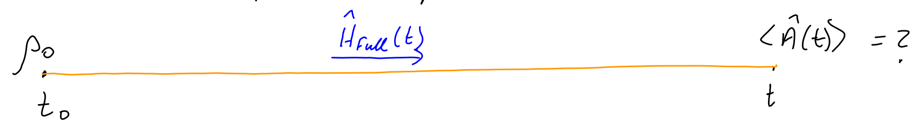
Kubo formula : linear response to a perturbation

GF24



Consider $\hat{H}_{full}(t) = \hat{H} + \hat{H}'(t)$ [in Schrödinger picture] (1)

Assume : $\hat{H}$ is time-independent, $\hat{H}|n\rangle = E_n |n\rangle$ (2)

$\hat{H}'$ is linear in an external field (absent before time t_0)

Examples : coupling to EM potentials

scalar potential couples to charge: $\hat{H}' = \int d\vec{r}\; \phi(\vec{r},t)\, \hat{n}(\vec{r})$ (3)

vector potential couples to current : $\hat{H}' = \int d\vec{r}\; \vec{A}(\vec{r},t)\, \hat{\vec{j}}(\vec{r})$ (4)

Zeeman energy in inhomogeneous magnetic field: $\hat{H}' = \int d\vec{r}\; \vec{B}(\vec{r},t) \left[\hat{\rho}_\uparrow(\vec{r}) - \hat{\rho}_\downarrow(\vec{r})\right]$ (5)

GF25

At times $t < t_0$, system is in thermal equilibrium, described by initial density matrix :

$$\langle \hat{O} \rangle \equiv \mathrm{Tr}[\hat{\rho}\, \hat{O}], \quad \hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}, \quad Z = \sum_n e^{-\beta E_n} \tag{1}$$

(for grand-canonical ensemble, $\hat{H}$ stands for $\hat{H} - \mu \hat{N}$)

Expectation value of an operator $\hat{A}$ at time $t > t_0$:

full time-ev. op.

$$\langle \hat{A}(t) \rangle \equiv \frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | \hat{U}^\dagger(t,t_0)\, \hat{A}_S(t)\, \hat{U}(t,t_0) | n \rangle \tag{2}$$

do thermal average using unperturbed energies, states, which are then time-evolved to time t.

weight | initial states, time t_0 | time evolution under action of full $\hat{H}_{full}(t)$ | time t

$e^{-\beta E_n}$ $|n\rangle$

$|n(t)\rangle = \hat{U}(t,t_0)|n\rangle$ (3)

Compact notation: $\langle \hat{A}(t)\rangle \overset{(25.2)}{=} Tr\left[\hat{\rho}\ \underbrace{\hat{U}^{\dagger}(t,t_0)\, \hat{A}_S(t)\, \hat{U}(t,t_0)}_{=\hat{A}_H(t)}\right] = \langle \hat{A}_H(t)\rangle$ (1) $\boxed{GF26}$

alternative form: (2)

$$\langle \hat{A}(t)\rangle = Tr\left[\hat{\rho}_H(t)\, \hat{A}\right], \quad \text{with } \hat{\rho}_H(t) \equiv \hat{U}(t,t_0)\, \hat{\rho}\, \hat{U}^{\dagger}(t,t_0) \qquad (3)$$

Note: for density matrix, time evolution (26.3) is <u>opposite</u> to usual definition for Heisenberg operators, (26.2)

Now, we want to expand (1) to <u>linear</u> order in $\hat{H}'$.

Interaction representation: $\hat{U}(t,t_0) \overset{(12.4)}{=} e^{-i\hat{H}(t-t_0)}\ \hat{U}_I(t,t_0)$ $(\hbar=1)$ (4)

where $\hat{U}_I(t,t_0) = \mathcal{T}\, e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, \hat{H}'_I(t')} \simeq 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \hat{H}'_I(t')$ (5)

time-dependence in interaction representation: $\hat{O}_I(t) \overset{(12.3)}{=} e^{i\hat{H}(t-t_0)}\ \hat{O}_S(t)\, e^{-i\hat{H}(t-t_0)}$ (6)

