (i\hbar)\left(-\frac{iE}{\hbar}\right) I - H \right\} \tilde{G} = 1$$

or $$\tilde{G}^r(E) = (E\,I - H)^{-1}$$

However, this form is not well defined when we do

inverse Fourier transform. we need to shift the

poles to lower part (negative imaginary) so

the correct formula is

$$\tilde{G}^r(E) = \left((E + i\eta) I - H \right)^{-1}$$

$\eta \to 0^+$.

If we use the same method to $G^<$, we get

$$(E \cdot I - H)\, \tilde{G}^< = 0$$

Does this mean $\tilde{G}^< = 0$? Of course not.

unless $E \cdot I - H \overset{?}{=} 0$

$$f(E) = \frac{1}{e^{\beta(E-\mu)}+1}$$

Formally we can write

$$\tilde{G}(E) = \text{const.}\ \delta(E-H)$$

In fact, this is correct except we cannot fix the constant. The correct expression is

$$\tilde{G}^{<}(E) = -f(E)\left(\tilde{G}^{r}(E) - \tilde{G}^{a}(E)\right) = i f(E)\hat{A}(E)$$

minus sign here

We prove this by different means. This is an important relation in equilibrium. It is called "fluctuation dissipation theorem". This relation does not hold in nonequilibrium as there is no fermi distribution f to talk about. Fortunately, there is a replacement to it. That is the Keldysh equation. So in summary

- For equilibrium systems we have fluctuation-dissipation:

$$\tilde{G}^{<} = -f(\tilde{G}^{r} - \tilde{G}^{a}) = i f \tilde{A}$$

- For nonequilibrium case, we get Keldysh equation

$$\tilde{G}^{<} = \tilde{G}^{r}\tilde{\Sigma}^{<}\tilde{G}^{a}$$

where $\Sigma^{<}$ is self-energy. The tilde ~ means we are in energy domain!

Note that both equations are in energy domain $\tilde{G} \rightarrow \tilde{G}(E)$. not in time domain $G(t)$.

The Keldysh equation is perhaps the most important equation in NEGF. It is a consequence of the contour variable Dyson equation.

We prove a very general fluctuatis. dissipatn theorem. We define

$$G^{>}_{AB}(t) = -\frac{i}{\hbar} \langle A(t) B(0) \rangle$$

$$G^{r}_{AB}(t) = -\frac{i}{\hbar} \theta(t) \langle A(t) B \pm B A(t) \rangle$$
$$= \theta(t) \left(G^{>}_{AB}(t) - G^{<}_{AB}(t) \right)$$

$$-i A_{AB}(t) = -\frac{i}{\hbar} \langle A(t) B \pm B A(t) \rangle = G^{>}_{AB}(t) - G^{<}_{AB}(t)$$
$$= G^{r}_{AB}(t) - G^{a}_{AB}(t)$$

These definites are consistent to those on page 7, 9, except that A and B are arbitray quantu operatr, hermitn or not. Now the $\pm$ sign. If A, B are fermio-like we take +, bosonic-like we take −. Think of $\frac{1}{e^{\beta(\varepsilon\cdots)} \pm 1}$ ← + fermi distribn − bose distribn.

Fermion-like means the operatr follows anti-comutatr relation like c and c^+, Bosoni-like means the operatr follows commutation relation. More precisely, under the time order or countour order sign T_τ, bosoni operatr commute, fermoin operatr anti commute. Even though we are dealing with fermions (electrons), we still have boson like operatr like local energy, current j, or charge ρ as the are pair of fermi operatrs like c^+c.

The idea of proof is to use Lehmann representation i.e. expand the expressiond Green's functions in the eigen state of $\hat{H}$ and then use the plemelj formula $\frac{1}{x+i\eta} = P\frac{1}{x} - i\pi\delta(x)$ where $P\frac{1}{x}$ stand for principle value

☐ Question. what is a "principle value"?

Let $\hat{H}|\mu\rangle = E_\mu|\mu\rangle \quad \mu = 1, 2, \ldots 2^N$

This is a "many-body" state. in Fock space. Since the dimensin of the Fock space is 2^N, we have 2^N differn states denoted by $|\mu\rangle$. This space is much larger that the single particle of eigen vectr of H, where $\hat{H} = c^+ H c$. The dimension of single partcle state is N. For such non-interacting system, standard procedure exists to build $|\mu\rangle$ for the single partcle state φ, where $H\varphi_i = \epsilon_i\varphi_i$ where ϵ is single partile energy. We leave this as a exercise.

☐ Question: How to build $|\mu\rangle$ from φ_i?

We'll work exclusively in $|\mu\rangle$, the many-body state. We work for $G^>$ where Heisenberg operator

$$A(t) = e^{\frac{i}{\hbar}\hat{H}t} A e^{-\frac{i}{\hbar}\hat{H}t}$$

$$B(0) = B$$

$$G^>(t) = \frac{1}{i\hbar}\langle A(t)B(0)\rangle = \frac{1}{i\hbar}\mathrm{Tr}\left(\frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z} e^{\frac{i}{\hbar}\hat{H}t} A e^{-\frac{i}{\hbar}\hat{H}t} B\right)$$

we use the fact that $\hat{H}$ and $\hat{N}$ commute, and so it is always possile that $\hat{N}|\mu\rangle = N_\mu|\mu\rangle$ is also an eigen state of $\hat{N}$.

