23 March 2017

Single spin-less electron and states

Let $|0\rangle$ denotes the vaccum, i.e., no electrons.

then $c^+|0\rangle = |1\rangle$ is a state with one electron.

Due to Pauli exclusion principles we cannot have two electrons in the same state, we have

$$(c^+)^2|0\rangle = 0$$

This is true for any state $|0\rangle$ or $|1\rangle$, so $(c^+)^2 = 0$ is an operator identity.

c is defined by c^+ as c^+'s hermitian conjugate.

i.e. $(\varphi, c^+\psi) = (c\varphi, \psi)$ ← define c.

take $\psi = |0\rangle$ $\rightarrow$ $\langle\varphi|(c^+|0\rangle) = \langle c\varphi|0\rangle$

$\rightarrow$ $\langle\varphi|1\rangle = \langle c\varphi|0\rangle$

If $\langle\varphi| = \langle 0|$ $\langle 0|1\rangle = 0$ $\Rightarrow$ $\langle c\varphi|0\rangle = 0$

$\rightarrow |\varphi\rangle = |0\rangle$ $c|0\rangle = 0$

$|c\varphi\rangle \equiv c|0\rangle = 0$

If $\langle\varphi| = \langle 1|$, $\langle 1|1\rangle = \langle c\varphi|0\rangle = 1$

so $c|\varphi\rangle = c|1\rangle = |0\rangle$ i.e. c annihilate electron

Thus for consistency we have the following rules for c^+ and c

$$\begin{cases} c^+|0\rangle = |1\rangle & \text{by definition} \\ c^+|1\rangle = 0 & \text{by } (c^+)^2 = 0, \text{ i.e. Pauli exclusion principle} \\ c|1\rangle = |0\rangle & \text{Also } (c)^2 = 0, \quad c^+c|n\rangle = n|n\rangle \\ c|0\rangle = 0 & n = 0, 1 \end{cases}$$

We can represent C^+ and C as 2×2 matrix in the basis of $|0\rangle, |1\rangle$, of the single electron Hilbert space as

$$\langle n|C^+|n'\rangle \rightarrow \begin{matrix} \\ 0 \\ 1 \end{matrix}\begin{matrix} \begin{matrix} 0 & 1 \end{matrix} \\ \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \end{matrix} \qquad C = \begin{matrix} \\ 0 \\ 1 \end{matrix}\begin{matrix} \begin{matrix} 0 & 1 \end{matrix} \\ \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \end{matrix}$$

$$\langle 1|C^+|0\rangle = 1 \qquad \langle 0|C|1\rangle = 1$$

then C and C^+ are related by transpose, or more generally hermitican conjugate $(C)^+ = C$ in the usual linear algebrain sense.

Brief summary, two states, vaccum $|0\rangle$, and one electron $|1\rangle$, are acted upon by the creation operator C^+, and annihilation operator C.

$\hat{n} = C^+C$ is the occupation number.

It is easy to verify $CC^+ + C^+C = \hat{1}$ is operator identity

$$C^+C = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \qquad CC^+ = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad \text{so} \quad CC^+ + C^+C = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Many operators case. i.e. more than one electron.

It is sufficient and necessary to demand

$$\begin{cases} C_iC_j + C_jC_i = 0, & C_i^+C_j^+ + C_j^+C_i^+ = 0 \\ C_iC_j^+ + C_j^+C_i = 1 \end{cases}$$

This takes care that the wave function is anti-symmetric with respect to partile exchage

Eg. $C_1^+C_2^+|0\rangle \equiv |1,2\rangle$

$C_2^+C_1^+|0\rangle = |2,1\rangle = -|1,2\rangle$

What is the 4×4 matrix representation if we have two electrons? This can be confusing since we need to take care, e.g. $c_1 c_2 = -c_2 c_1$!

What is the most general Hamiltn for a single electron (or no electron) state?

Take a polynomial in c and $c^\dagger$ we have

$$H = \varepsilon_0 + a c + b c^\dagger + d c^\dagger c$$

since $c^2 = c^{\dagger 2} = 0$ we have no high order terms. $c^3 = 0$

$c c^\dagger + c^\dagger c = 1$ so we don't need $cc^\dagger$ term. However, $H^\dagger = H$ need to be hermitian. so $\varepsilon_0^* = \varepsilon_0$ $(dc^\dagger c)^\dagger = d^* c^{\dagger} c^{\dagger}$

ε_0 and d must be real, and $b = a^*$.

$$H = \underbrace{\varepsilon_0}_{\varepsilon_0 \cdot \hat{1}} + ac + (ac)^\dagger + dc^\dagger c = \begin{bmatrix} \varepsilon_0 & 0 \\ 0 & \varepsilon_0 \end{bmatrix} + \begin{bmatrix} 0 & a \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ a^* & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & d \end{bmatrix}$$

$$= \begin{bmatrix} \varepsilon_0 & a \\ a^* & \varepsilon_0 + d \end{bmatrix}$$

We can always diagnolize H toget $\begin{bmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{bmatrix}$ by a linear transform of c and $c^\dagger$ by changing the basis $\varphi_1 = \alpha_1 |0\rangle + \alpha_2 |1\rangle$

$\varphi_2 = \beta_1 |0\rangle + \beta_2 |1\rangle$

Question: How does the operator change when the basis chage according to α_i, β_i? $e, c^\dagger$

Hint: If $S^\dagger H S = \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{pmatrix}$ diagnlize H, how S acts on c and $c^\dagger$. Let $d|\varphi_1\rangle = 0$ and $d^\dagger |\varphi_1\rangle = |\varphi_2\rangle$, $d^\dagger |\varphi_2\rangle = 0$. $d|\varphi_2\rangle = |\varphi_1\rangle$

How to relate the new creatn & annihilat to the old one?

The question is not so trivial. Clearly

$$S^\dagger c S = c' \qquad S^\dagger c^\dagger S = c'^\dagger \qquad \text{so that}$$

$S^\dagger H S$ is diagonal. But how to relate it to $d, d^\dagger$?

$$S^\dagger H S = \varepsilon_1 + \varepsilon_2 d^\dagger d \quad \text{by definition.}$$

What is the transformation for c to d? So that it is diagonal in d?