Insert (26.4-6) into (26.1): $\boxed{GF27}$

$$\langle \hat{A}_H(t)\rangle = \langle U^{\dagger}(t,t_0)\, \hat{A}_S(t)\, \hat{U}(t,t_0)\rangle \qquad (1)$$

$$\overset{(26.5)}{=} \left\langle \left(1 + \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \hat{H}_I(t')\right) \underbrace{e^{i\hat{H}(t-t_0)}\, \hat{A}_S(t)\, e^{-i\hat{H}(t-t_0)}}_{\hat{A}_I(t)} \left(1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \hat{H}_I(t')\right)\right\rangle \qquad (2)$$

$$= \langle \hat{A}_S(t)\rangle + \int_{t_0}^{\infty} dt'\ \underbrace{\frac{(-i)}{\hbar}\theta(t-t')\ \langle[\hat{A}_I(t), \hat{H}'_I(t')]\rangle}_{\equiv\ \mathcal{G}^R_{AH'}(t,t')} \qquad (3)$$

$Tr\, \rho_0\, e^{i\cancel{H_0}(\,)}\, A_S\, e^{-i\cancel{H_0}(\,)}$

reinstate $\hbar \neq 1$

"retarded", due to $\theta(t-t')$

time-evolution with/without perturbation

$$\delta\langle \hat{A}(t)\rangle \equiv \langle \hat{A}_H(t)\rangle - \langle \hat{A}_S(t)\rangle = \int_{t_0}^{\infty} dt'\ \mathcal{G}^R_{AH'}(t-t') \qquad (4)$$

where, in general: $\mathcal{G}^R_{AH'}(t-t') \equiv -\frac{i}{\hbar}\theta(t-t')\langle[\hat{A}_I(t), \hat{H}'_I(t')]\rangle$ (5)

Kubo formula

3-line summary of derivation of Kubo formula: $\boxed{\text{GF28}}$

$$\langle \hat{A}(t) \rangle = \langle \hat{U}^\dagger(t,t_0)\, \hat{A}\, \hat{U}(t,t_0) \rangle \tag{1}$$

$$\hat{U}(t,t_0) = e^{-i\hat{H}(t-t_0)/\hbar} \left(1 - \frac{i}{\hbar} \int_{t_0}^{t} dt'\, \hat{H}'(t') \right) \tag{2}$$

$$\delta \langle \hat{A}(t) \rangle = \int_{t_0 \to -\infty}^{\cancel{t}\ \infty} dt' \underbrace{\frac{-i}{\hbar}\, \theta(t-t') \langle \hat{A}(t)\, \hat{H}'(t') - \hat{H}'(t')\, \hat{A}(t) \rangle}_{G^R_{AH'}(t-t')} \tag{3}$$

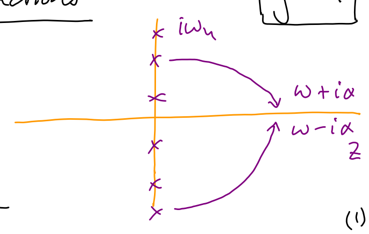
Important: <u>same</u> unperturbed Hamiltonian governs

thermal weighting $\langle \dots \rangle \overset{(25.1)}{=} \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta H} \dots \right]$ (5)

and time evolution: $\hat{A}(t) \overset{(26.6)}{=} e^{i\hat{H}t/\hbar}\, \hat{A}_S\, e^{-i\hat{H}t/\hbar}$ (6)

this will be assumed throughout in what follows.

General relations between various types of Green's functions $\boxed{\text{GF29}}$



Goal: to show that:

Fourier transform of retarded/advanced GF:
$$\mathcal{G}^{R/A}_{AB}(\omega) = \int d\bar{\omega}\, \frac{A_{AB}(\bar{\omega})}{\omega \pm i\alpha - \bar{\omega}} \tag{1}$$

Matsubara transform of thermal GF:
$$\bar{\mathcal{G}}_{AB}(i\omega_\ell) = \int d\bar{\omega}\, \frac{A_{AB}(\bar{\omega})}{i\omega_\ell - \omega} \tag{2}$$

analytical continuation to real axis, from above/below:
$$\mathcal{G}^{R/A}_{AB}(\omega) = \bar{\mathcal{G}}_{AB}(i\omega_\ell \to \omega \pm i\alpha) \tag{3}$$

spectral function:
$$A_{AB}(\bar{\omega}) = \frac{1}{Z} \sum_{nm} A_{nm} B_{mn} \left(e^{-\beta E_n} - \zeta e^{-\beta E_m} \right) \delta(\hbar\bar{\omega} - E_m + E_n) \tag{4}$$

$$= \frac{i}{2\pi} \left[\mathcal{G}^R(\omega) - \mathcal{G}^A(\omega) \right] = \text{discontinuity of } \bar{\mathcal{G}}(i\omega_n) \text{ across real axis} \tag{5}$$