Trace means $\sum_{\mu} \langle \mu | \cdots | \mu \rangle = \mathrm{Tr}(\cdots)$

$$G^{>}_{AB}(t) = \frac{1}{i\hbar} \sum_{\mu} \langle \mu | \frac{1}{Z} e^{-\beta(\hat{H} - \mu \hat{N})} e^{\frac{i}{\hbar}\hat{H}t} A \underset{\uparrow}{\;} e^{-\frac{i}{\hbar}\hat{H}t} B | \mu \rangle$$

$\sum |\nu\rangle\langle\nu| = \hat{1}$ insert complet set

$$= \frac{1}{i\hbar Z} \sum_{\mu\nu} e^{-\beta(E_\mu - \mu N_\mu)} \cdots$$

sorry for notatn confusi let use n & m instead

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

Go to energy space by Fourier transform

$$\tilde{G}^{>}_{AB}(E) = \int_{-\infty}^{+\infty} dt\, G^{>}_{AB}(t) e^{i\frac{Et}{\hbar}} = \frac{1}{i\hbar Z} \sum_{n,m} \langle n | A | m \rangle \langle m | B | n \rangle \left\{ 2\pi\, \delta\left(\frac{E_n - E_m + E}{\hbar}\right) \cdot e^{-\beta(E_n - \mu N_n)} \right\}$$

$$= \frac{1}{iZ} \sum_{n,m} \langle n | A | m \rangle \langle m | B | n \rangle e^{-\beta(E_n - \mu N_n)} \cdot 2\pi\, \delta(E_n - E_m + E)$$

we have use the formula $\int_{-\infty}^{+\infty} e^{ixt}\, dt = 2\pi\delta(x)$

notice the 2π here

and $\delta(ax) = \frac{1}{|a|}\delta(x)$.

$G^{>}$ is done, now let focus on $A_{AB}(t)$

$$A_{AB}(t) = i\left(G^{>}_{AB}(t) - G^{<}_{AB}(t)\right)$$

$$= \frac{1}{\hbar} \langle \underbrace{A(t) B}_{\text{already worked out}} \pm B A(t) \rangle$$

swap positn of A & B.

The Fourier transfm of A_{AB} is

$$\tilde{A}_{AB}(E) = \frac{1}{Z}\sum_{n,m}\Big\{ e^{-\beta(E_n-\mu N_n)} \cdot 2\pi\delta(E+E_n-E_m)\langle n|A|m\rangle\langle m|B|n\rangle$$

$$\pm\ e^{-\beta(E_n-\mu N_n)} \underbrace{2\pi\delta(E+E_m-E_n)\langle n|B|m\rangle\langle m|A|n\rangle}_{\text{swap indx } n\leftrightarrow m}\Big\}$$

$$= \frac{1}{Z}\sum_{n,m}\Big\{\left(e^{-\beta(E_n-\mu N_n)} \pm e^{-\beta(E_m-\mu N_m)}\right) 2\pi\delta(E+E_n-E_m)\langle n|A|m\rangle\langle m|B|n\rangle\Big\}$$

Due to the δ-fnctn constraints. we have $E+E_n-E_m=0$

we have $E_m = E+E_n$

Also if $\langle n|A|m\rangle \neq 0$ $N_n = N_m$, transitn betwn different N is possible if A is c or c^+. We need consider two case. if A or B is of the form c^+c then $N_n \equiv N_m$. if $A=c$, $B=c^+$ then $N_n = N_m - 1$ in order to have nonzero $\langle n|A|m\rangle\langle m|B|n\rangle$

For Bosonic case (A or B of the fm $c^+\ldots c$)

$$= \frac{1}{Z}\sum_{n,m}\left(e^{-\beta(E_n-\mu N_n)} - e^{-\beta(E+E_n-\mu N_n)}\right)\cdot 2\pi\delta(\cdots)\ldots\Big\}$$

$$= \left(1-e^{-\beta E}\right)\frac{1}{Z}\sum_{n,m} e^{-\beta(E_n-\mu N_n)}\cdot 2\pi\delta(E+E_n-E_m)\langle n|A|m\rangle\langle m|B|n\rangle$$

compare with $\tilde{G}^{>}_{AB}(E)$ we get

$$N(E) \equiv \frac{1}{e^{\beta E}-1}$$

$$\tilde{A}_{AB}(E) = \left(1-e^{-\beta E}\right)\cdot i\cdot \tilde{G}^{>}_{AB}(E)$$

or $$\tilde{G}^{>}_{AB}(E) = \frac{-i}{1-e^{-\beta E}}\tilde{A}_{AB}(E) = -i\left(\frac{1-e^{-\beta E}+e^{-\beta E}}{1-e^{-\beta E}}\right)\tilde{A}_{AB}(E)$$

$$= -i\left(1+N(E)\right)\tilde{A}_{AB}(E)$$

we get, for bosonic operator which conserve particle number (in the sense $A|n\rangle$ and $|n\rangle$ has the same num of electrons. We are dealing with electrons, not real boson particles)

$$\tilde{G}^{>} = -i(1+N)\tilde{A}$$

$\tilde{G}^{>} \to \tilde{G}^{>}_{AB}(E)$

$\tilde{A} \to \tilde{A}_{AB}(E)$

since $-i\tilde{A} = \tilde{G}^{>} - \tilde{G}^{<}$

$$\tilde{G}^{<} = \tilde{G}^{>} + i\tilde{A} = -i(1+N)\tilde{A} + i\tilde{A}$$

$$= -iN\tilde{A} = N(E)\left(\tilde{G}^{r}(E) - \tilde{G}^{a}(E)\right)$$

This is a correct result. since $-iA = G^r - G^a$.