Since adding a constant does not change physics, the "most general" Hamiltonian is really for a one state electron

$$H = \varepsilon_0 c^\dagger c$$

To define the Green's functions, we need to talk about the pictures. The schrödinger picture is used in elementary quantum-mechanics where the wave function follows the Schrödinger equation

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

while the operators such as c is time independent. We introduce Heisenberg picture such that

$$\langle \psi_S(t) | \hat{O} | \psi_S(t) \rangle \equiv \langle \psi_H | \hat{O}(t) | \psi_H \rangle$$

where the wave function does not vary with time and operators satisfies the Heisenberg equation of motion

$$i\hbar \frac{d\hat{O}(t)}{dt} = [\hat{O}(t), H]$$

$$\rightarrow \quad \hat{O}(t) = e^{\frac{i}{\hbar}Ht} \hat{O}\, e^{-\frac{i}{\hbar}Ht}$$

We use the convention that at $t=0$ $\quad |\psi_S(t=0)\rangle = |\psi_H\rangle$

and $\quad \hat{O}(t=0) = \hat{O}$.

i.e. the two pictures are cychronized at $t=0$. The Green's functions are defined in Heisenberg picture $c(t)$, $c^+(t)$ with statistical-mechanical averge $\langle \cdots \rangle = \mathrm{Tr}(\rho \cdots)$ where in equilibrium with grand-canonical ensemble we have

$$\rho = \frac{e^{-\beta(H-\mu N)}}{\mathrm{Tr}(e^{-\beta(H-\mu N)})} \qquad Z = \mathrm{Tr}(e^{-\beta(H-\mu)N} \qquad \mathrm{Tr}(\rho) = 1$$

$N = c^+c$ is # operator

However, in general nonequilibrium case the exact form of ρ is not known explicitly in advance. So the definition will be with respect to arbitrary ρ.

Greater : $$g^>(t) = -\frac{i}{\hbar}\langle c(t) c^+(0)\rangle$$

if time translational invariance does not hold, we use

$$g^>(t,t') = -\frac{i}{\hbar}\langle c(t)\, c^+(t')\rangle$$

lesser: $$g^<(t) = \frac{i}{\hbar}\langle c^+(0)\, c(t)\rangle$$

↑ sign change

retarded: $$g^r(t) = \theta(t)\left[g^>(t) - g^<(t)\right]$$

$$= \theta(t)\left[-\frac{i}{\hbar}\right]\langle \underbrace{c(t)\, c^+(0) + c^+(0)\, c(t)}_{\text{anti-commutator}}\rangle$$

advanced: $$g^a(t) = -\theta(-t)\left[g^>(t) - g^<(t)\right]$$

so that $$g^r - g^a = g^> - g^< = -iA$$

A is called spectrum function $\qquad \theta(t) + \theta(-t) = 1$

time ordered: $$g^t(t) = \theta(t)\, g^>(t) + \theta(-t)\, g^<(t)$$

anti-time ordered. $$g^{\bar{t}}(t) = \theta(t)\, g^<(t) + \theta(-t)\, g^>(t)$$

We see $$g^t + g^{\bar{t}} = g^> + g^<$$

We can also check $g^r + g^a = \theta(t)[g^> - g^<]$

$$(-\theta(-t))[g^> - g^<]$$

$$= \theta(t) g^> + \theta(-t) g^< - (\theta(t) g^< + \theta(-t) g^>)$$

$$= g^t - g^{\bar{t}}$$

and $g^t = \theta(t) g^> + \theta(-t) g^< = \theta(t) g^> + (1 - \theta(t)) g^<$

$$= \theta(t)(g^> - g^<) + g^< = g^r + g^< = g^a + g^>$$

Similarly $g^{\bar{t}} = g^< - g^a = g^> - g^r$

In summary we have the relations

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

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

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

$$g^t = g^< + g^r = g^> + g^a$$

$$g^{\bar{t}} = g^< - g^a = g^> - g^r$$

Question: How many independent Green's function do we really have?

In addition we define the Matsubara Green's function as

$$g^M(\tau, \tau') = -\frac{1}{\hbar} \langle T_\tau (C(\tau) C^+(\tau')) \rangle$$

here $it \equiv \tau$

$$C(\tau) = e^{\frac{\tau(H - \mu N)}{\hbar}} C e^{-\frac{\tau(H-\mu N)}{\hbar}}$$

However, I will not pursue in this direction.

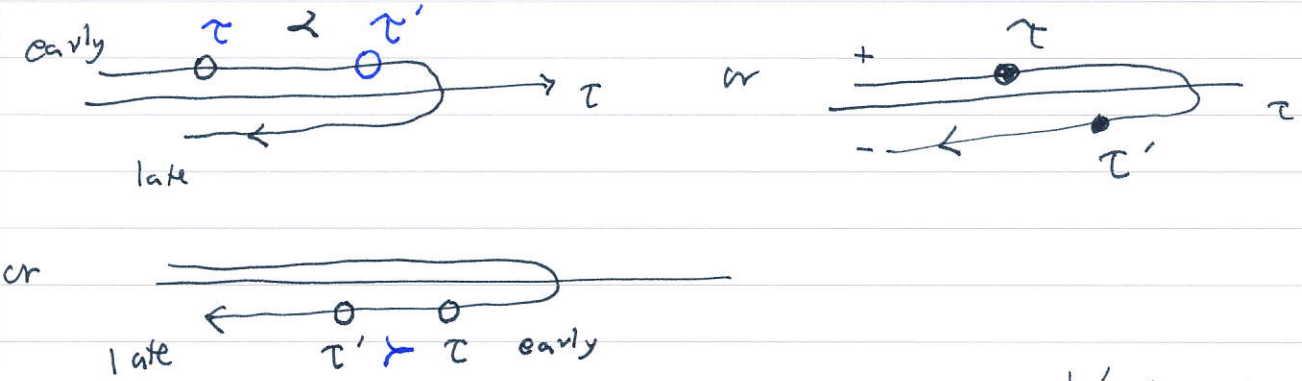
Contour ordered Green's function.

We define the contour as runing from $-\infty$ to $+\infty$ and then back from $+\infty$ to $-\infty$ as shown

This contour has nothing to do with complex numbers τ is real all the time. but it has the concept of brapiches. the top branch will be denoted as '+', botton branch '-'. So we also have

$$\tau \equiv (\sigma, t) \qquad \sigma = + \text{ or } -$$

The contour forms a linear order on τ if $\tau \prec \tau'$ we say τ is early, τ' is late and τ procede τ'. Eg.



It is clearly that contour time on the '+' branch is always early that that on the '-' branch. If both τ, τ' are on + brach contour order means the same as time order. If both on '-' branch contour order is the same as anti-time order. We define contour ordered Green's function as

$$g(\tau, \tau') = -\frac{i}{\hbar} \langle T_\tau \, c(\tau) \, c^\dagger(\tau') \rangle$$

So $T_\tau\, C(\tau)\, C^+(\tau') = \begin{cases} C(\tau)\, C^+(\tau') & \text{if } \tau > \tau' \\ \text{late} \leftarrow \text{early} & \text{i.e. } \tau \text{ is later than } \tau' \\ -C^+(\tau')\, C(\tau) & \text{otherwise} \\ & \text{i.e. } \tau \text{ is early} \end{cases}$

please note the minus sign here.