Building blocks of $\mathcal{G}^{R/A}$ are: $\boxed{GF30}$

$$\mathcal{G}^{>}_{AB}(t,t') \equiv -i/\hbar \langle \hat{A}(t)\, \hat{B}(t') \rangle \quad (1)$$

$$\mathcal{G}^{<}_{AB}(t,t') \equiv -\zeta\, i/\hbar \langle \hat{B}(t')\, \hat{A}(t) \rangle \quad (2)$$

mnemonic: $\gtrless$ corresponds to the order and sign produced by $\mathcal{T}[A(t)\, B(t')]$

"Retarded" and "Advanced" GF: (arise in linear response)

$$\mathcal{G}^{R/A}_{AB}(t,t') \equiv \mp i/\hbar\, \theta(\pm(t-t')) \langle \underbrace{[\hat{A}(t), \hat{B}(t')]_{\zeta}}_{AB - \zeta BA} \rangle \quad (3)$$

$$\overset{(1,2)}{=} \pm\, \theta(\pm(t-t')) \left(\mathcal{G}^{>} - \mathcal{G}^{<} \right)_{AB}(t,t') \quad (4)$$

$$\left(\mathcal{G}^{R} - \mathcal{G}^{A}\right)_{AB}(t-t') \overset{(3,4)}{=} \left[\theta(t-t') + \theta(t'-t)\right]\left(\mathcal{G}^{>} - \mathcal{G}^{<}\right)_{AB}(t,t') = \left(\mathcal{G}^{>} - \mathcal{G}^{<}\right)_{AB}(t,t') \quad (5)$$

For later use, we collect some useful relations: $\boxed{GF31}$

$$\mathcal{G}^{<}_{AB}(t,t') \overset{(29.2)}{=} \zeta\, \mathcal{G}^{>}_{B,A}(t',t) \quad (1)$$

$$\left[\mathcal{G}^{<}_{AB}(t,t')\right]^{*} \overset{(29.2)}{=} \zeta\, i/\hbar \langle A^{\dagger}(t)\, \hat{B}^{\dagger}(t') \rangle \overset{(29.1)}{=} -\zeta\, \mathcal{G}^{>}_{A^{\dagger},B^{\dagger}}(t,t') \overset{(29.2)}{=} -\mathcal{G}^{<}_{B^{\dagger}A^{\dagger}}(t',t) \quad (2)$$

$$\left[\mathcal{G}^{>}_{AB}(t,t')\right]^{*} \overset{(29.1)}{=} i/\hbar \langle B^{\dagger}(t')\, A^{\dagger}(t) \rangle \overset{(29.2)}{=} -\zeta\, \mathcal{G}^{<}_{A^{\dagger}B^{\dagger}}(t,t') \overset{(29.1)}{=} -\mathcal{G}^{>}_{B^{\dagger}A^{\dagger}}(t',t) \quad (3)$$

$$\mathcal{G}^{R}_{AB}(t,t')^{*} \overset{(30.4)}{=} \theta(t-t')\left(\mathcal{G}^{>*} - \mathcal{G}^{<*}\right)_{AB}(t,t') = -\theta(-t'+t)\left(\mathcal{G}^{>} - \mathcal{G}^{<}\right)_{B^{\dagger}A^{\dagger}}(t',t) \quad (4)$$

$$= \mathcal{G}^{A}_{B^{\dagger}A^{\dagger}}(t',t) \quad (5)$$

"Time-ordered" or "causal" GF: (arises from pert. theory on real-time axis) GF32

$$\mathcal{G}^{c}_{AB}(t,t') = -i/\hbar \langle T_t \hat{A}(t)\hat{B}(t')\rangle \tag{1}$$

$\theta(t-t')AB + \zeta\theta(t'-t)BA$

$$= \theta(t-t')\,\mathcal{G}^{>}_{AB}(t,t') + \theta(t'-t)\,\mathcal{G}^{<}_{AB}(t,t') \tag{2}$$

We will show below: its analytic continuation to imaginary axis gives

"Thermal" GF: (arises from pert. theory on imag. time axis)

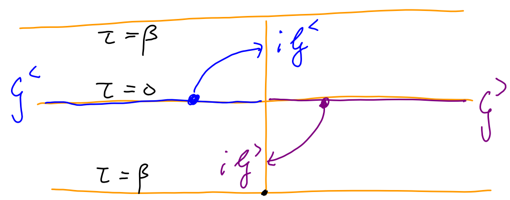
$$\mathscr{G}_{AB}(\tau,\tau') \overset{(20.2)}{=} -\frac{1}{\hbar}\langle T_\tau \hat{A}(\tau)\hat{B}(\tau')\rangle \tag{3}$$