$N(E) = \frac{1}{e^{\beta E}-1}$. is bose function.

Now we consider fermion case with + sign and

$N_n = N_m - 1$

we get
$$\tilde{A}_{AB}(E) = \frac{1}{Z}\sum_{n,m}\left\{e^{-\beta(E_n-\mu N_n)} + e^{-\beta(E+E_n-\mu(N_n+1))}\right\} 2\pi\delta(E+E_n-E_m)\langle n|A|m\rangle\langle m|B|n\rangle \}$$

$$= \frac{1+e^{-\beta(E-\mu)}}{Z}\sum_{n,m} e^{-\beta(E_n-\mu N_n)} 2\pi\delta(E+E_n-E_m) \cdot \langle n|A|m\rangle\langle m|B|n\rangle$$

$$= i\left(1+e^{-\beta(E-\mu)}\right)\tilde{G}^{>}_{AB}(E)$$

Omitting subscripts AB,

$$\tilde{G}^{>}(E) = \frac{-i}{1+e^{-\beta(E-\mu)}}\tilde{A}(E)$$

$$= -i(1-f(E))\tilde{A}(E) = (1-f(E))(\tilde{G}^{r} - \tilde{G}^{a})$$

$1-f$ means the occupation of holes.

similarly $\quad -iA = G^> - G^<$ and $G^> = (1-f)(-iA)$

gives $\quad G^< = G^> + iA = (1-f)(-iA) + iA$

fluctuation-dissipation theorem: $\quad = ifA = -f(G^r - G^a)$

Or $\quad \tilde{G}^<_{AB}(E) = i f(E) \tilde{A}_{AB}(E) = -f(E)\left(\tilde{G}^r_{AB}(E) - \tilde{G}^a_{AB}(E)\right)$

fermion case has a minus sign here.

$$f(E) \equiv \frac{1}{e^{\beta(E-\mu)}+1}$$

$$N(E) \equiv \frac{1}{e^{\beta E}-1}$$

N has no chemical potential μ.

The remain relations are $\tilde{A}$ and $\tilde{G}^r$, $\tilde{G}^r$ and $\tilde{G}^a$!

In proving the above relation $G^< = ifA = -f(G^r - G^a)$ we have used the fact the B operator create one particle and A operator annihilates one particle. If B operator happen to be creating two particles (two electrons) we would get $e^{\beta(E-2\mu)}$ instead! In practice this equation always mean

$$\tilde{G}^<_{c_j c_k^+}(E) \quad \text{for } A = c_j. \quad B = c_k^+.$$

The most important formula for electron Green's functions.

1) $$\tilde{G}^r(E) = \frac{1}{(E+i\eta)I - H}$$ ← matrix inverse $\eta \to 0^+$

2) $$\tilde{G}^<(E) = i f(E) \tilde{A}(E) = -f(E)\left(\tilde{G}^r(E) - \tilde{G}^a(E)\right)$$

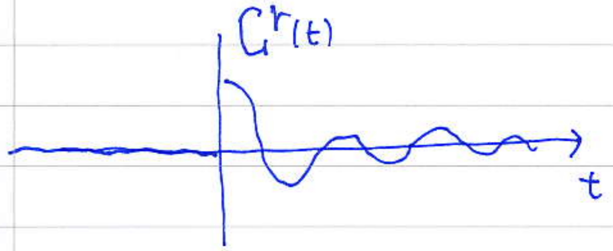
These two formulas should be memorized/learned by heart.

28 Nov 2015

We now discuss the relationship between the spectrum function A and retarded and advanced Green's function G^r and G^a. It is very simple in time domain

$$G^r(t) = \theta(t)\left(G^>(t) - G^<(t)\right)$$
$$= -i\,\theta(t)\,A(t) \qquad\qquad G^a(t) = i\,\theta(-t)\,A(t)$$

G^r takes positive t half of A, G^a takes negative half of A with a sign flip.



The feature that $G^r(t) \equiv 0$ for $t < 0$ is called causality.

This fact implies that $\tilde{G}^r(E)$ is an analytic functi of E is we analytically continues the retarded Green's function to the upper half plane z. The meaning of causality is best seen in the linear response theory. (See, eg. N. Pottier, "Nonequilibm Stat phys")

If the original Hamiltn $\hat{H}$ is perturbed by some external perturbation in the form

$$\hat{H}_{tot} = \hat{H} - b(t)\cdot\hat{B}$$

where b(t) is a scalar control field (like classical magnetic or electric field) and $\hat{B}$ is quantum operator then

$$\underset{\text{now}}{\langle \hat{A}(t)\rangle} = -\int_{-\infty}^{+\infty} dt'\, G^r_{AB}(t,t')\, \underset{\text{past}}{b(t')}$$

Since past can influence the future, but future cannot have effects to the past, we must have

$$G^r_{AB}(t,t') = 0 \quad \text{if} \quad t < t'$$

Under time indept Hamiltn $\hat{H}$ which has no explicit time

$G^r_{AB}(t,t') \equiv G^r_{AB}(t-t')$ depends on the time difference only. $t < t'$ means $G^r_{AB}(\Delta t)$ with $\Delta t = t - t' < 0$

Back to relation of A and G^r — since

$$G^r(t) = -i\,\theta(t)\,A(t)$$

is a product of two functions $\theta(t)$ and $A(t)$, we can compute $\tilde{G}^r(E)$, the Fourier space retarded Green's function by applying the convolution theorem in reverse: product in time domain becomes convolution in energy domain.