The relation to earlier real time green's function is

$$g(\tau, \tau') \equiv g^{\sigma\sigma'}(t, t') \qquad \text{where} \quad \tau \equiv (\sigma, t), \quad \tau' \equiv (\sigma', t')$$

$$g^{++}(t, t') = g^{++}(t - t') = g^{t}$$

if time translational invariance holds

$$g^{--} = g^{\bar{t}} \qquad g^{+-}(t, t') = g^{<}(t - t')$$

(early, late)

$$g^{-+}(t, t') = g^{>}(t - t')$$

(late, early)

or

$$g(\tau, \tau') \to \begin{matrix} \\ + \\ - \end{matrix} \begin{matrix} \begin{matrix} + & \quad - \end{matrix} \\ \begin{bmatrix} g^{t} & g^{<} \\ g^{>} & g^{\bar{t}} \end{bmatrix} \end{matrix}$$

We need to work with contour order because only contour ordered Green's function has a perturbation expansion theory.

Under what condition the Green's functions, and in general, correlation functions, are time translationally invariant?

Answer. $[\rho, H] = 0$

This certainly is the case for equilibrium $\rho \propto e^{-\beta H}$ or $e^{-\beta(H - \mu N)}$ and $[H, N] = 0$.

Proof. $\mathrm{Tr}[\rho e^{\frac{i}{\hbar}Ht} A e^{-\frac{i}{\hbar}Ht} e^{+\frac{i}{\hbar}Ht'} B e^{-\frac{i}{\hbar}Ht'}]$

$= F(t,t') = \langle A(t) B(t') \rangle \overset{?}{=} F(t-t')$

$= \mathrm{Tr}[\rho e^{\frac{i}{\hbar}Ht} A e^{-\frac{i}{\hbar}H(t-t')} B e^{-\frac{i}{\hbar}Ht'}]$

$= \mathrm{Tr}[e^{-\frac{i}{\hbar}Ht'} \rho e^{\frac{i}{\hbar}Ht} A e^{-\frac{i}{\hbar}H(t-t')} B]$

We have used the cyclic property of Trace. $\mathrm{Tr}(ABC) = \mathrm{Tr}(CAB)$

if $[\rho, H] = 0$ then $[\rho, e^{-\frac{i}{\hbar}Ht'}] = 0$

so $F(t,t') = \mathrm{Tr}[\rho e^{\frac{i}{\hbar}H(t-t')} A e^{-\frac{i}{\hbar}H(t-t')} B] = \langle A(t-t') B(0) \rangle$

$= F(t-t')$ is a funct of $t-t'$ only.

so we have translational invariance

$F(t-t') = \langle A(t) B(t') \rangle = \langle A(t+\Delta) B(t'+\Delta) \rangle$

for any Δ. In particular we can take $\Delta = -t'$.

"Well behaved" correlation function.

If $F(t) = \langle A(t) B(0) \rangle$ (assumes time translation invariant) for $|t| \to \infty$ we get

$\langle A(t) B(0) \rangle = \langle A(t) \rangle \langle B(0) \rangle = \langle A(0) \rangle \langle B(0) \rangle$

we say the correlation is well-behaved.

We now evaluate equilibrium Green's functions, defined on pages 227-229 for the single quantum dot and demanding the resulting Green's functions are well-behaved. using grand-canonical ensemble

$$\rho = \frac{e^{-\beta(H-\mu N)}}{\mathrm{Tr}(e^{-\beta(H-\mu N)})} \qquad H = \varepsilon c^\dagger c \qquad N = c^\dagger c$$

$C(t) = C(0)\, e^{-\frac{i}{\hbar}\varepsilon t}$

$C^+(0) \equiv C^+$

$$g^<(t) \equiv \frac{i}{\hbar} \langle C^+(0)\, C(t) \rangle$$

Note that there is no restriction on the domain of t

$$= \frac{i}{\hbar} \mathrm{Tr}\left(\frac{e^{-\beta(H-\mu N)}}{Z} C^+ e^{\frac{i}{\hbar}Ht} C\, e^{-\frac{i}{\hbar}Ht} \right) \qquad -\infty < t < +\infty$$

The partition function $Z = \mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right) = \mathrm{Tr}\left(e^{-\beta(\varepsilon-\mu)N}\right)$

$$= \langle 0 | e^{-\beta(\varepsilon-\mu)\hat{N}} |0\rangle + \langle 1 | e^{-\beta(\varepsilon-\mu)\hat{N}} |1\rangle$$

$$= 1 + e^{-\beta(\varepsilon-\mu)}$$

↑ trace over no particle and one electron "Fock" space.

$$g^<(t) = \frac{i}{\hbar} Z \Big[\langle 0 | e^{-\beta(\varepsilon-\mu)N} C^+ e^{\frac{i}{\hbar}\varepsilon N t} C\, e^{-\frac{i}{\hbar}\varepsilon N t} |0\rangle + \langle 1 | e^{-\beta(\varepsilon-\mu)N} C^+ e^{\frac{i}{\hbar}\varepsilon N t} C\, e^{-\frac{i}{\hbar}\varepsilon N t} |1\rangle \Big]$$

since $C\, e^{-\frac{i}{\hbar}\varepsilon N t} |0\rangle = C \cdot |0\rangle = 0$ we only get the 2nd term

($N|0\rangle = 0|0\rangle$ ↑)

$\hat{N}|1\rangle = |1\rangle$

$$g^<(t) = \frac{i}{\hbar\left(\underbrace{1 + e^{-\beta(\varepsilon-\mu)}}_{Z}\right)} \Big[e^{-\beta(\varepsilon-\mu)} \underbrace{\langle 1 | C^+}_{\langle 0|} e^{\frac{i}{\hbar}\varepsilon \hat{N} t} \underbrace{C}_{|0\rangle\langle 1|} \underbrace{e^{-\frac{i}{\hbar}\varepsilon \hat{N} t}}_{e^{-\frac{i}{\hbar}\varepsilon t}} |1\rangle \Big]$$

$\langle 1|1\rangle = 1$ $\qquad C^+|0\rangle = |1\rangle$

$$= \frac{i}{\hbar} \frac{1}{1 + e^{-\beta(\varepsilon-\mu)}} \Big[e^{-\beta(\varepsilon-\mu)} \underbrace{\langle 1 | C^+ e^{\frac{i}{\hbar}\varepsilon \hat{N} t} |0\rangle}_{|0\rangle} e^{-\frac{i}{\hbar}\varepsilon t} \Big]$$

$$= \frac{i}{\hbar} \frac{1}{e^{\beta(\varepsilon-\mu)} + 1} e^{-\frac{i}{\hbar}\varepsilon t} = \frac{i}{\hbar} f(\varepsilon)\, e^{-\frac{i}{\hbar}\varepsilon t}$$

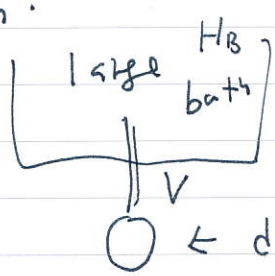
We define $f(\varepsilon) \equiv \langle C^+ C \rangle = \dfrac{1}{e^{\beta(\varepsilon-\mu)} + 1}$ which is the Fermi function at energy ε.

