Previous lecture :

Linear response theory

Introduce $G^{Ret}_{AB}(t,t') := -i\theta(t-t')\langle[A(t),B(t')]\rangle_0$

Heisenberg op.

Retarded Green's function.

$$\boxed{\Delta A_t = \frac{1}{\hbar}\int_{-\infty}^{\infty} dt' f_{t'} G^{Ret}_{AB}(t,t')}$$ Kubo formula

Another notation $G^{Ret}_{AB}(t,t') = \langle\langle A(t), B(t')\rangle\rangle^{Ret}$

Other (closely related) Green's functions appear naturally in other contexts:

$G^{Ret}_{AB}(t,t') = \langle\langle A(t), B(t')\rangle\rangle^{Ret} = -i\theta(t-t')\langle[A(t),B(t')]_{-\zeta}\rangle$ {We had $\zeta = 1$}

$G^{Adv}_{AB}(t,t') = \langle\langle A(t), B(t')\rangle\rangle^{Adv} = +i\theta(t'-t)\langle[A(t),B(t')]_{-\zeta}\rangle$ (Advanced Green's function)

$G^{C}_{AB}(t,t') = \langle\langle A(t), B(t')\rangle\rangle^{C} = -i\langle T_\zeta(A(t),B(t'))\rangle$ (Causal Green's function)

$S_{AB}(t,t') = \frac{1}{2\pi}\langle[A(t),B(t')]_{-\zeta}\rangle$ (Spectral density)

$\langle A(t)B(t')\rangle, \langle B(t')A(t)\rangle$ (Correlation functions)

In each case we consider: $X(t) = e^{i\frac{Ht}{\hbar}} X e^{-i\frac{Ht}{\hbar}}$ (Heisenberg picture)

For the GCE: $H \to \mathcal{H} = H - \mu N$ ("modified" Heisenberg picture)

$\langle X \rangle = \frac{1}{\Xi} \mathrm{Tr}\, e^{-\beta \mathcal{H}} X$; $\Xi = \mathrm{Tr}\, e^{-\beta\mathcal{H}}$ $\beta = \frac{1}{k_B T}$

$T_\zeta(A(t), B(t')) = \Theta(t-t') A(t) B(t') + \zeta \Theta(t'-t) B(t') A(t)$ – Wick ordering op.

A, B have no explicit time dependence.

Concentrate on the situation, where $\mathcal{H} = H - \mu N$ (GCE)

Demonstrate that $\frac{\partial \mathcal{H}}{\partial t} = 0$ implies $G^\alpha_{AB}(t,t') = G^\alpha_{AB}(t-t')$ $\alpha \in \{\mathrm{Ret}, \mathrm{Adv}, c\}$

and $S_{AB}(t,t') = S_{AB}(t-t')$

It suffices to show it for the correlation functions $\langle A(t) B(t') \rangle = \mathrm{Tr}(\varrho A(t) B(t'))$

with $\varrho = \frac{1}{\Xi} e^{-\beta\mathcal{H}}$, $\Xi = \mathrm{Tr}\, e^{-\beta \mathcal{H}}$.

$$\Xi \langle A(t) B(t') \rangle = \mathrm{Tr}\left\{ \varrho^{-\beta\mathcal{H}} A(t) B(t') \right\} = \mathrm{Tr}\left\{ e^{-\beta\mathcal{H}} e^{i\frac{\mathcal{H}t}{\hbar}} A e^{-i\frac{\mathcal{H}t}{\hbar}} e^{i\frac{\mathcal{H}t'}{\hbar}} B e^{-i\frac{\mathcal{H}t'}{\hbar}} \right\} =$$

$$= \mathrm{Tr}\left\{ e^{-\beta\mathcal{H}} e^{i\frac{\mathcal{H}}{\hbar}(t-t')} A e^{-i\frac{\mathcal{H}}{\hbar}(t-t')} B \right\} = \mathrm{Tr}\left\{ e^{-\beta\mathcal{H}} A(t-t') B(0) \right\}$$

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

Equations of motion for Green's functions

Recall the Heisenberg e.o.m. $i\hbar \frac{dA(t)}{dt} = [A(t), \mathcal{H}(t)]_- + i\hbar \frac{\partial A}{\partial t}(t)$

(true also for $H \longrightarrow \mathcal{H}$)