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

$$\theta(t) \rightarrow \hat{\theta}(E) = \int_{-\infty}^{+\infty} dt\, e^{i\frac{Et}{\hbar}} \theta(t) = \int_{0}^{+\infty} dt\, e^{i\frac{Et}{\hbar}}$$

Unfortunately the 2nd integral does not exists, and it's also not Lesbegues integrable as $\int^{+\infty} dt \left| e^{\frac{iEt}{\hbar}} \right| \rightarrow +\infty$.

physicist's way to solve this mathematical problem is to add artificial damping. i.e. change the problem to

$$\hat{\theta}_\eta(E) = \int_0^{+\infty} dt\, e^{\frac{i}{\hbar}Et - \frac{\eta}{\hbar}t} \qquad \eta \rightarrow 0^+$$

$$= \frac{e^{(\frac{i}{\hbar}E - \frac{\eta}{\hbar})t}}{\frac{i}{\hbar}E - \frac{\eta}{\hbar}}\Bigg|_0^{+\infty} = \frac{i\hbar}{E + i\eta}$$

Now we do the reverse convolution theorem

$$\tilde{G}^r(E) = -i \int_{-\infty}^{+\infty} dt \; \theta(t) A(t) e^{i\frac{E}{\hbar}t}$$

$$= -i \int_{-\infty}^{+\infty} dt \left[\underbrace{\int_{-\infty}^{+\infty} \frac{dE'}{2\pi\hbar} \tilde{\theta}_\eta(E') e^{-\frac{i}{\hbar}E't}}_{\theta(t)} \right] A(t) e^{i\frac{E}{\hbar}t}$$

$$= \int_{-\infty}^{+\infty} \frac{dE'}{2\pi\hbar} \tilde{\theta}_\eta(E') \, (-i) \int_{-\infty}^{+\infty} dt \, A(t) e^{i\frac{(E-E')}{\hbar}t} = \int_{-\infty}^{+\infty} \frac{dE'}{2\pi\hbar} \tilde{\theta}_\eta(E') \tilde{A}(E-E')$$

$$= \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \cdot \frac{\tilde{A}(E-E')}{E'+i\eta} \qquad = -\int_{+\infty}^{-\infty} \frac{dE''}{2\pi} \cdot \frac{\tilde{A}(E'')}{E-E''+i\eta}$$

No $\hbar$

$\hbar$ gets cancelled

let $E - E' = E''$

$$= \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\tilde{A}(E')}{E+i\eta-E'} \qquad \text{rename } E'' \text{ as } E'$$

This is the final expression for the spectrum represent. of $\tilde{G}^r(E)$

☐ Question. we get two expressions for $\tilde{G}^r$, one is

$\tilde{G}^r(E) = (E + i\eta - H)^{-1}$, and another is the above

spectrum integral. What is the difference? Which one more general. How to go from the one form to the other. i.e. their relationship?

☐ Show, by the same idea as above that

$$\tilde{G}^a(E) = \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\tilde{A}(E')}{E-i\eta-E'}$$

everything is the same except a sign change here.

ans: $G^a(t) = i\,\theta(-t)\,\hat{A}(t)$

sign differ for $G^r(t)$

$$\theta_\eta(-t) = \int \frac{dE'}{2\pi\hbar}\,\theta_\eta(E')\,e^{\frac{i}{\hbar}E't}$$

same + instead of −

so
$$\tilde{G}^a(E) = i\int_{-\infty}^{+\infty} dt\,\theta_\eta(-t)\,A(t)\,e^{i\frac{E}{\hbar}t}$$

$$= i\int \frac{dE'}{2\pi\hbar}\,\theta_\eta(E')\int_{-\infty}^{+\infty} dt\,A(t)\,e^{i\frac{E+E'}{\hbar}t}$$

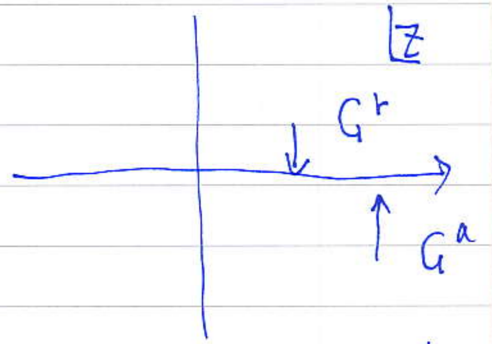
Let $E+E' = E''$

$$= i\int_{-\infty}^{+\infty} \frac{dE'}{2\pi\hbar}\,\frac{i\hbar}{E'+i\eta}\,\hat{A}(E+E')$$

$$= -\int_{-\infty}^{+\infty} \frac{dE''}{2\pi}\,\frac{\hat{A}(E'')}{E''-E+i\eta} = \int_{-\infty}^{+\infty} \frac{dE'}{2\pi}\cdot\frac{\hat{A}(E')}{E-E'-i\eta}$$ as claimed