Note: Heisenberg equation of motion for $C(t)$ gives $C(t) = e^{-\frac{i}{\hbar}\varepsilon t}$.

$$g^<(t) = \frac{i}{\hbar} f e^{-\frac{i}{\hbar}\varepsilon t}$$

According to our definition of well-behaved function, $g^<(t)$ is NOT well behaved as $g^<(t)$ does not go to 0 when $|t| \to \infty$. (not that $\langle c \rangle = \langle c^+ \rangle = 0$)

In order to make $g^<$ well-behaved, we introduce damping, or dissipation, in fact, this is compatible with the grand-canonical ensemble. If the dot is completely isolated, then the electron number cannot fluctuate, $\langle c^+ c \rangle = 0$ or 1, which is not a Fermi distribution at temperature $T = \frac{1}{k_B \beta} \neq 0$ So, we must allow the change of occupation so that $0 < f < 1$ if $T \neq 0$. This means the dot is not really isolated, it should have connected to electron bath.



$$H = \varepsilon c^+ c + V + H_B$$

The grand-canonical distribution is the limit $V \to 0$. If we keep a finite $V \neq 0$, then the electron will have a finite life time $\propto \frac{1}{|V|^2}$. We describe this phenomenologically as

$$e^{-\frac{i}{\hbar}\varepsilon t} \to e^{-\frac{i}{\hbar}\varepsilon t - \frac{\eta}{\hbar}|t|}$$

$[\eta] = [\varepsilon] =$ Joule, is related to life time by

$$\boxed{\eta = \frac{\hbar}{2\tau}}$$

The factor 2 will be explained when we relate to Boltzmann equation.

Roughly speaking $g^< \propto \psi \sim e^{-\frac{t}{2\tau}}$ is related to the wave function. but electron life-time is related to the probability $|\psi|^2 \propto e^{-\frac{t}{\tau}}$. That's why we need a $\frac{1}{2}$ there.

So our final formula for $g^<$ is

$$g^<(t) = \frac{i}{\hbar} \int e^{-\frac{i}{\hbar}\varepsilon t - \frac{\eta}{\hbar}|t|}$$

$g^<(t \to \pm\infty) \to 0$. We take the view that η may be small but finite and not zero. i.e. we may not take the limit $\eta \to 0^+$!

Greater Green's function

We note $g^<$ is related to $\langle c^+ c \rangle \to f$ particle

so $g^>$ is related to $\langle c\, c^+ \rangle \to 1-f$ hole

$$g^>(t) = -\frac{i}{\hbar}(1-f) e^{-\frac{i}{\hbar}\varepsilon t - \frac{\eta}{\hbar}|t|} \qquad cc^+ + c^+c = 1$$

We can obtain $g^>$ from $g^<$ by flipping the sign of temperature or β [I learned this from Jia-Huei]

$$f_\beta = \frac{1}{e^{\beta(\varepsilon-\mu)}+1} \qquad f_{-\beta} = \frac{1}{e^{-\beta(\varepsilon-\mu)}+1} = \frac{e^{\beta(\varepsilon-\mu)}}{1+e^{\beta(\varepsilon-\mu)}}$$

$$= 1 - f_\beta$$

so

$$\boxed{g^>_\beta(t) = -g^<_{-\beta}(t)}$$

This is computationally advantageous as we don't need to write $g^<$ and $g^>$ separately.

Code for $g^<$ is sufficient to compute $g^>$.

Retarded Green's function is important because it is related to the linear response theory.

$$g^r(t) = \theta(t)\left[g^>(t) - g^<(t)\right]$$

$$= \theta(t)\left(-\frac{i}{\hbar}\right)\left[(1-f)\,e^{-\frac{i}{\hbar}\varepsilon t - \frac{\eta|t|}{\hbar}} + f\,e^{-\frac{i}{\hbar}\varepsilon t - \eta\frac{|t|}{\hbar}}\right]$$

$$= -\frac{i}{\hbar}\,\theta(t)\,e^{-\frac{i}{\hbar}\varepsilon t\,\frac{-\eta|t|}{\hbar}}$$ we see f cancel.

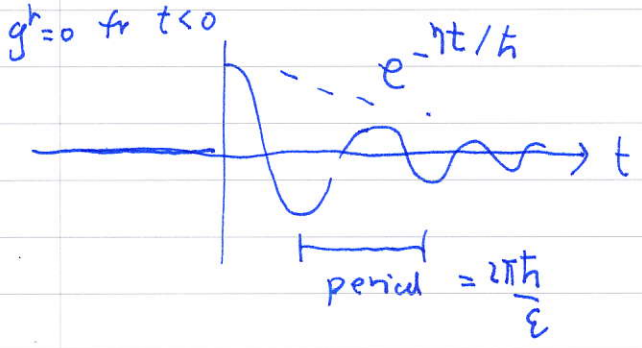
This is characteristic of free electrons. For interacting electrons (by that we mean the Hamiltn is not quadratic in $c, c^\dagger$), g^r may also depends on temperature.

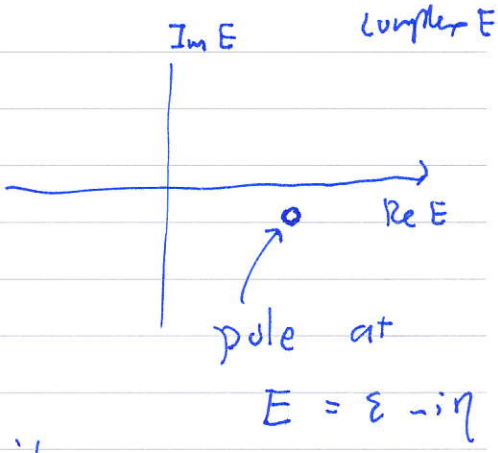
g^r is simpler in frequency or energy space, so we define

$$\tilde{g}^r(E) = \int_{-\infty}^{+\infty} dt\; g^r(t)\, e^{i\frac{Et}{\hbar}} = \int_0^{+\infty} \left(-\frac{i}{\hbar}\right) e^{-\frac{i}{\hbar}\varepsilon t - \frac{\eta t}{\hbar} + \frac{iEt}{\hbar}} dt$$

$$= \left(-\frac{i}{\hbar}\right) \frac{e^{-\frac{i}{\hbar}\varepsilon t - \frac{\eta t}{\hbar} + \frac{iEt}{\hbar}}\Big|_0^{\infty}}{-\frac{i}{\hbar}\varepsilon - \frac{\eta}{\hbar} + \frac{iE}{\hbar}} = \frac{1}{E - \varepsilon + i\eta}$$