$\theta(\tau-\tau')AB + \zeta\theta(\tau'-\tau)BA$

$$= \theta(\tau-\tau')\,\mathscr{G}^{>}_{AB}(\tau,\tau') + \theta(\tau'-\tau)\,\mathscr{G}^{<}_{AB}(\tau,\tau') \tag{4}$$

where

$$\mathscr{G}^{\gtrless}_{AB}(\tau,\tau') = -i\,\mathcal{G}^{\gtrless}_{AB}(t=-i\tau,\, t'=-i\tau') \tag{5}$$



When is analytic continuation allowed? (Negele & Orland, p.244) GF33

$$\mathcal{G}^{>}_{AB}(t,t') = -i/\hbar\ \frac{1}{Z}\mathrm{Tr}\Big[e^{-\beta\hat{H}}\, e^{i\hat{H}t}\hat{A}\, e^{-i\hat{H}t/\hbar}\, e^{i\hat{H}t'}\hat{B}\, e^{-i\hat{H}t'/\hbar}\Big] \tag{1}$$

(or $\hat{H}-\mu\hat{N}$)

$$= -i/\hbar\ \frac{1}{Z}\sum_n \langle n|\, e^{-\hat{H}(\beta - i(t-t')/\hbar)}\hat{A}\, e^{-i\hat{H}(t-t')/\hbar}\hat{B}|n\rangle \equiv \mathcal{G}^{>}_{AB}(t-t') \tag{2}$$

$$\mathcal{G}^{<}_{AB}(t,t') = -i\zeta/\hbar\ \frac{1}{Z}\sum_n \langle n|\, e^{-\hat{H}(\beta + i(t-t')/\hbar)}\hat{B}\, e^{+i\hat{H}(t-t')/\hbar}\hat{A}|n\rangle \equiv \mathcal{G}^{<}_{AB}(t-t') \tag{3}$$

Spectrum of $\hat{H}$ must satisfy $0 \le E_n < \infty$

(if $E_n < 0$, then $Z = \sum_n e^{-\beta E_n}$ does not exist for $\beta \to \infty$) (4)

$$\Rightarrow \sum_n \text{ in (2) exists only if } \overset{(5a)}{\mathrm{Re}(i(t-t')) \ge 0} \text{ and } \overset{(5b)}{\mathrm{Re}(\beta - i(t-t')/\hbar) \ge 0} \tag{5}$$

$$\text{(3)} \qquad \overset{(6a)}{\mathrm{Re}(-i(t-t')) \ge 0} \text{ and } \overset{(6b)}{\mathrm{Re}(\beta + i(t-t')/\hbar) \ge 0} \tag{6}$$

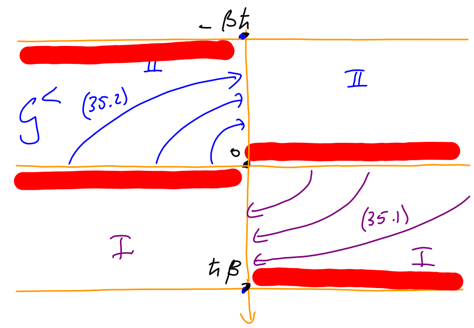
So, analytical continuation is possible for $\qquad [\mathrm{Re}(iz) = -\mathrm{Im}\, z]$ $\qquad \boxed{GF34}$

$$G^> \quad \text{if} \quad -\beta\hbar \overset{(33.5b)}{\le} \mathrm{Im}(t-t') \overset{(33.5a)}{\le} 0 \quad \xRightarrow{\mathrm{Im}(t-t') = -\tau} \quad 0 \le \tau \le \beta\hbar \qquad (1)$$

$$G^< \quad \text{if} \quad 0 \overset{(33.6a)}{\le} \mathrm{Im}(t-t') \overset{(33.6b)}{\le} \beta\hbar \quad \xRightarrow{\mathrm{Im}(t-t') = -\tau} \quad -\beta\hbar \le \tau \le 0 \qquad (2)$$

So, analytic continuation of $G^c_{AB}(t,t')$ is defined as

$$G^{c\to}_{AB}(t,t') \equiv \begin{cases} G^>_{AB}(t-t') & \text{if } t-t' \in \mathrm{I} \\ G^<_{AB}(t-t') & \text{if } t-t' \in \mathrm{II} \end{cases} \qquad (3)$$



$$\mathrm{I}: \{\mathrm{Im}(t-t') = 0 \text{ and } \mathrm{Re}(t-t') > 0\} \cup \{-\beta < \mathrm{Im}(t-t') < 0\} \qquad (4)$$

$$\mathrm{II}: \{\mathrm{Im}(t-t') = 0 \text{ and } \mathrm{Re}(t-t') < 0\} \cup \{0 < \mathrm{Im}(t-t') < \beta\} \qquad (5)$$