It is useful to define

$$G(z) = \int_{-\infty}^{+\infty} \frac{dE'}{2\pi}\cdot\frac{\hat{A}(E')}{z-E'}$$



then
$$G^r(E) = \lim_{\eta\to 0^+} G(E+i\eta)$$

$$G^a(E) = \lim_{\eta\to 0^+} G(E-i\eta)$$

If we approach the real axis from above we get G^r, from below we get $G^a(E)$. The limit is not the same since there is a discontinuity cross real axis.

Using the plemelj formula

$$\frac{1}{x+i\eta} = P\,\frac{1}{x} - i\pi\,\delta(x)$$

we can write

$$\tilde{G}^r(E) = P\int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\tilde{A}(E')}{E - E'} - i\frac{1}{2}\tilde{A}(E)$$

$$\tilde{G}^a(E) = P\int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\tilde{A}(E')}{E - E'} + i\frac{1}{2}\tilde{A}(E)$$

$i = \sqrt{-1}$

substract, we get

$$\tilde{G}^r(E) - \tilde{G}^a(E) = -i\tilde{A}(E)$$

this is nothing but the energy domain equtn for the definiti of A

$$A(t) = i\left(G^r(t) - G^a(t)\right)$$

or we write $A = i(G^r - G^a) = i(G^> - G^<)$

which works in t or E space.
as well as

Finally, we need to work out the relationship between $\tilde{G}^r$ and $\tilde{G}^a$. The usual formula is

$$\tilde{G}^a(E) = \left[\tilde{G}^r(E)\right]^\dagger$$ ← hermitian conjugate.

But it is tricker than you think if the operator A and B forming G^r_{AB} is arbitrary operator.

We start from the Lehman representation for $\tilde{G}^r_{AB}(E)$.

using

$$\tilde{G}^r_{AB}(E) = \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\tilde{A}_{AB}(E')}{E + i\eta - E'}$$

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and

$$\tilde{A}_{AB}(E') = \frac{1}{Z}\sum_{n,m}\left(e^{-\beta(E_n - \mu N_n)} \pm e^{-\beta(E_m - \mu N_m)}\right) \cdot 2\pi\delta(E' + E_n - E_m)\langle n|A|m\rangle\langle m|B|n\rangle$$

+ fermion-like
− boson-like

we can write

$$\tilde{G}^r_{AB}(E) = \frac{1}{Z}\sum_{n,m} \frac{\left(e^{-\beta(E_n-\mu N_n)} \pm e^{-\beta(E_m-\mu N_m)}\right)}{E+i\eta - (E_m - E_n)} \langle n|A|m\rangle\langle m|B|n\rangle$$

$\tilde{G}^a_{AB}(E)$ is obtained by replace $i\eta$ by $-i\eta$

Take the complex conjugate of $\tilde{G}^r_{AB}(E)$ we get

$$\left(\tilde{G}^r_{AB}(E)\right)^* = \frac{1}{Z}\sum_{n,m} \frac{\overset{\text{same}}{\cdots\cdots}}{E - i\eta - E'} \left(\langle n|A|m\rangle\langle m|B|n\rangle\right)^* \qquad E' = E_m - E_n$$

$$= \frac{1}{Z}\sum_{n,m} \frac{(e^{\cdots} \pm e^{\cdots})}{E - i\eta - E'} \langle n|B^+|m\rangle\langle m|A^+|n\rangle$$

we have used the genl relation

$$\langle \varphi|\hat{O}|\psi\rangle^* = \langle\psi|\hat{O}^+|\varphi\rangle$$

Note also $\quad \langle\varphi|\psi\rangle^* = \langle\psi|\varphi\rangle$

the result is not $G^a_{BA}(E)$ but

$$\boxed{\tilde{G}^r_{AB}(E)^* = \tilde{G}^a_{B^+A^+}(E)}$$

If A and B are hermitian operator then $A^+ = A$, $B^+ = B$

we get $\quad \tilde{G}^a = (\tilde{G}^r)^+ = (\tilde{G}^*)^T$ ← transpose means swap the index of the matrix

For the case of electron single particle Green's function $B = C^+_K$ $\quad A = C_j$, then

then $B^+ = (C^+_K)^+ = C_K$, $\quad A^+ = (C_j)^+ = C_j^+$,

$$\tilde{G}^{r*}_{C_j C_K^+}(E) = \tilde{G}^a_{C_K C_j^+}(E) \qquad \text{ie.} \quad [\tilde{G}^r]^+ = \tilde{G}^a \quad \text{still holds}$$

Matsubara Green's function is needed if we do dynamic mean-field. it is defined as

Only Matsubara, contour version has diagrammatic expansions.

$$G^M_{jk}(\tau, \tau') = -\frac{1}{\hbar} \langle T_\tau C_j(\tau) C_k^+(\tau') \rangle$$

where τ, τ' is not contour time but "imaginary time" $it = \tau$.

$$C_j(\tau) \equiv e^{\frac{1}{\hbar}(H-\mu N)\tau} c_j e^{-\frac{1}{\hbar}(H-\mu N)\tau}$$

In Matsubara approach, it is customary to include the chemical potential term $-\mu N$. so even if we take $\tau = it$. it is not Heisenberg operator.
The reason for this $-\mu N$ factor is that it make it the same as distribution$_{eq.}$ $\rho = \frac{e^{-\beta(H-\mu N)}}{Z}$.