$g^r(t)$





Since $g^r(t) = 0$ if $t < 0$, by Residue theorem, the poles for $g^r(E)$ must lay below real axis.

$$\tilde{g}^r(E) = g^r(E) = \frac{1}{E + i\eta - \varepsilon}$$

↑ omit $\sim$ for simplicity

We like to see how $g^<$ is related to g^r in E space.
This is known as fluctuation-dissipation theorem in equilibrium.

first $g^a(E) = \left(g^r(E)\right)^* = \dfrac{1}{E - i\eta - \varepsilon}$

Verify this explicitly using the definition on page 227,

i.e. $g^a(t) = -\theta(-t)\left[g^>(t) - g^<(t)\right]$.

$$\tilde{g}^<(E) = \int_{-\infty}^{+\infty} g^<(t)\, e^{\frac{i}{\hbar}Et}\, dt = \int_{-\infty}^{0} \left[e^{-\frac{i}{\hbar}\varepsilon t + \frac{\eta}{\hbar}t + \frac{i}{\hbar}Et} \right] dt \quad \left(f \to \tfrac{i}{\hbar} f\right)$$

$$+ \int_{0}^{+\infty} \left[e^{-\frac{i}{\hbar}\varepsilon t - \frac{\eta}{\hbar}t + \frac{i}{\hbar}Et} \right] dt \quad \left(f \to \tfrac{i}{\hbar} f\right)$$

$$= \frac{i}{\hbar} f \cdot \left\{ \frac{e^{-\frac{i}{\hbar}\varepsilon t + \frac{\eta}{\hbar}t + \frac{i}{\hbar}Et}}{-\frac{i}{\hbar}\varepsilon + \frac{\eta}{\hbar} + \frac{i}{\hbar}E} \Bigg|_{-\infty}^{0} + \frac{e^{-\frac{i}{\hbar}\varepsilon t - \frac{\eta}{\hbar}t + \frac{i}{\hbar}Et}}{-\frac{i}{\hbar}\varepsilon - \frac{\eta}{\hbar} + \frac{i}{\hbar}E} \Bigg|_{0}^{+\infty} \right\}$$

$$= f \cdot \left[\frac{1}{E - i\eta - \varepsilon} - \frac{1}{E + i\eta - \varepsilon} \right]$$

Compare with the expression for $\tilde{g}^r$ and $\tilde{g}^a$ we have

$$\tilde{g}^<(E) = -f(E)\left[\tilde{g}^r(E) - \tilde{g}^a(E)\right] = i f(E)\cdot \tilde{A}(E)$$

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

We observe that relation does not depend on $\eta \to 0^+$ or not.

Use the relation on page 241, $g^>_{\beta}(t) = -g^<_{-\beta}(t)$ we get

$$\tilde{g}^>(E) = \left(1 - f(E)\right)\cdot\left[\tilde{g}^r(E) - \tilde{g}^a(E)\right]$$

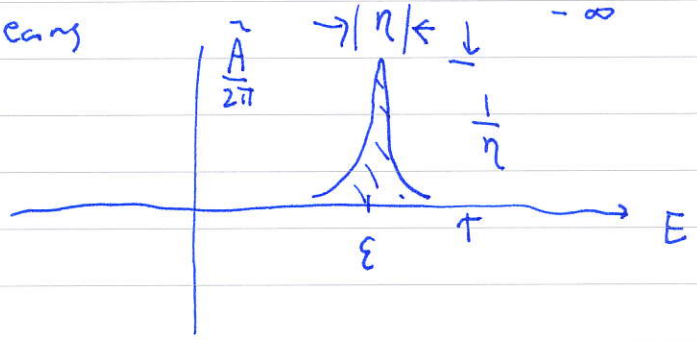
$$\tilde{A} = i\left(\tilde{g}^r - \tilde{g}^a\right) = i\left[\frac{1}{E + i\eta - \varepsilon} - \frac{1}{E - i\eta - \varepsilon}\right] = i\,\frac{E - i\eta - \varepsilon - E - i\eta + \varepsilon}{(E-\varepsilon)^2 + \eta^2}$$

$$= \frac{2\eta}{(E-\varepsilon)^2 + \eta^2} > 0 \quad \text{positive \& real.}$$

We note the "density of state" of the electron is given by $\frac{1}{2\pi}\tilde{A}(E) = \frac{1}{\pi}\frac{\eta}{(E-\varepsilon)^2+\eta^2} \to \delta(E-\varepsilon)$ $\eta \to 0^+$

we have used the fact of integral $\int_{-\infty}^{+\infty} \frac{dx}{x^2+1} = \pi$

finite η means



Taking the ratio of $g^<$ vs $g^>$

we get $\frac{\tilde{g}^<(E)}{\tilde{g}^>(E)} = -\frac{f(E)}{1-f(E)} = -\left[\frac{\frac{1}{e^{\beta(E-\mu)}+1}}{1-\frac{1}{e^{\beta(E-\mu)}+1}}\right]$

$= -e^{-\beta(E-\mu)}$. We may called this detailed balance equation. This is a relation discussed in the book by L. P. Kanahoff & G. Baym "Quantum Statistical Mechanics" (1962).

We now consider many electrons systems. They are still free electrons except Pauli exclusion principle is in operation but no electron-electron interaction or electron-phonon interaction. The Hamilton is still quadratic

$$\hat{H} = (c_1^+ c_2^+ \cdots c_N^+)\begin{pmatrix} H_{11} & H_{12} & & \\ & & & \\ & & & H_{NN} \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$$

With N possible electron states

$= \sum_{jk} c_j^+ H_{jk} c_k$. Here the indices

j and k are position, or momentum or spin labels.