$\mathcal{H} = H - \mu N$

our case: $\frac{\partial A}{\partial t} = 0$

Differentiate the definition of G^{α}_{AB} w.r.t. t

$$i\hbar \frac{\partial}{\partial t} G^{\alpha}_{AB}(t,t') = \hbar\delta(t-t')\underbrace{\langle [A(t), B(t')]_{-S} \rangle}_{\text{Depends on } (t-t') \text{ and is multiplied by } \delta(t-t') \to \text{ may drop } t\text{-dependencies.}} + \underbrace{\langle\langle [A,\mathcal{H}]_-(t), B(t') \rangle\rangle^{\alpha}}_{\text{A new ("higher order") Green's function with } A(t) \longrightarrow [A,\mathcal{H}]_-(t).} \qquad (*)$$

- The same equation for different α, but different boundary conditions.

  e.g. $G^{Ret}_{AB}(t,t') = 0$ for $t' > t$; $G^{Adv}_{AB}(t,t') = 0$ for $t' < t$.

- We could now write the e.o.m. for the new Green's function involving $[A,\mathcal{H}]_-(t)$. This would introduce another Green's function and so on...

  This generates a (typically infinite) hierarchy of e.o.m.

$G^{\alpha}_{AB}(t,t') \longrightarrow G^{\alpha}_{AB}(t-t')$, Fourier transform:

$$G^{\alpha}_{AB}(t-t') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dE\, G^{\alpha}_{AB}(E)\, e^{-i\frac{E}{\hbar}(t-t')}$$

$$\delta(t-t') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dE\, e^{-i\frac{E}{\hbar}(t-t')}$$

This transforms (*) to an algebraic form:

$$E\langle\langle A, B\rangle\rangle^{\alpha}_{E} = \hbar\langle [A,B]_{-S}\rangle + \langle\langle [A,\mathcal{H}]_-, B\rangle\rangle^{\alpha}_{E} \qquad \text{(e.o.m. in Fourier rep.)}$$

with $G^{\alpha}_{AB}(E) = \langle\langle A,B\rangle\rangle^{\alpha}_{E} = \int_{-\infty}^{\infty} d(t-t')\, G^{\alpha}_{AB}(t-t')\, e^{i\frac{E}{\hbar}(t-t')}$

Spectral representation of Green's functions

Conside the eigenstates of $\mathcal{H}$ $\quad \mathcal{H}|E_n\rangle = E_n|E_n\rangle$

- Correlation function: $\Xi\langle A(t)B(t')\rangle = \mathrm{Tr}\left\{e^{-\beta\mathcal{H}}A(t)B(t')\right\} =$

$$= \sum_n \langle E_n| e^{-\beta \mathcal{H}} A(t) B(t') |E_n\rangle =$$

$$= \sum_{mn} e^{-\beta E_n} \langle E_n| A(t) |E_m\rangle \langle E_m| B(t') |E_n\rangle =$$

$$= \left\{ \begin{array}{l} \text{definition of} \\ \text{Heisenberg op.} \\ A(t) = e^{i\mathcal{H}t/\hbar} A e^{-i\frac{\mathcal{H}t}{\hbar}} \\ B(t) = \ldots \end{array} \right\} = \sum_{mn} \langle E_n|A|E_m\rangle\langle E_m|B|E_n\rangle e^{-\beta E_n} \cdot$$

$$\cdot\, e^{\frac{i}{\hbar}(E_n - E_m)(t-t')} = \left\{ \begin{array}{l} \text{Dummy indices} \\ \text{change } n \leftrightarrow m \end{array} \right\} =$$

$$= \sum_{nm} \langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n} e^{-\beta(E_m - E_n)} e^{-\frac{i}{\hbar}(E_n - E_m)(t-t')}$$

The same way $\Xi\langle B(t')A(t)\rangle$

(replace $A \leftrightarrow B$, $t \leftrightarrow t'$, $n \leftrightarrow m$ in the calculation above).

$$\Xi\langle B(t')A(t)\rangle = \sum_{mn} \langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle \cdot$$

$$\cdot\, e^{-\beta E_n} e^{-\frac{i}{\hbar}(E_n - E_m)(t-t')}$$

- Spectral density:

$$S_{AB}(t,t') = \frac{1}{2\pi}\langle [A(t), B(t')]_{-\zeta}\rangle =$$

$$= \frac{1}{2\pi}\Big(\langle A(t)B(t')\rangle - \zeta\langle B(t')A(t)\rangle\Big)$$

Plug the derived expressions for $\langle A(t)B(t')\rangle$, $\langle B(t')A(t)\rangle$, Fourier transform.