The T_τ super operator arranges the order of operator according to the value of τ from small to large. i.e.

$$T_\tau A(\tau) B(\tau') = \begin{cases} A(\tau) B(\tau') & \text{if } \tau > \tau' \\ -B(\tau') A(\tau) & \text{if } \tau' > \tau \end{cases}$$

minus sign when A, B is fermi-like

large τ ← small

The value of τ cannot be arbitrarily large, combine ρ with the the factor in $C_j(\tau)$, we have

$$Tr\left(e^{-(\beta - \frac{\tau}{\hbar})(H-\mu N)} c_j e^{-(\frac{\tau - \tau'}{\hbar})(H-\mu N)} c_k e^{-\frac{\tau'}{\hbar}(H-\mu N)} \cdots \right)$$

if τ is larger than $\hbar\beta$, the factor $e^{-(\beta - \frac{\tau}{\hbar})(H-\mu N)}$ becomes unbounded since H usually has a lower bound but not upper bound.

So, we define the Matsubara Green's funct only in the interval $-\hbar\beta \leq \tau, \tau' \leq \hbar\beta$.

It can be shown that Matsubara function depends only on the difference, $\tau - \tau'$. also satisfies the anti periodic BC. for fermion.

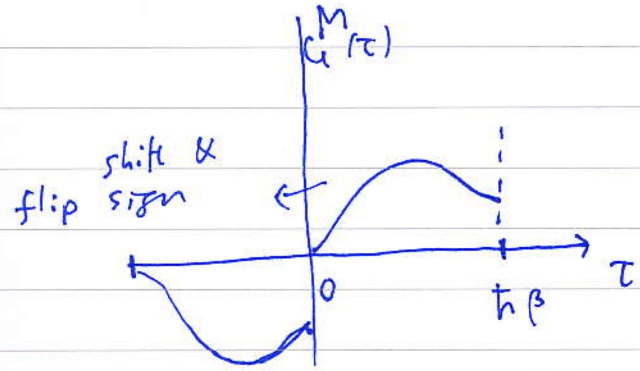
☐ Question/problem. prove the above statements explicitly.

We write $G^M(\tau, \tau') \equiv G^M(\tau - \tau')$, and

$$G^M(\tau) = - G^M(\tau - \beta\hbar)$$

minus sign for fermion
+ sign for boson

[See Piet Brouwer, 2005 lecture notes "Theory of Many-particles system. as well as Mahan's book]



In particular
$$G^M(\hbar\beta) = - G^M(0)$$
anti-periodic B.C.

Make can make Fourier series (not integral)

$$\tilde{G}^M(i\omega_n) \equiv \int_0^{\hbar\beta} d\tau \, e^{i\omega_n\tau} G^M(\tau)$$

$$\omega_n = \frac{(2n+1)\pi}{\hbar\beta} \qquad n = 0, \pm 1, \pm 2, \ldots$$ This is Matsubara frequency

Inverse is $$G^M(\tau) = \frac{1}{\hbar\beta} \sum_n e^{-i\omega_n\tau} \tilde{G}^M(i\omega_n)$$

☐ Question: Is $G^M(\tau)$ an odd function of τ?
ie $G^M(\tau) = - G^M(-\tau)$?

Since $\tau<0$ part is related to $\tau>0$ part by anti-symmetry, we focus on $0\leq\tau\leq\hbar\beta$ only, then

$$G^{M}_{AB}(\tau) = -\frac{1}{\hbar}\langle A(\tau)B(0)\rangle$$

No need for T_τ as $\tau>0$

$0\leq\tau\leq\hbar\beta$

$$= -\frac{1}{\hbar}\mathrm{Tr}\left(\frac{e^{-\beta(H-\mu N)}}{Z} e^{\frac{\tau}{\hbar}(H-\mu N)} A\, e^{-\frac{\tau}{\hbar}(H-\mu N)} B\right)$$

go to Lehmann representation

$\rightarrow$

$$= -\frac{1}{\hbar}\frac{1}{Z}\sum_{n,m} e^{-(\beta-\frac{\tau}{\hbar})(E_n-\mu N_n)-\frac{\tau}{\hbar}(E_m-\mu N_m)} \langle n|A|m\rangle\langle m|B|n\rangle$$

$$\tilde{G}^{M}_{AB}(i\omega_n) = \int_0^{\hbar\beta} e^{i\omega_n\tau} G^{M}_{AB}(\tau)\,d\tau$$

$$= -\frac{1}{\hbar}\frac{1}{Z}\sum_{n,m}\int_0^{\hbar\beta} d\tau\, e^{\frac{\tau}{\hbar}(E_n-E_m-\mu(N_n-N_m))+i\omega_n\tau} e^{-\beta(E_n-\mu N_n)} \langle n|A|m\rangle\langle m|B|n\rangle$$

