More Green Functions (Chap 10)

So far we have figured out how to calculate

\[ G(k, \omega) \quad D(k, \omega) \]

and their Fourier transforms. We have shown that the time-ordered quantities contain some physical information such as the electron density, kinetic energy, etc. There are many other quantities related to

- neutron scattering \( S(k, \omega) \)
- conductivity \( \sigma(k, \omega) \)
- magnetic susceptibility \( \chi_m(k, \omega) \)
- charge susceptibility \( \chi_c(k, \omega) \)

Fortunately each of these may also be expressed as Green functions describing the linear response to a small applied force.

Suppose the system described by a Hamiltonian \( H_0 \) is perturbed by \( f(t) A \)

\[ H = H_0 - f(t) A \]

Where \( f \) is a small field coupling to an operator \( A \), then in the Heisenberg representation...
\[ A^H(t) = U^+(t) A^z(t) U(t) \]

where, as usual

\[ U(t) = T \exp \left\{ i \int_{-\infty}^{+} dt' A^z(t') f(t') \right\} \]

Now, since \( f(t) \) is "small",

\[ U(t) \approx I + i \int_{-\infty}^{+} dt' A^z(t') f(t') \]

\[ U^+(t) \approx I - i \int_{-\infty}^{+} dt' A^+_z(t') f(t') \]

Then

\[ A^H(t) \approx A^z(t) + i \int_{-\infty}^{+} dt' [A^z(t), A^z(t')] f(t') \]

Let's drop the \( f \) suffix and assume \( \langle A(t) \rangle = 0 \) (i.e., suppose \( A = S^z \) and \( f = H^z \) and the system is non-magnetic), then

\[ A^H(t) = \int_{-\infty}^{+} dt' \chi_A(t-t') f(t') \]

\[ \chi_A(t-t') = i \langle [A(t), A(t')] \rangle \Theta(t-t') \]

The function \( \chi_A \) describes the linear response of the system to a small applied perturbation.
which couples to $A$ and contributes a term $-t A$ to $H$. The "R" refers to "retarded".

The retarded Green function $X_R$ describes the physics of the system quite well but it

does not look much like either $G$ or $D$

we have described thus far. These time

ordered or causal Green functions

$$X_c (t, t') = -i \langle T A(t) A(t') \rangle$$

may be calculated using FDT. We need to know the relation to $X_R$!

Relationship between Green Functions.

We may define many different Green functions.

Consider $(t, t')$ here.

**retarded**

$$G_R (t, t') = -i \langle \sum A(t), B(t') \rangle \Delta \Theta (t-t')$$

**advanced**

$$G_A (t, t') = +i \langle \sum A(t), B(t') \rangle \Delta \Theta (t'-t)$$

**causal**

$$G_c (t, t') = -i \langle T A(t) B(t') \rangle$$

$$= -i \langle A(t) B(t') \Theta (t-t') - C B(t') A(t) \Theta (t'-t) \rangle$$

**Matsubara**

$$G_{M} (\beta , \beta') = - \langle T A(-i\beta) B(-i\beta') \rangle$$

$$= - \langle A(-i\beta) B(-i\beta') \Theta (-\beta - \beta') - C B(-i\beta) A(-i\beta) \Theta (-\beta') \rangle$$
we will discuss the Matsubara $G_m$ at length next chapter (T≠0 FP PT) along with the associated formalism.