In matrix notation we have $\hat{H} = c^+ H c$

$c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$ H is $N \times N$ matrix. We can diagonalize H with a unitary rotation, say here

$$S^+ H S = \begin{pmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ 0 & & \ddots \\ & & & \varepsilon_N \end{pmatrix} \qquad S^+ S = S S^+ = I$$

We can construct S by column vectors of eigen states

$$H\psi_j = \varepsilon_j \psi_j \qquad \psi_j = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{pmatrix} = \begin{pmatrix} S_{1j} \\ S_{2j} \\ S_{3j} \\ \vdots \\ S_{Nj} \end{pmatrix}$$

Then $S = (\psi_1 \ \psi_2, \cdots \psi_N)$

and $H S = (H\psi_1, H\psi_2, \cdots H\psi_N)$

$$= (\varepsilon_1 \psi_1, \ \varepsilon_2 \psi_2, \cdots \varepsilon_N \psi_N) = S \begin{pmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ 0 & & \ddots \\ & & & \varepsilon_N \end{pmatrix}$$

$$= (\psi_1, \psi_2, \cdots \psi_N) \begin{pmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ 0 & & \ddots \\ & & & \varepsilon_N \end{pmatrix}$$

We can write for the many-body Hamiltonian

$$\hat{H} = c^+ H c = c^+ S \begin{pmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ 0 & & \ddots \\ & & & \varepsilon_N \end{pmatrix} S^+ c = d^+ \begin{pmatrix} \varepsilon_1 & & \\ & \varepsilon_2 & \\ & & \ddots \\ & & & d_N \end{pmatrix} d$$

Let the vector $d = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{pmatrix} = S^+ c \qquad d^+ = c^+ (S^+)^+ = c^+ S$

$$\hat{H} = \sum_j \varepsilon_j d_j^+ d_j$$ ← a collection of non interacting electrons.

The Green's function defined in too d_j is the same as before e.g.

$$g_j^r(E) = -\frac{i}{\hbar} \int_{-\infty}^{\infty} \theta(t) \langle d_j(t) d_j^+(0) + d_j^+(0) d_j(t) \rangle \, e^{i \frac{E}{\hbar} t} \, dt$$

Consider define $G^{>}_{jK}(t) = -\frac{i}{\hbar} \langle C_j(t) C^{+}_{K}(0) \rangle$ as matrix

$N \times N$ matrix $\rightarrow G^{>}(t) = -\frac{i}{\hbar} \langle C(t) C^{+}(0) \rangle$

$$\begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_N \end{pmatrix} \left(C_1^{+} C_2^{+} \cdots C_N^{+} \right)$$

$N \times 1$ $\quad 1 \times N$

but $\hat{H}$ is diagonal in d so $C = Sd$

$C^{+} = d^{+} S^{+}$

$$G^{>}(t) = -\frac{i}{\hbar} \langle S\, d(t)\, d^{+}(0)\, S^{+} \rangle$$

$$= -\frac{i}{\hbar} S \langle d(t) d^{+}(0) \rangle S^{+}$$

Clearly $\langle d(t) d^{+}(0) \rangle$ is diagonal $\quad \langle d_j(t) d^{+}_{K}(0) \rangle \propto \delta_{jK}$

we can write $\quad \langle d_1 d_2^{+} \rangle = 0$

$G^{>}(t) = S \{ g^{>}_j(t) \} S^{+}$ we use $\{ \cdots \}$ to denote

the diagonal matrix $\{ g^{>}_j \} \equiv \begin{pmatrix} g^{>}_1 & & 0 \\ & g^{>}_2 & \\ 0 & & \ddots \\ & & & g^{>}_N \end{pmatrix}$

This works for all the Green's function

$$G^{>,<,a,r,t,\bar{t}}(t) \text{ or } E = S \{ g^{>,<,a,r,t,\bar{t}}(t) \text{ or } E \} S^{+}$$

Question:
Why works also for $G^{<}$ as $G^{<}$ need swap the position of the operator?

This means all the relation worked out for small g also works for big G if the relation is linear

e.g. $\{ g^{r}_j - g^{a}_j \} = \{ g^{>}_j - g^{<}_j \} \Rightarrow$ multiply S from left, multiply S^{+} from right

$G^r - G^a = G^> - G^<$ etc. The fluctuation-dissipation theorem is

$$G^<(E) = -f(E)\left(G^r(E) - G^a(E)\right)$$

$$G^>(E) = \left(1 - f(E)\right)\left(G^r(E) - G^a(E)\right)$$

since $\{ g_j^r(E) \} = \left\{ \frac{1}{E + i\eta - \varepsilon_j} \right\}$ ← { } means diagonal matrix with diagonal element indicated inside

we have

$$G^r(E) = S \left\{ \frac{1}{E + i\eta - \varepsilon_j} \right\} S^+ \qquad S S^+ = I \quad S^{-1} = S^+$$

$$= \left[S^{+-1} \{ E + i\eta - \varepsilon_j \} S^{-1} \right]^{-1}$$

$$= \left[S \{ E + i\eta - \varepsilon_j \} S^+ \right]^{-1} = \left[(E + i\eta) S S^+ - S \{ \varepsilon_j \} S^+ \right]^{-1}$$

$$= \left[(E + i\eta) I - H \right]^{-1} \qquad I = \begin{bmatrix} 1 & & 0 \\ & 1 & \\ 0 & & \ddots \\ & & & 1 \end{bmatrix} \text{ is identity matrix}$$

$$S \{ \varepsilon_j \} S^+ = S \begin{pmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ 0 & & \ddots \\ & & & \varepsilon_N \end{pmatrix} S^+ = H$$

Thus we get the well-known result for retarded Green's function

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

we can consider more generally

$$G(z) = (zI - H)^{-1} \qquad z \in \mathbb{C} \text{ is}$$

complex. This is called resolvant of Operator H.

then $G^r(E)$ is obtained if $z \to E + i0$

$G^a(E)$ " " $z \to E - i0$

Matsubara Green's function is obtained if $z \to i\hbar\omega_n + \mu$

$\omega_n = \frac{(2n+1)\pi}{\hbar\beta}$ $\quad n = 0, \pm 1, \pm 2, \cdots$

25 Nov 2015

NEGF is a very useful tool for many part of condensed matter physics. Students of this group should know this theory / formulism very well in order to do good work. This note is intended to give a solid fundation ~~of basic~~ 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 $i\hbar \frac{d}{dt} C = H C$

where C is a colum vector of complex numbers.
H is the single particle Hamilton 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 $\hat{}$ on c

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

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

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

that is grand-canonical distribution where

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

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

$|n_1 n_2 \cdots n_N\rangle$ 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 avgs $\langle \cdots \rangle_{eq}$.

In nonequilibrium open quantum systems, we don't have a nice formula for ρ, at best we can compute reduced density matrix. With the exception 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 definition

t: Heisenberg evolution

Greater: $$G^{>}_{jk}(t,t') = -\frac{i}{\hbar}\langle c_j(t)\, c^{\dagger}_k(t')\rangle$$

create 1st

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

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

since we swap a fermi operator we need + sign here. For Boson operator we do not have sign change

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

$$G^{>}(t,t') = -\frac{i}{\hbar}\langle c(t)\, c^{\dagger}(t')\rangle$$

$$= -\frac{i}{\hbar}\left\langle \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \left(c_1^{\dagger} c_2^{\dagger} \cdots c_N^{\dagger}\right)\right\rangle$$

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

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

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

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

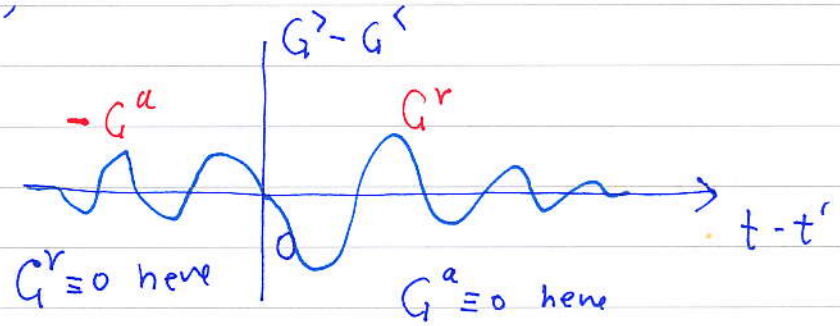
For bosm, we use commutator.