$$= -\frac{1}{\hbar}\frac{1}{Z}\sum_{n,m}\frac{e^{-\beta(E_n-\mu N_n)}\left[e^{\frac{\hbar\beta}{\hbar}(E_n-E_m-\mu(N_n-N_m))+i\omega_n\hbar\beta}-1\right]}{\frac{1}{\hbar}(E_n-E_m-\mu(N_n-N_m))+i\omega_n} \times\langle n|A|m\rangle\langle m|B|n\rangle$$

$$i\omega_n\hbar\beta = i\frac{(2n+1)\pi}{\hbar\beta}\hbar\beta = i2\pi n + i\pi$$

$$e^{i\omega_n\hbar\beta} = -1$$

$$= +\frac{1}{Z}\sum_{n,m}\frac{e^{-\beta(E_m-\mu N_m)}+e^{-\beta(E_n-\mu N_n)}}{E_n-E_m-\mu(N_n-N_m)+i\hbar\omega_n}\langle n|A|m\rangle\langle m|B|n\rangle$$

If we compare this expression with that of Lehmann representation for $\tilde{G}^{r}_{AB}(E)$ we see that they are the same except the denominator is different.

We assume $A = c$, $B = c^{\dagger}$, so $N_n - N_m = -1$

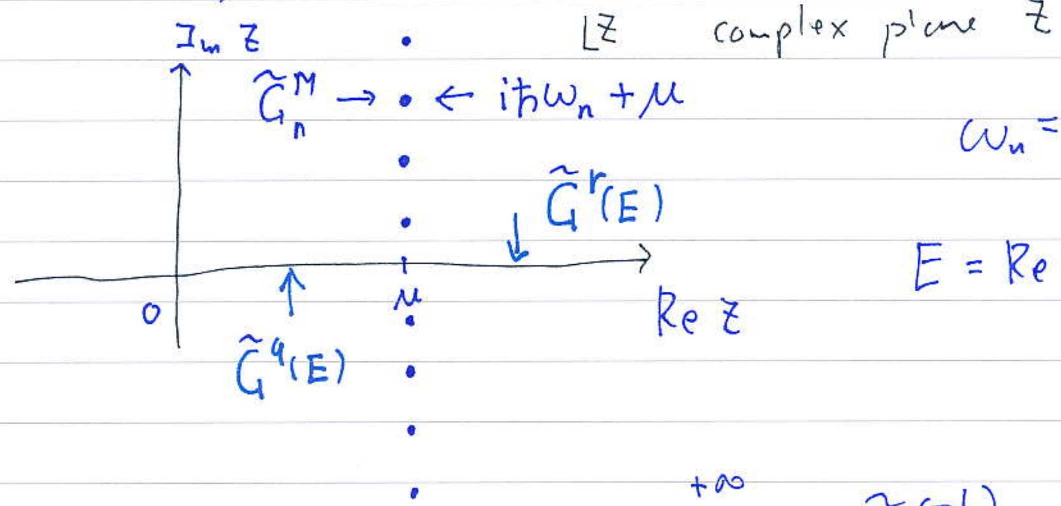
(see page 23) so $E + i\eta \leftrightarrow i\hbar\omega_n + \mu$

We have now obtain an important relation betwn retarded Green's function and Matsubara Green's function. i.e.

$$\tilde{G}^r(E\ \ ) = \tilde{G}^M(i\hbar\omega_n + \mu \to E + i\eta)$$

or $$G(z \to i\hbar\omega_n + \mu) = \tilde{G}^M(i\omega_n) \equiv \tilde{G}_n \qquad n = 0, \pm1, \pm2, \ldots$$

picturically this means



$\omega_n = \frac{(2n+1)\pi}{\hbar\beta}$

$E = \mathrm{Re}\, z$

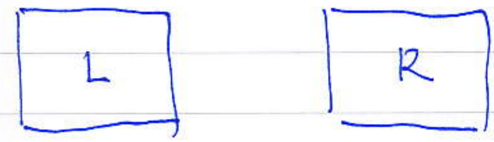
If we already know $G(z) = \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\tilde{A}(E')}{z - E'}$

which means we know $\tilde{A}$,
then if we approach the real axis from above ~~we~~ get retarded Green's func $\tilde{G}^r(E)$, if we approach from below we get $\tilde{G}^a(E)$. if we sit at the discrete points $i\hbar\omega_n + \mu$, where μ is chemical potential of the electron, we are at the values of Matsubara Green's function $\tilde{G}^M(i\omega_n)$. In this sense, $\tilde{A}$ is the most important quantity for equilibrium Green's functions.

"NEGF"

After a long preparation for the equilibrim Green's functions, we are ready to talk about the nonequilibm ones. The reason that we need a thorough understanding of equilibm one fibe is that it is always the case that we "build" nonequilbm Green's functn from equilibm ones. Without a equilibm system to start with, we don't know how to make a nonequilibm one.

The idea of NEGF is that we prepare constrainted equilibrim states at $t \to -\infty$. But seperated and non interacting. at $t \to -\infty$.



non interacting betwen L and R

left system in equilibm at $\beta_L = \frac{1}{K_B T_L}$, μ_L

and right system in equilibm at different β_R μ_R.