These Green functions are related to each other via the Feynman representation. Remember this choice of basis employed the full set of states of $H$. First let's prove some preliminaries. All 4 of these Green functions are functions of $t-t'$ so long as $H$ is time independent. Consider the common building block

$$C(t-t') = \langle A(t) B(t') \rangle$$

$$= \frac{1}{Z} \text{Tr}\{e^{-\beta H} e^{i H t} A e^{-i H t} e^{i H t'} B e^{-i H t'} \}$$

then as $[e^{-\beta H}, e^{i H t}] = 0$, this is

$$= \frac{1}{Z} \text{Tr} e^{-\beta H} A e^{i H (t-t')} B e^{-i H (t-t')}$$

$$= \langle A(0) B(t-t') \rangle$$

Since all 4 of $G_A, G_B, G_c, G_m$ are made of these components, all only depend on $t-t'$ (or $2\pi-t'$)
The Advanced and Retarded Green Functions

$G_R$ and $G_A$ differ in that $G_R$ is analytic in the upper half complex plane and $G_A$ is analytic in the lower. Consider for example

\[ G_\text{analytic} (w) = \int_{-\infty}^{\infty} dt \ e^{i(w(t-t'))} G_R (t-t') \]

\[ G_\text{analytic} = -i \int_{-\infty}^{\infty} dt \ e^{i\omega(t-t')} \langle [A(t), B(t')]_e \rangle \times \Theta(t-t') \]

\[ \approx -i \int_{+\infty}^{\infty} dt \ e^{i\omega(t-t')} \langle [A(t), B(t')]_e \rangle \]

It is reasonable, for a stable system, to assume that the part in $\langle \rangle$ does not grow exponentially with time. Let $\omega = \omega_0 + i\omega_c$ so we may explore the properties of $G(\omega)$ in $\omega$. If $\omega_c > 0$, then the integral is convergent so that $G(\omega > 0)$ is analytic since its derivatives also exist since they just add factors of $t$ to the integrand of

\[ G(\omega) = -i \int_{-\infty}^{\infty} dt \ e^{i\omega t} e^{-i\omega_c t} \langle [A(t), B(0)]_e \rangle \]

which would converge for any $\omega_c > 0$ and finite $\langle \rangle$. 
Then $G_R(w)$, the proper Fourier transform of $G(t-t')$ is then

$$G_R(w) = \lim_{w_i \to 0^+} G(w_i + iw)$$

Then as we have seen, $G_R(t)$ gives the response of the system to a force $f(t)$, it means that $G_R(w)$ is the linear response of a system to one Fourier component, i.e., the response of a system to a sinusoidal force $F(w)$ of frequency $w$.

A very similar argument applied to $G_A(w)$ shows that it is analytic in the lower half plane.

Let's investigate $G(w)$ further in the Lagrangian representation, i.e., we introduce a complete set $\{|n>\}$ of states of $H$ with eigenvalues $E_n$

$$H|n> = E_n|n>$$

Then

$$G(w) = -\frac{i}{\pi} \int_0^\infty dt \exp(-it) \sum_m e^{-iE_m t} \langle H(t), \phi(0) | m \rangle |n>$$
\[ \frac{1}{2} \sum_n H e^{i\omega t} \sum e^{-BE_n} \langle n | A(4) B(0) + eB(0) A(4) | n \rangle \]

Now insert \( I = \sum_n \ln x_n \)

\[ \frac{1}{2} \int_0^\infty dt e^{i\omega t} \sum_{nn} e^{-BE_n} \left\{ A_{nn} B_{nn} e^{i(E_n - E_n)t} + e^{B_{nn} A_{nn} e^{i(E_n - E_n)t}} \right\} \]

let \( n \rightarrow m \) in the second term

\[ \frac{1}{2} \int_0^\infty dt e^{i\omega t} \sum_{nm} (e^{-BE_m} + e^{-BE_n}) A_{nm} B_{nm} e^{i(E_n - E_m)t} \]

Now integrating over time, we obtain

\[ G(\omega) = \frac{1}{2} \sum_{nm} \frac{e^{-BE_n} + e^{-BE_m}}{E_n - E_m - \omega} A_{nm} B_{mn} \]