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

Let define $$G^> - G^< = G^r - G^a = -i A$$

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 fourr transfm is 2π x density of states. A is the speefm 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

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

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

$$c^\dagger_k(t')\, i\hbar\frac{\partial c_j(t)}{\partial t}\rangle$$

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

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

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

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

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

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

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 clear $G^r(t,t') \equiv G^r(t-t')$ in practice equilibrium Green's func is always time translationally invariant. we have only one argument

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

$I = \begin{pmatrix} 1 & & 0 \\ & 1 & \\ 0 & & 1 \end{pmatrix}$ N-dimensional identity matrix

become. in E-space

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

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

However, this form is not well defined when we do inverse Fourier transfm. we need to shift the poles to lower part (negative imag) so the correct formula is

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

$\eta \to 0^+$.

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

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

(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:

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

- For nonequilibrium case, we get Keldysh equation

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

where $\Sigma^{<}$ is self-energy.

The tilde $\sim$ means we are in energy domain!

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

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

We prove a very general fluctuation-dissipation theorem. We define

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

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

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

These definitions are consistent to those on pages 7, 9, except that A and B are arbitrary quantum operators, hermitian or not. Now the $\pm$ signs. If A, B are fermion-like we take $+$, bosonic-like we take $-$. Think of $\frac{1}{e^{\beta(\varepsilon\cdots)} \pm 1}$ ← $+$ fermi distribution, $-$ bose distribution.

Fermionic-like means the operators follows anti-commutator relation like c and $c^\dagger$, Bosonic-like means the operator follows commutation relation. More precisely, under the time order or contour order sign T_τ, bosonic operators commute, fermionic operators anti commute. Even though we are dealing with fermions (electrons), we still have bosonic like operators like local energy, current j, or charge ρ as the are pair of fermionic operators like $c^\dagger c$.

The idea of proof is to use Lehmann representation i.e. expand the — expressions Green's functions in the eigen state of $\hat{H}$ and then use the

plemelj formula $\frac{1}{x \pm i\eta} = P\frac{1}{x} \mp i\pi\delta(x)$ 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 dimension of the Fock space is 2^N, we have 2^N diffrent state denoted by $|\mu\rangle$. This space is much larger that the single particle eigen vector of H, where $\hat{H} = C^+ H C$. the dimension of single particle state is N. For such non-interacting system, standard procedure exists to build $|\mu\rangle$ for the single particle state φ, where $H\varphi_i = \epsilon_i \varphi_i$ where ϵ is single particle 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

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

$$B(\omega) = B$$

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

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

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

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

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

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

sorry for notation confusion let use n & m instead

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

Go to energy space by Fourier transform

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

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

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

note the 2π here

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

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

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

$$= \frac{1}{\hbar} \langle A(t)B \pm BA(t) \rangle$$

already worked out

$\Leftarrow$ swap position of A & B.

The Fourier transform of A_{AB} is

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

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

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

Due to the δ-function constraint, we have $E + E_n - E_m = 0$

we have $E_m = E + E_n$

Also if $\langle n|A|m\rangle \neq 0$ $N_n = N_m$, transition between different N is possible if A is c or $c^\dagger$. We need consider two cases. if A or B is of the form $c^\dagger c$ then $N_n = N_m$. if $A = c$, $B = c^\dagger$ 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 form $c^\dagger \cdots c$)

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

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

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

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

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

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

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

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)

$$\tilde{G}^{>} = -i(1+N)\tilde{A} \qquad \tilde{G}^{>} \to \hat{G}^{>}_{AB}(E), \quad \tilde{A} \to \hat{A}_{AB}(E)$$

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 fraction.

Now we consider fermi case with + sign and

$N_n = N_m - 1$

we get $\tilde{A}_{AB}(E) = \frac{1}{Z}\sum_{n,m}\{ e^{-\beta(E_n - \mu N_n)} +$

$e^{-\beta(E + E_n - \mu(N_n+1))}\} 2\pi\delta($

$E + E_n - E_m)\langle n|A|m\rangle\langle m|B|n\rangle \}$

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

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

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

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

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

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

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

In proving the above relation $G^< = ifA = -f(G^A - G^a)$ 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 means

$$\tilde{G}^<_{C_j C_k^\dagger}(E) \quad \text{for } A = C_j,\ B = C_k^\dagger.$$

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

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

$$G^r(t) = \theta(t)\left(G^>(t) - G^<(t)\right)$$

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

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

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

This fact implies that $\tilde{G}^r(E)$ is an analytic function 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, "Nonequilibrium Stat Phys")

If the original Hamiltonian $\hat{H}$ 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

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

($\hat{A}(t)$: now; t': past)

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.

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

$$\theta(t) \to \tilde{\theta}(E) = \int_{-\infty}^{+\infty} dt\, e^{i\frac{Et}{\hbar}}\,\theta(t) = \int_0^{+\infty} dt\, e^{i\frac{Et}{\hbar}}$$

Unfortunately the 2nd integral does not exists, and it is also not Lesbesgues integrable as $\int_0^{+\infty} dt \left| e^{i\frac{Et}{\hbar}} \right| \to +\infty$.

physicists' way to solve this mathematical problem is to add artificial dampin. i.e. change the problem to

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

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

Now we do the reverse convolution theorem

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

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

$\theta(t)$

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

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

No $\hbar$ — $\hbar$ gets cancelled

let $E - E' = E''$

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

rename E'' as E'

This is the final expression for the spectral representation 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 spectral integral. What is the difference? Which one more general. How to go from the one form to the other. ie. 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: $G^a(t) = i\,\theta(-t)\,\tilde{A}(t)$