$\longrightarrow$ SPECTRAL REP. OF $S_{AB}(E)$

$$S_{AB}(E) = \frac{Z^{-1}}{2\pi}\int_{-\infty}^{\infty} d(t-t')\Big[\sum_{mn}\langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n}\left(e^{-\beta(E_m-E_n)} - \zeta\right)\Big]\cdot$$

$$\cdot\, e^{-\frac{i}{\hbar}(E_n - E_m - E)(t-t')}$$

$$S_{AB}(E) = \frac{\hbar}{Z}\sum_{mn}\langle E_n|B|E_m\rangle\langle E_m|A|E_n\rangle e^{-\beta E_n}\left(e^{\beta E} - \zeta\right)\cdot$$

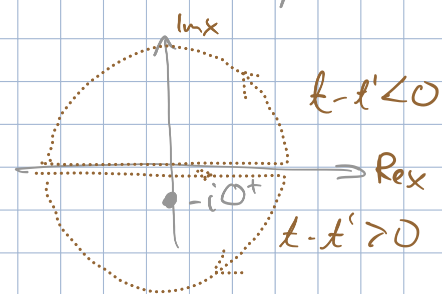
$$\cdot\,\delta\big(E - (E_n - E_m)\big)$$

Relation between $S_{AB}(E)$ and $G^{Ret}_{AB}(E)$:

In time representation: $G^{Ret}_{AB}(t-t') = -2\pi i\,\Theta(t-t')\,S_{AB}(t-t')$

An identity: $\Theta(t-t') = \frac{i}{2\pi}\int_{-\infty}^{\infty} dx\,\frac{e^{-ix(t-t')}}{x + i0^+}$ (prove as homework)

$$S_{AB}(t-t') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dE'\,S_{AB}(E')\,e^{-\frac{i}{\hbar}E'(t-t')}$$



$$G^{Ret}_{AB}(E) = \int_{-\infty}^{\infty} d(t-t')\, e^{\frac{i}{\hbar}E(t-t')} \left(-2\pi i\right) \Theta(t-t') S_{AB}(t-t') =$$

$$= \int_{-\infty}^{\infty} dE' \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} d(t-t')\, \frac{1}{2\pi\hbar} \frac{S_{AB}(E')}{x+i0^+}\, e^{-\frac{i}{\hbar}(\hbar x + E' - E)(t-t')} \overset{\int d(t-t')}{=}$$

$$= \frac{1}{\hbar} \int_{-\infty}^{\infty} dE' \int_{-\infty}^{\infty} dx\, \frac{S_{AB}(E')}{x+i0^+}\, \delta\left(x - \frac{E-E'}{\hbar}\right)$$

$$\boxed{G^{Ret}_{AB}(E) = \int_{-\infty}^{\infty} dE' \frac{S_{AB}(E')}{E-E'+i0^+}}$$

Spectral representation of the retarded Green's function.

Analogous calculation for $G^{Adv}_{AB}(E)$ leads to

$$G^{Adv}_{AB}(E) = \int_{-\infty}^{\infty} dE' \frac{S_{AB}(E')}{E-E'-i0^+}$$

We may plug $S_{AB}(E)$ in the spectral rep. and do the integration

$$G^{Ret/Adv}_{AB} = \frac{\hbar}{\Xi} \sum_{mn} \langle E_n | B | E_m \rangle \langle E_m | A | E_n \rangle e^{-\beta E_n} \frac{e^{\beta(E_n - E_m)} - \zeta}{E - (E_n - E_m) \pm i0^+}$$

Remark: we expressed the Green's function via the spectral density. The inverse is also possible $\longrightarrow$ $S_{AB}(E) = \mp \frac{1}{\pi} \operatorname{Im} G^{RET/ADV}_{AB}(E)$

PRESENT AIM: BUILD A CONNECTION TO THERMODYNAMICS

Recall:

$$\langle B(t') A(t) \rangle = \frac{1}{\Xi} \sum_{mn} \langle E_n | B | E_m \rangle \langle E_m | A | E_n \rangle e^{-\beta E_n} e^{-\frac{i}{\hbar}(E_n - E_m)(t-t')}$$

$$S_{AB}(E) = \frac{\hbar}{\Xi} \sum_{nm} \langle E_n | B | E_m \rangle \langle E_m | A | E_n \rangle e^{-\beta E_n} \left(e^{\beta E} - \zeta\right) \delta\left(E - (E_n - E_m)\right)$$

Notation $S_{AB}(E) \longrightarrow S^{\zeta}_{AB}(E)$

Focus on $\zeta = -1$.

$$\langle B(t') A(t) \rangle = \frac{1}{\hbar} \int_{-\infty}^{\infty} dE \, \frac{S^{-}_{AB}(E)}{e^{\beta E} + 1} \, e^{-\frac{i}{\hbar} E (t - t')}$$

(SPECTRAL THEOREM FOR $\zeta = -1$)