Note \( E_n, \omega, e \) are real, so let

\[ G(\omega) = \frac{1}{2} \int_0^\infty dx \sum_{nm} \frac{e^{-BE_n} + e^{-BE_m}}{w - x} A_{nm} B_{mn} \delta(x - E_n + E_m) \]

\[ = \int_0^\infty dx \frac{A(x)}{w - x} \]

where

\[ A(x) = \frac{1}{2} \sum_{nm} e^{-BE_m} A_{nm} B_{nm} \delta(x - E_n + E_m) \]

is the spectral function of \( A \) and \( B \) operators with the properties
\[ \sum_{m} \int_{0}^{\infty} \frac{A(x)}{1 + e^{-\beta x}} = \frac{1}{2} \sum_{mn} e^{-\beta E_n} A_{mn} B_{mn} = \langle A, B \rangle \]

\[ \int_{-\infty}^{\infty} dx \ A(x) = \langle [A, B]_e \rangle \]

more significantly

\[ G(w) = \int \frac{A(x)}{w-x} \sim \frac{1}{w} \int dx \ A(x) = \frac{\langle [A, B]_e \rangle}{w} \]

That is, if \( A = G_x \) and \( B = G^+ \) and \( e = -1 \) for all

\[ G_x(w) \sim \frac{1}{w} \]

Now suppose we repeat this, starting with

\[ G'(w) = \int_{-\infty}^{\infty} dt \ e^{i \omega(t-t')} G_A(t-t') \]

then since \( G_A(t-t') \propto \theta(t'-t) \), we would find that the integral converges provided that \( \omega < 0 \), so \( G_A(w) \) is analytic in the lower half plane, we would also find that

\[ G'(w) = \int_{-\infty}^{\infty} dx \ \frac{A(x)}{w-x} \]

with the same A!
I.e., \( G'(w) = G(w) \) and

Note that:

\[
\begin{align*}
G_R(w) &= G(w + i\delta) \\
G_A(w) &= G(w - i\delta)
\end{align*}
\]

\( \delta = \epsilon^+ \)

So that \( G(w) \) is analytic in the upper half plane and equal to \( G_R \); and also analytic in the lower plane and equal to \( G_A \)

\[
G = G_R \quad \text{analytic}
\]

\[
G = G_A \quad \text{analytic}
\]

The branch cut separating the two regions is

\[
G_R(w) - G_A(w) = \lim_{\delta \to 0} \left\{ G(w + i\delta) - G(w - i\delta) \right\}
\]

\[
= \lim_{\delta \to 0} \int_{-\infty}^{\infty} dx \, A(x) \left\{ \frac{1}{w + i\delta - x} - \frac{1}{w - i\delta - x} \right\}
\]

\[
= -2\pi i \int_{-\infty}^{\infty} dx \, A(x) \delta(w - x)
\]

\[
= -2\pi i \, A(x)
\]
Now what about the time ordered $G_c(w)$ that we can calculate using FDPT. If we repeat the same steps, in introduce $1/n < h$ ... then we find

$$G_c(w) = \int_{-\infty}^{\infty} dx \, A(x) \left\{ \frac{P}{w-x} - \frac{1-\mathrm{e}^{-\beta x}}{1+\mathrm{e}^{-\beta x}} \delta(x-w) \right\}$$

the term

$$I = \int_{-2}^{2} f(x) \, e^x \, \frac{1}{1+\mathrm{e}^{-\beta x}}$$

I.e from $A$ we can get $G_R$, $G_c$ and $G_R$. Thus is significant, since we may calculate $G_c$ using FDPT, take its imaginary part & extract $G_R$ which describes the physics, the linear response of the system.