Periodicity in complex time-direction

$\boxed{GF35}$

For $\quad -\beta \le \mathrm{Im}(t-t') \le 0$, where $G^>$ is defined: $\qquad (1)$

$$G^>_{AB}(\overbrace{t-t'}^{\in \mathrm{I}}) \overset{(34.2)}{=} -\frac{i}{\hbar}\,\frac{1}{Z}\,\mathrm{Tr}\left[e^{-(\beta - i(t-t')/\hbar)\hat H}\,\hat A\, e^{-i(t-t')\hat H/\hbar}\,\hat B\right] \qquad (2)$$

rewrite as
$$= -\frac{i}{\hbar}\,\frac{1}{Z}\,\mathrm{Tr}\left[e^{-\hat H(\beta + i(t-t'+i\beta\hbar))/\hbar}\,\hat B\, e^{+i(t-t'+i\beta\hbar)\hat H/\hbar}\,\hat A\right] \qquad (3)$$

$$\overset{(34.3)}{=} \zeta\, G^<_{AB}(\underbrace{t-t'+i\beta\hbar}_{\in \mathrm{II}}) \qquad (4)$$

$0 \le \mathrm{Im}(t-t'+i\beta\hbar) \le \beta$, so $G^<_{AB}$ is defined.

So: if $t-t' \in \mathrm{I}$

$$G^{c\to}_{AB}(\overbrace{t-t'+i\beta\hbar}^{\in \mathrm{II}}) = G^<_{AB}(t-t'+i\beta\hbar) = \zeta\, G^>_{AB}(t-t') = \zeta\, G^{c\to}_{AB}(\overbrace{t-t'}^{\in \mathrm{I}}) \qquad (5)$$

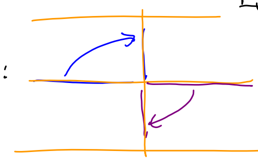
so $G^{c\to}$ is anti-periodic in imaginary time direction.

This is one of the major advantages of combining $G^>$ and $G^<$ into a single function.

Relation to thermal functions:

GF36

Consider analytic continuation onto imaginary axis itself:



$t \to -i\tau \qquad \mathrm{sgn}(t) \to \mathrm{sgn}(\tau)$

Then $$\hat{A}(t) = e^{it\hat{H}/\hbar}\,\hat{A}_S\, e^{-it\hat{H}/\hbar} \longrightarrow \hat{\tilde{A}}(\tau) \overset{(16.6)}{\simeq} e^{\tau\hat{H}/\hbar}\,\hat{A}_S\, e^{-\tau\hat{H}/\hbar} \qquad (1)$$

$(-i)(-i\zeta) = -\zeta$

Define: $$\mathcal{G}^{\gtrless}_{AB}(\tau,\tau') \equiv \begin{Bmatrix} -\frac{1}{\hbar}\langle \hat{\tilde{A}}(\tau)\,\hat{\tilde{B}}(\tau')\rangle \\ -\zeta/\hbar\,\langle \hat{\tilde{B}}(\tau')\,\hat{\tilde{A}}(\tau)\rangle \end{Bmatrix} \overset{(30.1,2)}{=} -i\, G^{\gtrless}_{AB}(t=-i\tau,\, t'=-i\tau') \qquad (2)$$

analytic continuation of real-time $G^{\gtrless}$

Then $$\mathcal{G}_{AB}(\tau,\tau') \overset{(20.2)}{=} -\frac{1}{\hbar}\langle T_\tau\, \hat{A}(\tau)\,\hat{B}(\tau')\rangle \qquad (3)$$

$\theta(\tau-\tau')AB + \zeta\theta(\tau'-\tau)BA$

$$\overset{(2)}{=} \theta(\tau-\tau')\,\mathcal{G}^{>}_{AB}(\tau,\tau') + \theta(\tau'-\tau)\,\mathcal{G}^{<}_{AB}(\tau,\tau') \qquad (4)$$

$$= -i\, G^{c\to}_{AB}(t=-i\tau,\, t'=-i\tau') \qquad (5)$$

thermal GF is analytic continuation of causal GF

Periodicity: (35.5) implies: $\mathcal{G}_{AB}(\tau-\beta\hbar) = \zeta\,\mathcal{G}_{AB}(\tau) = (22.4)$ ✓ (6)