There nothing in betwen. So the Green's functn is

$$G_0 = \begin{bmatrix} G_L & 0 \\ 0 & G_R \end{bmatrix} .$$

G_0 is a matrix, indexed by positions like, j, k or states μ, ν.

We let the system interact as we go to $t \approx 0$, the time of interest.

$$H_{tot}(t) = H_L + H_R + V e^{\epsilon t}$$

$e^{\epsilon t} \to 0$ as $t \to -\infty$, $\epsilon \to 0^+$. ϵ is known as adiabatic switch-on parameter.

For the electron-photon system, we may consider

$$H_{tot} = \underbrace{H_L^e + H_R^e}_{\text{free electrons}} + \underbrace{H_\gamma}_{\text{free photons}} + V$$

electron-photon interaction term

The effect ~~of~~ the interaction is encapsulated in the self-energy.

encapsulated

$$G = G_0 + G_0 \Sigma G$$ or more explicitly

[this defined the meaning of self energy Σ]

for electrons

$$G_{jk}(\tau, \tau') = G^0_{jk}(\tau, \tau') + \int d\tau_1 \int d\tau_2 \sum_{lm} G^0_{jl}(\tau\, \tau_1)\, \Sigma_{lm}(\tau_1, \tau_2)\, G_{mk}(\tau_2\, \tau')$$

so $G_0 \Pi G$ means matrix multiplication for the site index j, k, and contour integrals for the contour time τ.

For continuous variables like photon, we need integrals for space and contour time, like $\int dx \int d\tau$

The "NEGF technowleges" is discussed in many places including two of my reviews, I don't what to repeat here. In any case, I don't have new insight and cannot make it better than before. So please refere to the literature for this. Just highlight few important points here.

$$G(\tau, \tau') \to \begin{array}{c c} & \begin{array}{cc} + & - \end{array} \\ \begin{array}{c} + \\ - \end{array} & \begin{bmatrix} G^{++} & G^{+-} \\ G^{-+} & G^{--} \end{bmatrix} \end{array} = \begin{bmatrix} G^t & G^< \\ G^> & G^{\bar{t}} \end{bmatrix}$$

$\tau \equiv (t, \sigma)$

$\sigma = +$ or $-$

G^t is time order.

$\bar{t}$ anti-time order

A single G in countour order means 4 Gs in the usual time t, $G^t, G^{\bar t}, G^>, G^<$. However out of the 4, only two are considered indepnt. since we have many linear relations, such as

$$G^t - G^{\bar t} = G^r + G^a$$

$$G^> - G^< = G^r - G^a = -iA$$

$$G^r = G^t - G^<, \qquad G^a = G^< - G^{\bar t}$$

$$G^t + G^{\bar t} = G^> + G^<$$

These linear relations can be proved from the basic definition. i.e.

$$G^t(t,t') = \theta(t-t')\, G^>(t,t') + \theta(t'-t)\, G^<(t,t')$$

Now for the Dyson equation on contour

$$G(\tau,\tau') = G^0(\tau,\tau') + \int d\tau_1 \int d\tau_2\, G^0(\tau,\tau_1) \underbrace{\Sigma(\tau_1,\tau_2)\, G(\tau_2,\tau')}_{\text{still matrix multiplicn is implied.}}$$

we cannot do Fourier transform and taking advantage of time translational invariance which gives us convolution theorem, which is

convolution in time t is multiplication in ω or E.

□ Problem: prove the convolution theorem

$$C(t-t') = \int_{-\infty}^{+\infty} A(t-t_1)\, B(t_1-t')\, dt_1 \implies \tilde C(\omega) = \tilde A(\omega)\, \tilde B(\omega)$$

$$\tilde A(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t} A(t), \quad \text{etc.}$$

translational invariance in time, $A(t,t') \equiv A(t-t')$ is needed here.

Go back to real time, the Dyson equation on contour becomes pair of two equations

$$G^r(t, t') = G_0^r(t, t') + \int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{+\infty} dt_2 \, G_0^r(t, t_1) \Sigma^r(t_1, t_2) * G^r(t_2 t')$$

Applying convolution theorem, we get

$$\tilde{G}^r(E) = \tilde{G}_0^r(E) + \tilde{G}_0^r(E) \tilde{\Sigma}^r(E) \tilde{G}(E)$$

This equation is easily solved to give

$$\tilde{G}^r(E) = \left\{ \tilde{G}_0^r(E)^{-1} - \tilde{\Sigma}^r(E) \right\}^{-1}$$

This is a matrix equation including all relevant degrees of freedom (ie. left and right).

The 2nd equation is the Kedysh equation

$$G^< = G^r \Sigma^< G^a$$

or

$$G^<(t, t') = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} G^r(t, t_1) \Sigma^<(t_1 t_2) G^a(t_2 t') \, dt_1 dt_2$$

or Apply convolution theorem again

$$\tilde{G}^<(E) = \tilde{G}^r(E) \tilde{\Sigma}^<(E) \tilde{G}^a(E)$$

matrix multiplication implied.

This form of Kedysh equation is valid only in steady state, as we have dropped a transient term. For photon Green's function D, we have similar equations $D = D_0 + D_0 \Pi D$. How to find Σ and Π? We need Feynman diagramatic expansions. I refer to read Fetter & Walecka, or AGD (Abrikosov) or some of the recent ones such as H. Bruus & K Flensberg.