What about $G_m$? Matsubara introduced $G_m(\tau)$ as a convenient way to generalize the $T=0$ formalism to finite $T$. If we can write it in terms of $A$, then we can calculate the finite $T$ linear response physics! Generally let $0 < \varepsilon < \beta$ then
\[ G(\tau - \beta) = -\langle T e^{-i(\tau - \beta)} A(\tau - \beta) B(0) \rangle \]
\[ = \epsilon \langle B(0) A(-i(\tau - \beta)) \rangle \]
\[ = \epsilon \frac{\text{Tr} e^{-\beta H} B e^{(\tau - \beta) H} A e^{-(\tau - \beta) H}}{\text{Tr} e^{-\beta H} A e^{\tau H} B e^{-\tau H}} \]
\[ = \epsilon \langle A(0) B(\tau) \rangle = \epsilon \langle A(-i\tau) B(0) \rangle \]
\[ = -\epsilon G(\tau) \]

That is that \( G_n(\tau) \) is a periodic function of \( \tau \), with period \( \beta \).

\begin{align*}
\text{Fermions} & \quad e = -1 \\
\text{G}(\tau) & \quad \begin{array}{c}
\text{G}(\tau - \beta) = -\text{G}(\tau)
\end{array}
\end{align*}

Since \( G \) is an (anti)periodic function, it
has a discrete Fourier transform.

\[ \text{Fermion} \]
\[ G(\omega) = T \sum_n e^{-i\omega n \beta} G(i\omega_n) \]
\[ \text{Since} \quad G(\tau) = -G(\tau + \beta) \quad \omega_n = (2n+1)\pi T \]
\[ G(i\omega_n) = \frac{1}{\sqrt{\beta}} \int_0^\beta e^{i\omega_n \tau} G(\tau) \]

\[ \text{Bosons} \]

Similarly if \( e = -1 \), Bosons

\begin{align*}
\text{Boson} & \quad e = -1 \\
\text{G}(\tau) & \quad \begin{array}{c}
\text{G}(\tau) = \text{G}(\tau)
\end{array}
\end{align*}
Then
\[ G(\tau) = T \sum_{n} e^{-i\kappa_{n}\tau} G(\kappa_{n}) \quad \kappa_{n} = 2\pi nT \]
\[ G(\kappa_{n}) = \int_{0}^{\beta} d\tau e^{i\kappa_{n}\tau} G(\tau) \]

Now, can we write \( G_{m} \) in terms of \( A \)?

\[ G_{m}(\kappa_{n}) = -\frac{1}{2} \int_{0}^{\beta} d\tau e^{i\kappa_{n}\tau} \text{Tr} e^{-\beta H} e^{\tau H} A e^{-\tau H} \]

Insert \( \sum_{\kappa} \text{Im} \kappa = i\pi \)

\[ G(\kappa_{n}) = -\frac{1}{2} \int_{0}^{\beta} d\tau e^{i\kappa_{n}\tau} \sum_{nm} e^{-\beta E_{n}} A_{mn} B_{nm} c_{n}^{\dagger} e_{m}^{\dagger} \]

\[ = -\frac{1}{2} \sum_{nm} A_{mn} B_{nm} \frac{e^{-\beta E_{n}} + e^{-\beta E_{m}}}{E_{n} - E_{m} - i\kappa_{n}} \]

\[ = \int dx \frac{A(x)}{i\kappa_{n} - x} \]

Thus, knowledge of \( A \)

\[ A(x) \rightleftharpoons \begin{cases} G_{0}(w) \\ G_{R}(w) \\ G_{I}(w) \\ G_{m}(w) \end{cases} \]

Furthermore, given any \( G \), we may calculate \( A \) and hence any other \( G \). Note that

\[ G_{R}(w) = \int G_{m}(i\kappa_{n} \rightarrow w + i\epsilon) \]
Fluctuation-Dissipation theorem relates fluctuations of A to the linear response to a force which couples to A

\[ \langle A^2 \rangle \leftrightarrow \langle A(t) \rangle \]

Remember, we assumed \( \langle A \rangle = 0 \)

This intuitively makes sense. The more fluctuations a system experiences, the larger the response to an external force.