↑ sign differ fm $G^r(t)$ ↗

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

↑ same ↑ $+$

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

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

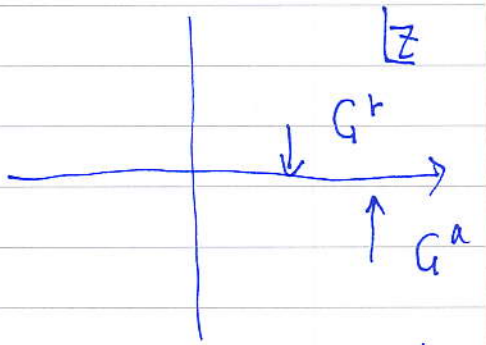
let $E+E' = E''$

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

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

It is useful to define

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



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. 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 equation for the definition of A

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

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

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

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

But it is trickier 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 $$\tilde{G}^r_{AB}(E) = \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\tilde{A}_{AB}(E')}{E + i\eta - E'}$$ page 33

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

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

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

we have used the general relation

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

Note also $\langle g|\psi\rangle^* = \langle\psi|g\rangle$

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

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

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

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

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 "imaging 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 e factor in $C_j(\tau)$, we have

$$\mathrm{Tr}\left(e^{-(\beta-\frac{\tau}{\hbar})(H-\mu N)} C_j\, e^{-(\frac{\tau-\tau'}{\hbar})(H-\mu N)} C_k\, e^{-\frac{\tau'}{\hbar}(H-\mu N)} \cdots \right)$$

if τ is large 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 $-\hbar\beta \le \tau, \tau' \le \hbar\beta$.

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

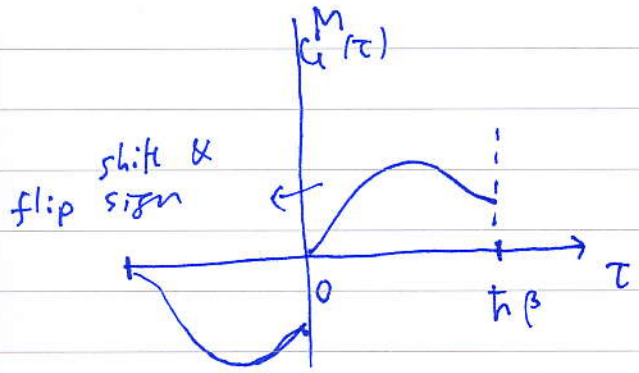
☐ Question/problem. prove the above statements explicitly.

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 note "Theory of Many-particle 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 $0\le\tau\le\hbar\beta$ only, then

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

No need for T_τ as $\tau>0$

$$0\le\tau\le\hbar\beta$$

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

go to Lehmann representation

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

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

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

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

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

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

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

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 $N_n - N_m = -1$

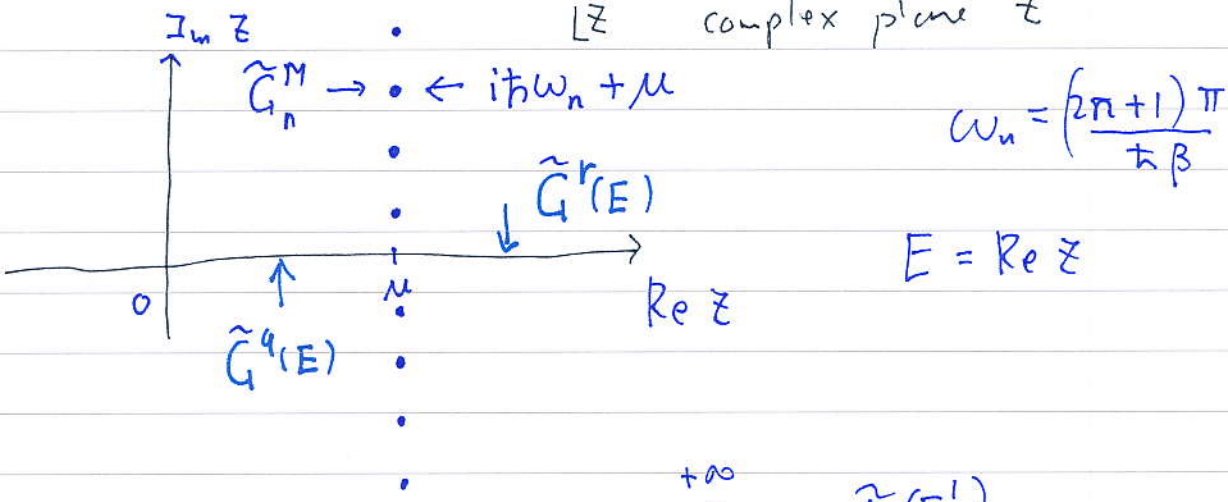
(see page 23) so $E + i\eta \leftrightarrow i\hbar\omega_n + \mu$

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

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

or $$G(z \to i\hbar\omega_n + \mu) = \tilde{G}^M(i\omega_n) \equiv \tilde{G}^M_n \qquad n = 0, \pm 1, \pm 2, \ldots$$

pictorically this means



If we already know $G_1(z) = \int_{-\infty}^{+\infty} \frac{dE'}{2\pi} \frac{\tilde{A}(E')}{z - E'}$

which means we know $\tilde{A}$,

then if we approach the real axis from above we get retarded Green's fucm $\tilde{G}^r(E)$, 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 Matubara Green's function $\tilde{G}^M(i\omega_n)$. ∴ In this sense, $\tilde{A}$ is the most important quantity for equilibrium Green's functions.

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

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

non interacting between L and R

left system in equilibrium at $\beta_L = \frac{1}{k_B T_L}$, μ_L and right system in equilibrium at different β_R μ_R. There nothing in between. So the Green's function 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 $t \gtrsim 0$, 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

$$H_{tot} = \underbrace{H_L^e + H_R^e}_{\text{free electrons}} + \underbrace{H_\gamma}_{\text{free photons}} + V \quad \leftarrow \text{electron-photon interaction term}$$

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

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

for electrons [this defined the means of self energy Σ]

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

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 high light few important points here.

$$G(\tau,\tau') \rightarrow \begin{matrix} & + & - \\ + & G^{++} & G^{+-} \\ - & G^{-+} & G^{--} \end{matrix} = \begin{bmatrix} G^t & G^< \\ G^> & G^{\bar{t}} \end{bmatrix}$$

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

$\sigma = +$ or $-$

G^t is time order.

$\bar{t}$ anti-time order

A single G in contour 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. ie.

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

Now for the Dyson equation on contour

$$G(\tau,\tau') = G^0(\tau,\tau') + \int d\tau_1 \int d\tau_2\, G^0(\tau,\tau_1)\, \Sigma(\tau_1,\tau_2)\, G(\tau_2,\tau')$$

(still matrix multiplication 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

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

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

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

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

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

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 (i.e. left and right).

The 2nd equation is the Kedysh equation

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

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

matrix multiplication implied.

or apply convolution theorem again

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

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 expansion. I refer to read Fetter & Walecka, or AGD (Abrikosov) or some of the recent ones such as H. Bruus & K Flensberg.