If \( X(w) \) is the response function, so that

\[ \langle A(t) \rangle = \int_0^\infty dt' X(t+t') \langle f(t') \rangle = \langle A(w) \rangle = X(w) f(w) \]

and \( C(t-t') \) describes the fluctuations about equilibrium

\[ C(t-t') = \frac{1}{2} \langle \{ A(t), A(t') \} \rangle = \int_0^\infty \frac{dw}{2\pi} e^{-i\omega(t-t')} C(w) \]

according to the FDT

\[ C(w) = \frac{\gamma}{\hbar} \left[ 1 + 2N(w) \right] X^2(w) \]

Fluctuations quantum thermal dissipation \( (\hbar \omega_0 = \hbar \omega) \)

When \( \omega \ll k_B T / \hbar \), \( \hbar \omega \approx k_B T / \hbar \omega \), then we recover the classical result.
\[ C(\omega) = \frac{2kT}{\omega} X''(\omega) \]

Let's prove this, starting with the classical result. Imagine we have a classical oscillator.

\[ \mathcal{A} \text{ssuming} \]
\[ \langle X(\omega) X(\omega') \rangle = 2kT \int \frac{d\omega}{2\pi} \omega e^{-i\omega t} \]
\[ X(\omega) = X'(\omega) + iX''(\omega) \]

\[ \text{E.O.M. } m(\ddot{x} + \omega^2 x) + \eta \dot{x} = f(t) \]
\[ \text{spring force } \frac{m}{\eta} \text{ applied force} \]

After we Fourier transform
\[ X(\omega) = \mathcal{F}(x(t)) \quad \mathcal{F}(\omega) = \frac{1}{m(\omega^2 - \omega_0^2) - i\eta \omega} \]
\[ X''(\omega) = \frac{\eta \omega}{(m(\omega^2 - \omega_0^2))^2 + \eta^2 \omega^2} = |X(\omega)|^2 \eta \omega \]

According to the equipartition theorem
\[ \frac{1}{2} \omega_0^2 \langle x^2 \rangle = \frac{kT}{2} \]
\[ \langle x^2 \rangle = \int \frac{d\omega}{2\pi} (X(\omega))^2 |\mathcal{F}(\omega)|^2 = \frac{kT}{\hbar \omega_0} \]
If the damping is weak, \( n \ll \omega_0 \) then

\[
\frac{\vert X'(\omega) \vert^2}{\vert X(\omega) \vert^2} = \frac{H(\omega)}{H(\omega_0)}
\]

An adiabatic approximation to the integral is possible. Let \( \vert X(\omega) \vert^2 = \frac{1}{\omega_0} X''(\omega) \)

\[
K_0 T/(m\omega_0^2) = \frac{H(\omega_0)}{2\pi} \int_0^{\omega_0} d\omega \frac{X''(\omega)}{\omega} = \frac{H(\omega_0)^2}{2m\omega_0^2 n}
\]

That is \( \vert f(\omega_0) \vert^2 = 2nK_0 T \). Since \( \omega_0 \) is arbitrary, this must apply for all \( \omega_0 \).

\[
\vert f(\omega) \vert^2 = 2nK_0 T
\]

Thus

\[
C(\omega) = \langle X(\omega)X(-\omega) \rangle = \vert X(\omega) \vert^2 \vert f(\omega) \vert^2
\]

\[
C(\omega) = \left( \frac{\vert f(\omega) \vert^2}{\omega} \frac{X''(\omega)}{\omega_n} \right) = \frac{2K_0 T}{\omega} X''(\omega)
\]

\[
C(\omega) = \frac{2K_0 T}{\omega} X''(\omega) \quad \text{Classical Fluctuation}
\]

\[
\text{Dissipation Theorem}
\]
We will now prove the Quantum FDP again using the Lehmann representation. I.e. we employ the complete set of states of $H$

$$H |n\rangle = E_n |n\rangle \quad \mathbb{1} = \sum_n |n\rangle \langle n|$$

and

$$\langle n| A(t) |m\rangle = \langle n| e^{iHt} A e^{-iHt} |m\rangle$$

$$= e^{i(E_n - E_m)t} A_{nm}$$

We apply this to $\chi(t-t')$, $\chi(t)$ and $C(t-t')$

$$\chi(t-t') = i \langle A(t) A(t') - A(t') A(t) \rangle \Theta(t-t')$$

$$= i \sum_{nm} e^{-BE_n} \left\{ \langle n| A(t) |m\rangle \langle m| A(t') |n\rangle - \langle n| A(t') |m\rangle \langle m| A(t) |n\rangle \right\} \Theta(t-t')$$

$$= i \sum_{nm} (e^{-BE_n} - e^{-BE_m}) |n\rangle \langle m| A |n\rangle \langle m| \chi(t-t')$$

We now introduce the spectral function $A(\omega) = -\frac{i}{\pi} \text{Im} C(\omega)$ or in this case $A(\omega) = -\frac{i}{\pi} \chi^\prime(\omega)$

$$\chi'(\omega) = \frac{1}{\pi} \sum_{nm} |n\rangle \langle m| A |n\rangle \langle m| e^{-BE_n} \delta(\omega - (E_n - E_m))$$

$$= \frac{1}{\pi} \sum_{nm} (e^{-BE_n} - e^{-BE_m}) |n\rangle \langle m| A |n\rangle \langle m| \delta(\omega - (E_n - E_m))$$

This is very close in form to $\chi(t-t')$
In fact we may write

\[ X(t) = i \int_0^\infty \Theta(t) \sum n \left[ e^{-i(En-Em)t} \left( e^{-BEn} - e^{-EBm} \right) \right] \left| \langle m \mid A(t) \rangle \right|^2 \]

by its definition

\[ = \int_0^\infty \Theta(t) dw \ e^{-i\omega t} X''(w) \]

Then we use i \int_0^\infty e^{-i\omega t} dw = \frac{1}{\omega+i\delta} \text{ and we get}

\[ X(\omega) = \int \frac{dw}{\pi} \frac{1}{\omega+i\delta-\omega} X''(\omega) \]

We may do roughly the same thing with the fluctuation function.

\[ C(t-t') = \frac{1}{2} \left\langle \left[ A(t), A(t') \right]^2 \right\rangle \quad \text{no } \Theta(t-t') \]

\[ = \frac{1}{2} \sum_{nm} e^{-BEn} \left\{ \langle n \mid A(t) \mid m \rangle^* \langle m \mid A(t') \mid n \rangle + \langle n \mid A(t') \mid m \rangle^* \langle m \mid A(t) \mid n \rangle \right\} e^{-i(En-Em)(t-t')} \]

\[ = \frac{1}{2} \sum_{nm} \left( e^{-BEn} + e^{-BEm} \right) \left| \langle n \mid A(t) \rangle \right|^2 \left( e^{-i(En-Em)(t-t')} \right) \]

\[ = \frac{1}{2} \sum_{nm} e^{-BEn} \left( 1 + e^{-B(E_{m}-E_n)} \right) \left| \langle n \mid A(t) \rangle \right|^2 e^{-i(En-Em)(t-t')} \]

Again note the similarity to the definition of \( X'' \). They only differ by the sign so that (by inspection)

\[ C(t) = \frac{1}{2\pi} \int \frac{dw}{1-e^{-i\omega t}} \left( \frac{1+e^{-B\omega}}{1-e^{-B\omega}} \right) X''(w) \]
\[ C(t) = \int \frac{d\omega}{2\pi} \ e^{-i\omega t} \ (1 + 2n(\omega)) \ \chi''(\omega) \]

\[ n(\omega) = \frac{1}{e^{\omega/kT} - 1} \]

Hence

\[ C(\omega) = 2\hbar \left\{ \frac{\chi''(\omega)}{1 + n(\omega)} \right\} \chi''(\omega) \]

Quantum
Fluctuation
Dissipation
Theorem